

ENERIFE

SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022 www.shifttenerife.com

Program



Servicio Canario de la Salud









COLLABORATORS







"It is not an S, on my world it means hope"





TENERIFE, CANARY ISLANDS, SPAIN, 10-14TH OCTOBER, 2022

WELCOME TO THE SHIFT 2022

Dear colleagues



Since last time we met at SHIFT 2017, it's been tough years for everyone. Pandemic, lockdowns, war....But we keep hope. We have gathered here again at Tenerife to share the best of our science. We are really proud to present this impressive program which has been possible because each of you! It is really an honor and privilege to welcome you in person at Tenerife, around 80 universities of 29 countries. Let us meet, share our time and discuss science together again. Let us SHIFT!

It will be an unforgettable week with a quite attractive scientific content, completely assured with your outstanding participation, and also with a stunning social program. We are convinced that SHIFT 2022 implies also the importance of returning to scientific inperson meetings! Scientific conferences have been, and will continue to be, instrumental in the progress of science. It is not only about the talks, the papers published, the posters, the presentations. It is about the personal face-to-face encounters, the discussions during the coffee breaks, by the networking lunches and the gala dinner. It is that brilliant idea or those synergies that could appear sharing the Conference lunch during the excursion to El Teide volcano National Park or during a nice walk through the historical UNESCO World Heritage venue city of La Laguna. Unexpected inspiring ideas and connections, new visions, new approaches are gestated in those moments. Shining a light on biomedical and energy applications: with news insights into the biomedical field to "cure the people", and with groundbreaking achievements in renewable energies to "heal the world", with attention to critical raw materials and strategic minerals. You are making the SHIFT possible! Let us SHIFT again after these uncertain times! SCIENCE will lead the way!

Thank you very much on behalf of my colleagues at the Organizing Committee, and welcome to Tenerife, welcome to the SHIFT!

Dr. Jorge Méndez-Ramos Conference Chairman SHIFT2022 Universidad de La Laguna, Tenerife, Canary Islands, Spain





NAZARIO MARTÍN UNIV COMPLUTENSE MADRID - SPAIN



AMADOR MENÉNDEZ CENTRO TECNOLÓGICO IDONIAL - ASTURIAS SPAIN



MAURIZIO FERRARI

TERESA GIRALDEZ UNIV. LA LAGUNA TENERIFE - SPAIN



HUESO

KINGDOM

JOSÉ MARQUÉS-

UNIV. HERIOT WATT

EDINBURGH - UNITE

ANDREW PLESTED HUMBOLDT UNIVERSIT BERLIN - GERMAN







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Md. K. Nazeeruddin EPFL Lausanne (S



	Friday, 14 (ULL-Central)	PLENARY: Luis Liz-Marzán (campus Central Paraninfo-ULL)	Coffee Break	10:15 - 11:15 h	Xiaogang Liu			11:15 - 12:15 h DI ENARV	Sara Skrabalak	12:30-13:00h Closing ceremony	Farewell cocktail 13:00h Campus Central	and a	THE BLE THE			Shift ²²	TENERIFE					Saturday, 15 th 7:30-21:00h	Trip to La Palma			Sub Palma	
Canary Islands)	-Guajara)	PLENARY: Kentaro Nakamura (Campus ULL- Guajara)	.u	Satellite SHIFT-DBL (3)		INV: R. Henriques		INV: B. Baker INV-1 1			0.5					INV: B. Judkewitz Z. Gidden	Ua	-	17:30-19:00h	awiviaterial		4	enerife)				
	Thursday, 13 (ULL-Guajara	PLENARY: Ke	Coffee Break	Energy session 7 KNI-1 B Galán		illa INV: F. Wall	INV: F.Leon - R.Ortuño	E. Andresen	INN	Lunch Guajara)	uis Carlos Suajara)	Coffee Break	Energy session 8		INV: E.	ed R.Campana	F. A	Refreshment break (5 min,	ession G		1. 13th	20:30h Conference Gala Dinner	Real Casino Santa Cruz de Tenerife)	3			
(10-14th OCTOBER, 2022, Tenerife,				Bio session 5	KN: F. Vetrone	ty INV: M. Quintanilla UE	¥	J. Casar I. Conta Mantine		k Networking Lunch (Campus ULL- Guajara)	PLENARY: Luis Car (Campus ULL-Guajara)		Bio session 6	KN: A. Dennis	INV:	Z	E. Martín-Rodríguez Ce A. Skrioka		Poster session	(Flash poster "karaoke") (17:30-18:30h)	Thursday 13th	100	(Real Cas				
th OCTOBER	Wed, 12	World Heritage Excursion				 (Historical city center of La Laguna, venue 			Heritage city) - El Teide	National Park (UNESCO	World Heritage		I EIDE	- Lunch	erti	FI Teide"	- Conference	photo		A DEPARTMENT		SOCIAL PROGRAM	ļ	1			
	jara)	gemann		Satellite SHIFT-DBL (1)	Inter	roop INV: M.Barroso	4	no INV: B. Chanda			une			1999	INV	ambi M. Krieg gattil S. Mischke		"karaoke")			4	Science	0		No.	Hattory Theater	te to Blas Cabrera
Conference Schedule	Fuesday, 11 (ULL-Guajara)	PLENARY: Peter Hegemann (Campus ULL- Guajara)	Coffee Break	Energy session (3/4)	NV: I. García INV: Schweizer	NV:A.Ródenas INV: R.Schroop	N	NV:S. Pietralunga A. Rubino		Networking Lunch Campus ULL - Guajara)	PLENARY: Jennifer Dionne (Campus ULL-Guajara)	Coffee Break	Energy session (5/6)	INV: N.Stingelin INV:T.Welsch		M. Runowski A.Asaithambi W. Li A.Panangattil	Refreshment break (5 min	Poster session (Flash poster "karaoke")	(17:00-18:00h)			Music"	ED.	Adgrace	SIC	And a second	
SHIFT 2022 Confe	Tueso	ED)		Bio session 3 KN·H Lin	-	KN: A.B. Seddon	wicz	INV: K.Soga INV:	ero	N CC	PLENAI (C		Bio session 4	5	P.Formentín	2	Refi	Poster sessi			Tuesday 11th	19:30-21:30h "Talks and Music"	- C	(Teatro Leal, La Laguna) 🦿	ALKS&MUSI	the second second	LEAL
SHIF	Ctec/ULL-Guajara)	k (8:00-9:15h) 9:00-9:15h) :ri Odom) (IACtec)	0:15-10:30h)	Meijerink	Ntech-Tenerife)	0	17	ez, Toyota Canarias Inc.	MARYISLANDS	N	PLENARY: (14:15h)	5.15-15.30h)	Energy session (1/2)	KN: J. Concepción	a 2	D. Avram INV:R. Almeida Z. Curbelo E. Ximendes	JG.Sánchez M.Hernández E.Martinez A.Carneiro	reak (5 min)	E. Palmero S. Zanella D. González F. Maturi		Tueco	19:30		NO 31			
	Monday, 10 (MCtec/ULL-Guajara)	Registration Desk (8:00-9:00h) Opening ceremony (9:00-9:15h) PLENARY: Teri Odom (9:15-10:15h) (IACtec)	Coffee Break (10:15-10:30h)	10:30 - 11:30 h PLENARY: Andries Meijerink	(Parque Científico IACtec INtech-Tenerife)	T		11:30-11:45h J.M. Méndez, Toyota Canarias Inc. 11:45 - 12-15h Round table	INVEST R+D IN CANARYISLANDS	Networking lunch	(Campus ULL-Guajara) PLENARY: Michael Graetzel (14:15h)	Coffee Break (15:15-15:30h)	Bio session (1/2) E	<u>e</u> e		INV:Ramos INV:T.Grzyb D INV: J.Y.Son NV:Roscini Z.			N. Jurga M. Díaz E. P. Camarerd S. Marnues D. C	MacKenzie F.Sigoli P	oth 20.00L	Monday, 10°°, 20:00n Welcome reception	inarias	ito)	SAN CRISTON LA LAGU		
V	~	9:00 - 10:00 h	10:00 h			10:15 - 12:30 h	1			12:30 - 14:00 h	14:00 - 15:00 h	15:00 h		15:15-	17:30 h			10100000-0000	24 . 2023	18:30 h		Welcome	(Instituto de Canarias	Cabrera Pinto)		None-	

	SESSION CHAIRS (PLENAR)	Y TALKS)
Speakers	SESSION CHAIR	Schedule
Teri W. Odom	Eva Hemmer	Monday 10th, 9:15h
Andries Meijerink	Jose Marqués-Hueso	Monday 10th, 14:00h
Michael Graetzel	Nazario Martín	Monday 10th, 10:30h
Peter Hegemann	Teresa Giráldez	Tuesday 11th, 9:00h
Jennifer Dionne	Eva Hemmer	Tuesday 11th, 14:00h
Kentaro Nakamura	Jorge Méndez-Ramos	Thursday 13th, 9:00h
Luis D. Carlos	Eva Hemmer	Thursday 13th, 14:00h
Luis M. Liz-Marzán	Nazario Martín	Friday 14th, 9:00h
Xiaogang Liu	Andries Meijerink	Friday 14th, 10:15h
Sara E. Skrabalak	Eva Hemmer	Friday 14th, 11:15h
	SESSION CHAIRS (KEYNOT	E TALKS)
	Speakers (Bio session)	
Daniel Jaque	Luis Carlos	Monday 10th, 15:30h
Teresa Pellegrino	Luis Carlos	Monday 10th, 16:00h
Haichun Liu	Jose Marqués-Hueso	Tuesday 11th, 10:15h
Angela Seddon	Jorge Méndez-Ramos	Tuesday 11th, 10:45h
Ana Paula Pêgo	Luis Carlos	Tuesday 11th, 15:15h
Fiorenzo Vetrone	Luis Liz-Marzán	Thursday 13th, 10:15h
Allison Dennis	Jose Marqués-Hueso	Thursday 13th, 15:15h
	peakers (Energy session)	
Javier Concepción	Jose R. Galán-Mascarós	Monday 10th, 15:30h
Mohammad Nazzerudin	Nazario Martín	Tuesday 11th, 10:15h
José R. Galán-Mascarós	Nazario Martín	Thursday 13th, 10:15h
Fernando Martín	Andries Meijerink	Thursday 13th, 15:15h
	SESSION CHAIRS (Parallel s	sessions)
Monday 10th	Session chairs	

Monday 10th		
Bio session 1	Eva Hemmer / Amador Menéndez	Monday 10th, pm
Bio session 2	Amador Menéndez / Eva Hemmer	Monday 10th, pm
Energy session 1	Antonio García-Martín /Alberto Bollero	Monday 10th, pm
Energy session 2	Jose Marqués-Hueso / Emilio Palomares	Monday 10th, pm

Tuesday 11th		
Bio session 3	Daniel Jaque	Tuesday 11th, am
Energy session 3	Nazario Martín /Jorge Méndez-Ramos	Tuesday 11th, am
Energy session4	Jose Marqués-Hueso / Eva Hemmer	Tuesday 11th, am
Bio session 4	Luis Carlos	Tuesday 11th, pm
Energy session 5	Alberto Bollero	Tuesday 11th, pm
Energy session 6	Ruud Schropp	Tuesday 11th, pm

Thursday 13th		
Bio session 5	Luis Liz-Marzán / Jose Marqués Hueso	Thursday 13th, am
Energy session 7	Jorge Méndez-Ramos	Thursday 13th, am
Bio session 6	Eva Hemmer /Jose Marqués Hueso	Thursday 13th, pm
Energy session 8	Andries Meijerink/ Nazario Martín	Thursday 13th, pm

MAPS AND CONFERENCE LOCATIONS





C. Alvaron ntech 00,101 T nn <u>Universidad de La Laguna conference sites</u> X pələı Rectora Mari (Mon, 10th Oct, am, 9:00-12:15h) **Opening session** Parque Científico IACtec **Opening day lunch** (Mon, 10th Oct, 12:30-14:00h) Finca Mac-Kay 14 B 9 Neurdre * Plenary and parallel sessions Campus Guajara) ULL – Campus Guajara (Mon. 10th, pm to Thurs 13th, Oct) fram stop Calle ENERI To ULL - Central Campus C. Frat To La Laguna city center **Closing session** Tram stop (La Trinidad) C.H C.N

Universidad de La Laguna (ULL)

ULL – Campus Guajara

Plenary talks and parallel sessions (from Mon, 10th, pm to Thurs, 13th, Oct)



Universidad de La Laguna (ULL)

ULL – Campus Guajara

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Aulario General de Guajara Conference rooms location



Parallel rooms (first floor)



SOCIAL PROGRAM

- WELCOME RECEPTION (Monday, 10th October, 20:00h, Instituto de Canarias, Cabrera Pinto)





- CONFERENCE EXCURSION (Wednesday, 12th October):

*(9:00h, <u>Plaza del Adelantado</u>) La Laguna (Route: Historical city center of La Laguna, UNESCO World Heritage city)



*10:30 h, Coffee break at <u>Hotel Laguna Nivaria</u> *11:00 h, Departure from La Laguna (<u>Plaza del Adelantado</u>) to <u>"EL TEIDE" NATIONAL PARK</u> (Conference lunch and SHIFT2022 photo), back to La Laguna at 18:00h



- GALA DINNER (Thursday, 13th October, 20:30h, <u>Real Casino Santa Cruz de Tenerife</u>)



OUTREACH ACTIVITIES:

-"<u>Talks and Music</u>" (<u>Teatro Leal</u>, La Laguna, Tuesday 11th October, 19:30-21:30h)



Science divulgation (public open lectures) & Music & Theater (Tribute to <u>Blas Cabrera Felipe</u>, "father of Spanish Physics", born in Canary Islands)



-CRITICAL RAW MATERIALS ROUND TABLE

(Thursday, 13th October, 17:30h-19:00h, Conference Venue)



A round table ("critical raw materials round table") on Thursday 13th october, 17:30-19:00h, in the main plenary speaker room of SHIFT2022 conference venue. With the participation of: Tom Lograsso (Director, Critical Materials Institute CMI, USA), Frances Wall (University of Exeter, UK), Kentaro Nakamura (The University of Tokyo, Japan), Pier Luigi Franceschini and Roland Gauss from EIT RawMaterials (Europe), Alberto Bollero (IMDEA-Nanociencia, Spain), Jose Luis Costa Kramer (IMN-CSIC, Spain) and Jose Manuel Rodríguez Ramos (CEO Wooptix Inc, Spain). Moderated and presented by Jorge Méndez (Universidad de La Laguna, Chairman of SHIFT2022)

Round table summary: Decarbonification, circular economy, and self-sufficiency will require a considerable effort from Europe in the next few years. This round table will enable an open discussion with international experts on the need of strategic materials in key sectors such as information technologies, energy and transportation to make possible achieving the European Green Deal objectives. Semiconductor chips, permanent magnets and batteries are main elements to achieve environmental, social and economic goals, but they require the use of raw materials currently under risk of shortage. This critical situation and possible alternatives will be discussed.



POST-CONFERENCE EXCURSION

TOUR TO LA PALMA - SATURDAY 15th OCTOBER (7:30-21:30h)

1 day return trip by domestic flight, 40 min, to the neighbor island, La Palma, the most western Canary Island with stunning views and a National Park and also first world-class Astrophysics Observatory "Roque de los Muchachos". And of course we will be able to see the volcano at "Cumbre Vieja" area that ended its activity just very recently (December 2021). It is absolutely spectacular to see the landscape after this eruption, how Earth is born.





TRIP TO LA PALMA

Post-conference excursion, Saturday, 15th October 2022

<u>"Optical Materials" Special Issue</u> SHIFT: SHINING A LIGHT ON BIOMEDICAL AND ENERGY APPLICATIONS

Selected papers with science presented by our very relevant speakers at **SHIFT 2022** will be published in a forthcoming **Special Issue of Optical Materials** published by Elsevier. More details can be found at: https://www.journals.elsevier.com/optical-materials/forthcoming-special-issues/call-for-paper-on-special-issue-shift-shining-a-light-on-biomedical-and-energy-applications

Call for Paper for "Optical Materials" Special Issue on – SHIFT: SHINING A LIGHT ON BIOMEDICAL AND ENERGY APPLICATIONS

We can proudly announce the launch of a special issue to be published in "Optical Materials" (Elsevier, I.F: 3.754) with selected papers from very relevant colleagues (Plenary, Keynote and Invited speakers) and also contributed authors presenting their works at SHIFT 2022 Conference

Submission Deadline: 15-Dec-2022

Editorial Acceptance Deadline: 01-Mar-2023



	PLENARY SPEAKERS							
Presenting author	Affiliation	Title	Schedule					
Teri W. Odom	Northwestern University, USA	Resolving Single-Particle Nano-Bio Interactions in Real Time	Monday 10th, 9:15h					
Andries Meijerink	Utrecht University, The Netherlands	Measuring Temperature with Light	Monday 10th, 14:00h					
Michael Graetzel	EPFL Lausanne, Switzerland	Mesoscopic photosystems for the generation of electricity and chemical fuel from sunlight	Monday 10th, 10:30h					
Peter Hegemann	Humboldt University, Germany	Engineered and unexpected natural rhodopsins for new optogenetic application	Tuesday 11th, 9:00h					
Jennifer Dionne	Stanford University, USA	Bridging atomic and reactor scales in plasmon catalysis for efficient, selective, and sustainable chemistry	Tuesday 11th, 14:00h					
Kentaro Nakamura	University of Tokyo, Japan	REY-rich mud: a key for sustainable development of our society	Thursday 13th, 9:00h					
Luis D. Carlos	University of Aveiro, Portugal	How hot are living cells?	Thursday 13th, 14:00h					
Luis M. Liz-Marzán	CIC biomaGUNE, Spain	Plasmonic Nanomaterials for Biosensing and Bioimaging	Friday 14th, 9:00h					
Xiaogang Liu	National University of Singapore	Luminescent Nanoparticles: A Wonderful Toolbox for Imaging and Assistive Technologies	Friday 14th, 10:15h					
Sara E. Skrabalak	Indiana University, USA	Nanocrystal Conversion Pathways to Compositionally Complex Nanocrystal Catalysts	Friday 14th, 11:15h					

KEYNOTE SPEAKERS								
Presenting author Affiliation		Title	Schedule					
	Bio session							
Daniel Jaque	Universidad Autónoma de Madrid, Spain	Nanomaterials for brain thermometry	Monday 10th, 15:30h					
Teresa Pellegrino	Istituto Italiano di Tecnologia, Italy	Nanomaterials for magneto-photo thermia to treat cancer	Monday 10th, 16:00h					
Angela Seddon	University of Nottingham, UK	Shining light on life	Tuesday 11th, 10:45h					
Ana Paula Pêgo	i3S - INEB, Portugal	nanoBiomaterials: a shining tool in the field of neurosciences	Tuesday 11th, 15:15h					
Haichun Liu	KTH Royal Institute of Technology, Sweden	Lanthanide upconversion nanoparticles for infrared photodetection and super-resolution microscopy	Thursday 13th, 10:15h					
Fiorenzo Vetrone	Université du Québec, Canada	Rare Earth Doped Nanoparticles: Manipulating their Architecture for Theranostics	Tuesday 11th, 10:15h					
Allison Dennis	Northeastern University, USA	Engineering Semiconductor Quantum Dots for Biosensing and Imaging Applications	Thursday 13th, 15:15h					
	Energy session							
Javier Concepción	Brookhaven National Laboratory, USA	Selective and efficient conversion of CO to methanol: Towards cascade strategies for CO2 reduction to liquid fuels	Monday 10th, 15:30h					
Mohammad Nazzerudin	EPFL, Switzerland	Development of Efficient and Stable Perovskite Solar Cells and Modules	Tuesday 11th, 10:15h					
José Ramón Galán-Mascarós	Institute of Chemical Research of Catalonia-ICIQ, Spain	Artificial photosynthesis: state-of-the-art, perspectives and catalysis	Thursday 13th, 10:15h					
Fernando Martín	IMDEA - Universidad Autónoma de Madrid, Spain	Real-time imaging and control of electron currents: towards attochemistry	Thursday 13th, 15:15h					

INVITED SPEAKERS							
Presenting author	Affiliation	Title	Schedule				
	Bio session						
Jose M. Rodríguez Ramos	Wootpix Inc., Spain	Quantitative phase imaging using hte WFPI technique with the SEBIQ-phase camera	Monday 10th, pm				
Jung-Young Son	Konyang University, Korea	Spectral image for detecting green mold pathogen on lemon	Monday 10th, pm				
Tomasz Grzyb	Adam Mickiewicz University, Poland	Upconverting nanoparticles sensitized by Er3+ or Tm3+ ions and their applications	Monday 10th, pm				
Claudio Roscini	Catalan Institute of Nanoscience and Nanotechnology, Spain	Wax-based photothermoresponsive switches	Monday 10th, pm				
Artur Bednarkiewicz	Institute of Low Temperature and Structure Research, Poland	New concept of subdiffraction imaging and sensing with photon avalanche materials	Tuesday 11th, am				
Kohei Soga	Tokyo University of Science, Japan	Polarity Based Nanostructure Design for Near Infrared Luminescence	Tuesday 11th, am				
Anna Lukowiak	Institute of Low Temperature and Structure Research, Poland	Luminescent bioactive nanoglasses and composites	Tuesday 11th, pm				
Marta Quintanilla	Universidad Autónoma de Madrid, Spain	Developing Sensors and Actuators for Biological Environments: Luminescence Thermometry and Plasmonic Heating	Thursday 13th, am				
Sidney J.L. Ribeiro	São Paulo State University, Brazil	Fluorescent Dyes Based On Pyrylium and Azo-compound Structures: Synthesis, PhotoinducedIsomerization, Solvathocromism and Fluorescent Probes For Selective Microenvironment Systems	Thursday 13th, pm				
Antonio Benayas	Universidad Autónoma de Madrid, Spain	Lifetime-thermometry for real time monitoring of liver inflammation: addressing the "tissue-issue" when measuring temperature in vivo	Thursday 13th, pm				
Riccardo Marín	Universidad Autónoma de Madrid, Spain	In pursue of a brighter future for silver sulfide nanocrystals in fluorescence imaging and thermal sensing	Thursday 13th, pm				

	Energy session		
Ilka Kriegel	Italian Institute of Technology, Italy	Hybrid nanoscale materials for light-energy conversion and storage	Monday 10th, pm
Alberto Bollero	IMDEA Nanoscience Madrid, Spain	From the Cosmos to the Nanoscale: Nanostructured Permanent Magnets for a Green Energy Transition	Monday 10th, pm
Kasper Moth-Poulsen	Chalmers University of Technology, Sweden	Solar Thermal Management Materials	Monday 10th, pm
Peter J. Skabara	University of Glasgow, United Kingdom	Novel organic semiconductors as downconverters for photonic applications and low power lighting	Monday 10th, pm
Rui M. Almeida	Universidade de Lisboa, Portugal	Phosphor-Up-converted white LEDs assisted by 1-D photonic crystals	Monday 10th, pm
Inés García-Benito	Universidad Complutense de Madrid, Spain	Searching for renewable energies: the breakthrough of perovskites.	Tuesday 11th, am
Airán Ródenas	Universidad de La Laguna, Spain	Seamless integration of photonics within harsh-environment resistant crystals with 3D laser nanolithography: Towards real-world advanced optical sensors	Tuesday 11th, am
Cecilia Noguez	Universidad Nacional Autónoma de México	Plasmonic response of nanoparticles arrays and its potential applications	Tuesday 11th, am
Stefan Schweizer	South Westphalia University, Germany	Lanthanide-doped Glass Light Guides with Bright Luminance in the Green Spectral Range	Tuesday 11th, am
Ruud E.I. Schropp	University of the Western Cape, South Africa	Freedom of spectrum utilization and customization of color and print in solar cell technology	Tuesday 11th, am
Silvia M. Pietralunga	CNR-IFN, Italy	Flexible photonic systems: from 1D photonic crystals to active planar waveguides	Tuesday 11th, am
Daniela Fontani	CNR-INO, Italy	Field optimization for bifacial modules	Tuesday 11th, am
Natalie Stingelin	Georgia Institute of Technology, USA	Phase Diagrammes of Complex Materials: From the Katana, Swiss Chocolates to Organic Semiconductors	Tuesday 11th, pm
Antonio García-Martín	IMN-CNM, CSIC (Spain)	Nanostructure strategies towards performance-enhanced perovskite solar cells	Tuesday 11th, pm
Tory Welsch	University of Delaware, USA	Colloidal Quantum Dot Heterostructures for Photon Upconversion	Tuesday 11th, pm
Tom Lograsso	Critical Materials Institute, USA	Bioleaching critical minerals from end-of-life feedstocks	Thursday 13th, am
Frances Wall	University of Exeter, United Kingdom	Responsible rare earths: circular economy approaches including life cycle assessment	Thursday 13th, am
Fernando León/ Rubén Ortuño	Banknote Production Control Department of Banco de España (Spain)	Materials for banknotes security	Thursday 13th, am
Miguel Anaya	University of Cambridge (UK)	Halide perovskites for next generation optoelectronic devices	Thursday 13th, am
Emilio Palomares	ICIQ-BIST, Spain	Molecular Solar Cells. From Dyes to Hybrid Semiconductors	Thursday 13th, pm
Dirk Guldi	Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany	Porphyrinoid-Based Charge and Photon Management	Thursday 13th, pm
Emilio Nieto	National Hydrogen Centre – CNH2, Spain	Hydrogen: present and Future	Thursday 13th, pm
Jose Manuel Méndez	General Manager, Marketing Department, Toyota, Spain	Toyota roadmap towards carbon neutrality and sustainable mobility for all	Monday 10th, am

CONTRIBUTED "ORAL"			
		ENERGY AND OTHER APPLICATIONS	
Presenting author	Category	Title	Code
Daniel Avram	Senior / Dr.	Upconversion emission properties in transition metal, lanthanide co-doped systems: a spectral selective, time-resolved investigation	1 OE
Zaida Curbelo	Student	Synthesis of MnAIC / Hydrogel Inks for Fabricating Alternative Permanent Magnets by Bonding and 3D-printing	2 OE
José G. Sánchez	Senior / Dr.	Effect of Chalcogen Substitution Atom on the Performance Parameters of PM6:Y6-based Ternary Solar Cells	3 OE
Eugenia Martinez-Ferrero	Senior / Dr.	Self-Assembled Molecules as Selective Contacts in CsPbBr3 Nanocrystal Light Emitting Diodes	4 OE
Ester M. Palmero	Senior / Dr.	Understanding the Role of Particle Size in the Development of Flexible Permanent Magnet-Polymer Filaments for Additive Manufacturing	5 OE
Dora A. González	Student	Novel Carbazole-Based Conjugated Molecules as Self-Assembled Hole Transporting Monolayers for Inverted Perovskite Solar Cells	6 OE
Przemysław Woźny	Senior / Dr.	Upconversion luminescence of novel FeS2@NaYF4: Yb3+, Er3+ nanocomposites	7 OE
Erving Ximendes	Senior / Dr.	Machine learning and the improvement of readouts provided by luminescent thermometers	8 OE
Miguel A. Hernández-Rodríguez	Senior / Dr.	Designing all-photonic molecular analogues of electrical components: a molecular filter based on Ln3+	9 OE
Albano N. Carneiro Neto	Senior / Dr.	Simulating the emission of co-doped Yb3+/Er3+ upconverting nanoparticles	10 OE
Sofia Zanella	Student	Upconverting luminescent material as an all-photonic platform for molecular logic: from basic to more complex logic operations	11 OE
Fernando E. Maturi	Student	Understanding the anomalous behavior of liquid water through upconversion nanothermometry	12 OE
Fengchan Zhang	Student	Enhancement of single nanoparticle luminescence and trapping force by surface plasmon polaritons	13 OE
Joaquín Sanchiz	Senior / Dr.	Down-shifting layers for silicon-based PV module applications	14 OE
Albenc Nexha	Senior / Dr.	Composites with lanthanide doped fluorescent particles for flying, seed-like soft robots that monitor environmental temperature	15 OE
Adilet Zhakeyev	Senior / Dr.	Multi-material and multi-colour 3D printing enabled by upconversion and metallic catalyst	16 OE
Marcin Runowski	Senior / Dr.	New Frontiers for High-sensitivity Luminescence Manometry	17 OE
Wenhui Li	Senior / Dr.	From Polymer Films to Self Assembling Molecular Electrodes for Efficient and Stable Inverted Perovskite Solar Cells	18 OE
Andrea Rubino	Senior / Dr.	Hybrid nanosystems for new solar-based technology solutions	19 OE
Wilfried van Sark	Senior / Dr.	Outdoor performance of nanocrystal luminescent solar concentrators	20 OE
Carlos Brites	Senior / Dr.	Lanthanide-based logic: a venture for the future of molecular computing	21 OE
Bryce S. Richards	Senior / Dr.	Upconversion for photovoltaics: can it ever really work?	22 OE
Michal Žitňan	Senior / Dr.	The study of three types of materials for "green" hydrogen production by water splitting: TiO2, ZnO and CdS.	23 OE
Aswin Asaithambi	Senior / Dr.	Free carrier generation via photo-induced energy transfer in Perovskite-TMDC (0D-2D) Hybrid System	24 OE
Anjana Panangattil Muraleedharan	Student	Spectroelectrochemical investigations for photodoping of colloidaltin doped indium oxide nanocrystals	25 OE
Elina Andresen	Senior / Dr.	Upconversion for security tags and future applications	26 OE
Yazhi Liu	Student	Fabrication of Anti-counterfeiting Nanocomposites with Multiple Security Features via Integration of a Photoresponsive Polymer and Upconverting Nanoparticle	27 OE
Roberto Campana	Senior / Dr.	CNH2's recent advances in reversible solid oxide devices using scalable and cost-effective manufacturing processes	28 OE
Fernando Arteaga-Cardona	Senior / Dr.	Unprecedented atomic-scale details of the interface in lanthanide-based core@shell nanocrystals: when the interface controls the "device"	29 OE
A. Turshatov	Senior / Dr.	Application of Upconversion and Downshifting Luminescence of Lanthanide-based Phosphors in Plastic Recycling	30 OE

CONTRIBUTED "ORA	L"		
		BIO APPLICATIONS	
Presenting author	Category	Title	Code
Rodolfo N. Silva	Student	Novel and high-sensitive primary and self-referencing thermometers based on the excitation spectra of lanthanide ions	1 OB
Maria Méndez	Senior/Dr.	Synthesis and Characterization of Persistent Blue Light Luminescence Nanoparticles for Photodynamic Therapy (PDT)	2 OB
Natalia Jurga	Student	Luminescence of different up-converting nanoparticles in blood	3 OB
Pablo Camarero	Student	Handling of single multicellular spheroids: a 3D tumor model	4 OB
Lewis E. MacKenzie	Senior/Dr.	Straight-forward synthesis of upconversion nanoparticles for biosensing applications using a polymer-assisted open-air modest-temperature method: control of shape and emission	5 OB
Fernando Lahoz	Senior/Dr.	Optical molecular detection trough fluorescence quenching	6 OB
Jose J. Velázquez	Senior/Dr.	Effect of Al2O3 on the crystallization of NaYF4 in oxyfluoride silicate glass-ceramics for optical thermometer	7 OB
Mario Díaz	Senior/Dr.	FLTX2: The novel ALL IN ONE Tamoxifen Derivative: Antiestrogen, Fluorescent and Photosensitizer	8 OB
Sergio Antonio Marques de Lima	Senior/Dr.	The influence of experimental parameters on the luminescent properties of red-emitting hybrids for bioimaging	9 OB
Fernando Aparecido Sigoli	Senior/Dr.	Dual magnetic field and temperature optical probes based on lanthanide-doped NaREF4 nanoparticles containing hierarchically structured heterogeneous crystalline phases	10 OB
Dasheng Lu	Senior/Dr.	Improving stability and thermal sensitivity of an optically trapped upconversion nanoparticle by coating with a thermo-sensitive polymer	11 OB
Elisa Ortiz Rivero	Student	Rare-earth-doped microspinner for non-invasive sensing	12 OB
Pilar Formentín	Senior/Dr.	Polymeric Surfaces based on Template Replica for Cell Culture	13 OB
Adolfo Speghini	Senior/Dr.	Nanocomposite films of α -synuclein with inorganic nanoparticles	15 OB
Jason Casar	Student	Hybrid polymer-ceramic mechanosensors for near-IR induced, color responsive pressure sensing in vivo	16 OB
Joana Costa Martins	Student	Er3+-doped nanoparticles as primary thermometers and NIR radiation sensors	17 OB
Parivash Moradifar	Senior/Dr.	Ultrafast decay alkaline-earth rare-earth fluoride nanoparticles for novel X-ray and gamma-ray scintillators	18 OB
Natalie Fardian-Melamed	Senior/Dr.	Seeing the Force: Single Avalanching Upconverting Nanoparticles as Ultrasensitive Local Force Transducers	19 OB
Emma Martín Rodríguez	Senior/Dr.	Influence of cell incubation parameters on molecular imaging of atherosclerosis with functionalized gold nanoshells	20 OB
Artiom Skripka	Senior/Dr.	Expanding the Library of Photon Avalanching Nanoparticles	21 OB

			POSTER CONTRIBUTION	
Presenting author	Category	Area	Title	Code
Ivet Maqueira Albo	Student	Energy	Understanding of light-driven chemical reactions using in situ Raman spectroscopy	1 PE
Nastaran Kazemi Tofighi	Student	Energy	Exfoliation and transferring of 2D materials for potential energy conversion and storage applications	2 PE
Nicola Curreli	Dr.	Energy	Depletion Layer Engineering in Core-Shell Metal Oxide Nanocrystals	3 PE
Nicolò Petrini	Student	Energy	Multi-Layer Optical Model for Metal Oxide Nanocrystals	4 PE
Luca Rebecchi	Student	Energy	Solar energy applications for Doped Transparent Metal Oxides	5 PE
Franzette Paz-Buclatin	Student	Energy	Diffractive microlenses inside laser crystals by 3D fs-laser nanolithography	6 PE
Wiebke Alex	Student	Energy	Photoisomerization of Push-pull Functionalized Norbornadiene/Quadricyclane Couples for Solar Energy Storage	7 PE
Peter R. Schol	Student	Energy	Investigation of Rylene-Based Dyes for Application in Dye-Sensitized Solar Cells	8 PE
Alexander Zika	Student	Energy	Photo-Switchable Polymer Nano-Assemblies	9 PE
Marcin Bilewicz	Dr.	Energy	Multilayer PE film with recycled filler	10 PE
Sylwia Ryszczyńska	Student	Energy	Temperature-dependent up-conversion luminescence in core/shell nanoparticles doped with Ho3+ and Er3+ ions upon 1151 nm excitation	11 PE
Paweł Jarka	Student	Energy	Investigation of the composite structures for organic solar cells (OSCs) based on bulk heterojunction (BHJ)	12 PE
Marta Zaborowska	Student	Energy	Electrospinning and optical characterization of RE-doped ZnO nanofibers	13 PE
Lidiya M. Muhammad	Student	Energy	Anthracene for Molecular Solar Thermal Systems (MOST)	14 PE
Fernando Déniz	Student	Energy	Synthesis and characterization of mixed oxides with rare earth	15 PE
Selene Díaz-González	Student	Energy	Synthesis, structural characterization and optical studies on the perovskite-type mixed oxide SrFe1-xCoxO3 (x=0.25, 0.50, 0.75) doped with rare-earth elements.	16 PE
Gabriela Brito-Santos	Student	Energy	Degradation analysis of highly UV-resistant down-shifting layers for applications on photovoltaics devices	17 PE
Weronika Smok	Student	Energy	Hybrid TiO2 NPs-SnO2 NWs photoanode for developing the performance of DSSC	18 PE
Tomasz Tański	Dr.	Energy	Zirconia nanofibers – from synthesis to optical properties characterization	19 PE
Miguel Medina-Alayón	Student	Energy	Shifting NIR photons into UV-VIS radiation with rare-earth doped materials for photocatalytic pollutant degradation and water-splitting	20 PE
Sheila Torres-García	Student	Energy	Anti-counterfeiting using colour tuneable upconversion photonic materials for codification of luminescent patterns	21 PE
Wojciech M Piotrowski	Student	Energy	The influence of vanadate host material on the relative sensitivity and brightness in the single band ratiometric thermometry	22 PE
Kyohei Okubo	Dr.	Bio	Near infrared hyperspectral imaging for biomedical applications including lipid visualization in liver and submucosal tumor detection	1 PB
Leyre Aldaz-Caballero	Student	Bio	CuinS2 quantum dots as pressure nanosensors	2 PB
Ely Bravo	Student	Bio	Tracking the development of cholestasis rat model with autofluorescence and emitting Ag2S NPS	3 PB
Chiara Cressoni	Student	Bio	From Thermometry to Bioimaging: Lanthanide Activated Nanoparticles as Multifunctional Tools for Biomedical Applications	4 PB
Patryk Fałat	Student	Bio	Lanthanide-doped core-shell nanostructures with enhanced VIS-to-UVC upconverted emission for biomedical applications	5 PB
Evelina Voronovic	Student	Bio	Every particle with a crown: protein corona guided accumulation of upconverting nanoparticles in cancer cells	6 PB
Adrian Drozdowski	Student	Bio	NIR to UV up-converting nanoparticles for PDT applications	7 PB
Santi Gené-Marimon	Dr.	Bio	Dispersion of Persistent Luminescent Particles using Different Strategies to Enhance their Antimicrobial Properties	8 PB
Liyan Ming	Student	Bio	Infrared emitting nanoparticles for thermal control in the brain	9 PB
Luis Felipe Morales-Curiel	Student	Bio	Volumetric bioluminescence imaging of cellular dynamics with deep learning based light-field reconstruction	10 PB
Maja Szymczak	Student	Bio	Novel luminescence manometer based on Cr3+ emission in Li2Mg3TiO6	11 PB
Kamila Maciejewska	Student	Bio	The strategy for enhancement the thermometric performance of Ln3+ based luminescence thermometry	12 PB
Liangliang Liang	Dr.	Bio	Mid-infrared Detection with Lanthanide Nanotransducers	13 PB
Zichao Luo	Dr.	Bio	Lanthanide-nucleotide Coordination Nanoparticles for STING Activation	14 PB
Zhuang Liu	Student	Bio	Highly Stable Lead-Free Perovskite Single Crystals with NIR Emission beyond 1100 nm	15 PB

			POSTER CONTRIBUTION (SHIFT - DBL- DOING BIOLOGY WITH LIGHT)		
Presenting author	Category	Area	Title	Code	
Anna Ekner-Grzyb	Dr.	DBL	Wheat seedlings' bioimaging and dependence of phytotoxicity on size and functionalization of upconverting NaYF4:Yb,Er@NaYF4 nanoparticles	P-DBL	1
David Bartolomé-Martín	Dr.	DBL	Development and optimization of calcium fluorescent sensors based on BK ion channels	P-DBL	2

		SHIFT - DBL- DOING BIOLOGY WITH LIGHT (Satellite meeting)	
KEYNOT	E	Title	
Justin Taraska		Imaging the nanoscale structure of the cell with correlative super resolution light and electron microscopy	Tuesday, 11th, am
Elizabeth M. C. Hillman		High-speed 3D microscopy for life-science applications	Tuesday, 11th, pm
Valentina Emiliani		Holographic manipulation of neuronal circuits	Thursday, 13th, am
Thomas Blanpied		The nanodomain basis of synaptic function	Thursday, 13th, pm
INVITED		Title	
Presenting author			
Margarida Barroso		Morphology, topology and function of endosome-mitochondria Interactions in breast cancer cells	Tuesday, 11th, am
Melike Lakadamyali		Super-resolution imaging of cellular processes	Tuesday, 11th, am
Baron Chanda		Role of membrane environment on binding allostery in pacemaker ion channels at single molecule resolution	Tuesday, 11th, am
Sandrine Leveque-Fort		Engineering fluorescence emission for enhanced super-resolution microscopy	Tuesday, 11th, pm
Ricardo Henriques		Super-Resolution and Machine-Learning enabled Live-Cell Biolmaging	Thursday, 13th, am
Stephan Pless		Deciphering location of ligand-induced conformational changes and ligand-binding sites in an ion channel	Thursday, 13th, am
Bradley Baker		Tracing electrical circuits in neural networks and in proteins	Thursday, 13th, am
Luke Lavis		Designing Brighter Dyes for Advanced Fluorescence Microscopy	Thursday, 13th, am
Barbara Di Ventura		The power of LOV	Thursday, 13th, pm
Benjamin Judkewitz		The smallest vertebrate brain knows how to sing	Thursday, 13th, pm
CONTRIBUTED "ORAL"			
Presenting author	Category	Title	Code
Carlos Renero-Lecuna	Senior/Dr.	Fluorescent Nd3+-based nanoparticles for NIR nanothermometry	DBL-O1
Niccolò Caselli	Senior/Dr.	Holographic optical tweezers for dynamic control of erythrocyte flickering	DBL-O2
Michael Krieg	Senior/Dr.	Neural engineering with photons as neurotransmitters	DBL-O3
Sabrina Mischke	Student	Seeing AMPA receptor complexes in a new light	DBL-O5
Dirk H. Ortgies	Senior/Dr.	Autofluorescence-free in vivo imaging in the time domain: Tailoring nanoparticles towards their application as contrast agents in the infrared	DBL-O4
Zoe Gidden	Student	Seeing inside the cell using LIVE-PAINT: A new way to image proteins in live cells using super-resolution microscopy	DBL-O6



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Resolving Single-Particle Nano-Bio Interactions in Real Time

<u>Teri W. Odom</u>¹

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Nanotechnology offers unique strategies for minimally invasive and localized approaches to diagnose and treat diseases. For example, nanoparticles have been explored in a range of applications, including as drug delivery vehicles, imaging probes, and therapeutic agents. Although increased therapeutic efficacy has been realized, direct visualization of how engineered nanoparticles interact with specific organelles or cellular components has been limited. Such interactions will have implications for fundamentals in cancer biology as well as in the design of translational therapeutic agents. This talk will describe how drug-loaded gold nanostars can behave as optical probes to interrogate how therapeutic nanoconstructs interact with cells at the nanoscale. We will focus on model cancer cell systems that can be used to visualize how gold nanoconstructs target cells, rotate, and translate on the plasma membrane, are endocytosed, and are trafficked intracellularly. Critically, differences in translational and rotational motion between spherical and star-shaped nanoconstructs indicate that the nanoparticle scaffold geometry affects how targeting ligands present and bind to cell-membrane receptors. That nanoparticle shape can preserve ligand activity of nanoconstructs in vitro will have important implications for engineering designer nanoconstructs for nanomedicine.

Representative publications:

- 1. P. Choo, T. Liu, and T.W. Odom, *J. Am. Chem. Soc.* **143**, 4550 (2021). "Nanoparticle Shape Determines Dynamics of Targeting Nanoconstructs on Cell Membranes."
- 2. E.E. Coughlin, J. Hu, A. Lee, and T.W. Odom, *J. Am. Chem. Soc.* **143**, 3671 (2021). "Light-Mediated Directed Placement of Different DNA Sequences on Single Gold Nanoparticles."
- 3. J. Hu, T. Liu, P. Choo, S. Wang, T. Reese, A. Sample, and T.W. Odom, *ACS Cent. Sci.* **6**, 2339 (2020). "Single-Nanoparticle Orientation Sensing by Deep Learning."
- 4. D. Bhowmik, K.S.B. Culver, T. Liu, and T.W. Odom, *ACS Nano* **13**, 13637 (2019). "Resolving Single-Nanoconstruct Dynamics during Targeting and Nontargeting Live-Cell Membrane Interactions."
- 5. K.S.B. Culver, T. Liu, A.J. Hryn, N. Fang, and T.W. Odom, *J. Phys. Chem. Lett.* **9**, 2886 (2018). "In Situ Identification of Nanoparticle Structural Information Using Optical Microscopy."
- H. Lee, D.H.M. Dam, J.W. Ha, J. Yue, and T.W. Odom, ACS Nano 9, 9859 (2015). "Enhanced Human Epidermal Growth Factor Receptor 2 Degradation in Breast Cancer Cells by Lysosome-Targeting Gold Nanoconstructs."
- 7. D.H.M. Dam, J. Lee, P. Sisco, D. Co, M. Zhang, M.R. Wasielewski, and T.W. Odom, *ACS Nano* **6**, 3318 (2012). "Direct Observation of Nanoparticle-Cancer Cell Nucleus Interactions."



SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Measuring Temperature with Light

Andries Meijerink^{*}, Markus Suta, Thomas van Swieten, Robin Geitenbeek and Freddy Rabouw

CMI, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands

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Please indicate preference: __Poster _X_Oral Specify Technical Area: _X_Biomedical __ Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Luminescence thermometry has rapidly developed in the past decades to a powerful method for remote temperature sensing. More recently, nanothermometry relying on the temperature dependent luminescence of lanthanide ions doped into nanocrystals has emerged, especially in biological applications for accurate sensing and mapping of temperature profiles in the range 270-330 K and also at higher temperatures.^{1,2} Here we first discuss fundamental aspects of luminescence thermometry, especially the role of Boltzmann equilibrium and a new theoretical approach to understand and predict the optimum single ion (nano)thermometer.^{3,4} Maximizing thermal sensitivity will be demonstrated with real-case examples based on these predictions and a careful analysis actual temperature accuracy that can be realized will be shown to strongly depend on the brightness of the luminescent temperature probes.⁵ Some pitfalls will also be discussed and warnings will be given!^{4, 5} All the considerations finally lead to clear guidelines for optimizing ratiometric lanthanide-based luminescent thermometer for a specific application. The temperature accuracy of luminescence thermometers is often directly related to relative sensitivity rather than including crucial aspects of systematic errors and noise. We will show what determines the actual temperature accuracy and how photonic effects and Poissonian noise are more important and need to be considered to determine temperature accuracy, which is especially important in biological systems.

In the second part of the talk examples of the unique capabilities of luminescence nanothermometry will be given, including temperature mapping with μ m resolution to probe temperature variation in microheaters used in synchrotron and TEM experiments and applications in microfluidics where measuring temperature variations inside the microchannels is notoriously difficult.² An outlook will be given towards the future of lanthanide doped nanoparticles temperature sensing.

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[2] a) R. G. Geitenbeek *et al., ACS Catal.* **2018**, *8*, 2397-2401; b) R. G. Geitenbeek *et al., Chem. Eng. Sci.* **2019**, *198*, 235-240; c) R. G. Geitenbeek, *Lab Chip* **2019**, *19*, 1236-1246.

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Mesoscopic photosystems for the generation of electricity and chemical fuel from sunlight

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Over the last 10 years mesoscopic photovoltaics, such as dye sensitized cells (DSCs) and perovskite solar cells (PSCs) have emerged as credible contenders to conventional p-n junction photovoltaics. Their certified power conversion efficiency currently attains 25.7 %, exceeding that of polycrystalline silicon. This lecture covers the genesis and recent evolution of DSCs and PSCs, describing their operational principles and current performance. DSCs have now found commercial applications for ambient light harvesting and electric power producing glazing. The scale up and pilote production of PSCs are progressing rapidly but challenges remain that still need to be met to implement PSCs on a large commercial scale. PSCs can produce high photovoltages rendering them attractive for applications in tandem cells, e.g. with silicon and for the generation of fuels from sunlight. Examples are the solar generation of hydrogen from water and the conversion of CO2 to chemical feedstocks such as ethylene, mimicking natural photosynthesis.



SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Engineered and unexpected natural rhodopsins for new optogenetic application

<u>Peter Hegemann</u>, Rodrigo Fernandez, Johannes Vierock and Enno Peter Humboldt Universität zu Berlin, Germany

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During the recent 20 years an enormous volume of microbial rhodopsins has been discovered and further engineered and employed in combination with fluorescent marker proteins for a flexible control of neuronal networks by all-optical electrophysiology. However, two types of channelrhodopsins (ChRs) were expected but not available, Ca^{2+} -selected ChRs for the activation of Ca^{2+} -mediated signaling processes and, second, K⁺-selected ChRs for short term cells hyperpolarization and inactivation. I will report about a set of engineered ChRs that conduct Ca^{2+} better than Na⁺ and H⁺ and will explain the underlaying voltage dependent Ca^{2+} -conducting mechanism and possible applications. Second, I will report about the recent discovery and characterization of a set of K⁺-selected ChRs that are highly efficient for short term cell inactivation. Third, I will report about a spectacular group of bestrhodopsins that are rhodopsins or rthodopsin-tandems C-terminally linked to a bestrophin domain and are forming large homopentameric clusters. We have characterized these channels in a large collaborative network between Israelian, Japanize and German research groups. We have demonstrated that Bestrophins work as light-activated anion channels.



10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Bridging atomic and reactor scales in plasmon catalysis for efficient, selective, and sustainable chemistry

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Chemical manufacturing is critical for industries spanning construction, clothing, plastics, pharmaceuticals, food, and fertilizers, yet remains among the most polluting and energy-demanding practices. Our vision is to enable sustainable chemical production with atomically-architected photocatalysts that precisely control molecular interactions for high-efficiency and product-selective chemistry. Controlling photochemical transformations requires bridging the length-scale between a catalyst's atomic-scale structural features that influence dynamics and the macroscale extrinsic parameters that can be controlled (e.g., illumination, temperature, pressure). Optical excitation of plasmons offers a solution for overcoming this size mismatch - creating nanoscopic regions of high electromagnetic field intensity that can modify electronic and molecular energy levels, enable access to excited-state dynamics, and open new reaction pathways that are impossible to achieve under typical conditions. Further, plasmons can be efficiently excited with sunlight or solar-driven LEDs, for sustainable chemical transformations.

Here, we present our research advancing plasmon photocatalysis from the atomic to the reactor scale. First, we describe advances in in-situ atomic-scale catalyst characterization, using environmental opticallycoupled transmission electron microscopy (OTEM). With both light and reactive gases introduced into the column of an electron microscope, we can monitor chemical transformations under various illumination conditions, gaseous environments, and at controlled temperatures, correlating three-dimensional atomicscale catalyst structure with photo-chemical reactivity. Then, we describe how these atomic-scale insights enable optimized reactor-scale performance. As model systems, we consider two reactions: 1) acetylene hydrogenation with Ag-Pd catalysts and 2) CO2 reduction with Au-Pd catalysts. Here, Au/Ag acts as a strong plasmonic light absorber while Pd serves as the catalyst. We find that plasmons modify the rate of distinct reaction steps differently, increasing the overall rate more than ten-fold. Secondly, reaction nucleation occurs at electromagnetic hot-spots – even when those hot-spots do not occur in the preferred nucleation site. Finally, plasmons open new reaction pathways that are not observed without illumination, enabling both high-efficiency and selective catalysis with tuned bimetallic composition. Our results help elucidate the combined roles of optical, electronic and chemical contributions to plasmon photocatalysis, en-route to record efficiency and selectivity.





TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

REY-rich mud: a key for sustainable development of our society

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Rare-earth elements and yttrium (REY) are widely recognized as strategic materials (U.S. Department of the Interior and U.S. Geological Survey, 2013; European Commission, 2020), which are crucial for hightechnology applications (e.g., laptop computers, cell phones, and flat screen televisions) and green energy technologies (e.g., electric/hybrid vehicles, wind power generators, and fuel cells). World demand for REY is increasing rapidly (Humphries, 2010, Roskill Information Services Ltd., 2007; Alonso et al., 2012; Goodenough et al., 2018, Elshkaki, 2021) and a stable supply of REY is a key to future development of technology and the global economy (Alonso et al., 2012; Goodenough et al., 2018, Elshkaki, 2021).

However, several problems currently exist with rare-earth resources at present. For example, more than half of the world's production of REY is from China (USGS 2021). Moreover, China's overwhelming dominance is particularly evident in heavy rare-earth elements (HREE) that are critically important materials for high-technology products including electronic, clean energy, and military technological devices (Service, 2010; Goodenough et al., 2018). Indeed, known HREE reserves are almost all in ion-adsorption-type ore deposits in southern China (e.g., Longnan and Xinxiu ore deposits), even though light rare-earth elements (LREE) can be obtained from carbonatite/alkaline igneous complexes in many countries (Goodenough et al., 2018). Thus, diversification of sources and increased access to REY resources, especially HREE, are required to maintain stable supply of meeting the ever-rising demand for the elements. Another problem is that most onshore REY deposits have high concentrations of radioactive elements such as U and Th (Murakami and Ishihara, 2006; Sørensen et al., 2011; Yang et al., 2009; Goodenough et al., 2018) due to the behavior of these elements during magma genesis similar to that of LREE. Therefore, production of REY from onshore LREE deposits produces massive amounts of radioactive waste, resulting in a serious and persistent environmental problem in REY mining.

In 2011, we have discovered that deep-sea muds enriched in REY (termed as REY-rich mud) are distributed over large areas of the Pacific Ocean, including the high seas (Kato et al., 2011). REY-rich mud has also been reported from the Indian Ocean (Yasukawa et al., 2014). Furthermore, a recent study has shown that REY-rich mud is also a promising resource for Sc that is an important element for leading-edge technologies in the energy and environmental fields (Yasukawa et al., 2018).

REY-rich mud has five notable advantages as a mineral resource: (1) tremendous resource potential because of their extensive distribution, (2) high REY concentrations with HREE enrichment, (3) ease of exploration, (4) very low radioactive element concentrations, and (5) high and easy recovery of REY by acid leaching. These facts clearly indicates that REY-rich mud is a promising resource for REY that are extremely important to create future sustainable development of our society. To exploit this new promising resource, there is an urgent need to establish mining technology from deep-sea with water depth of more than 4000m.



TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

How hot are living cells?

L. D. Carlos

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Specify Technical Area: Biomedical

The emergence of luminescent nanothermometry during the last decade opened up the possibility of measuring thermal flows at spatial scales below 10 μ m, unreachable by conventional electrical methods [1]. Diverse phosphors capable of providing a contactless thermal reading through their light emission properties have been examined, e.g., polymers, DNA or protein conjugated systems, organic dyes, quantum dots, and trivalent lanthanide (Ln3+) ions incorporated in organic-inorganic hybrids, multifunctional heater-thermometer nanoplatforms, upconverting, downconverting and downshifting nanoparticles. The implementation of these Ln3+-based phosphors (with an emphasis on upconverting nanoparticles) as ratiometric thermometers was extensively reviewed in the past five years [1].

In the last couple of years, the focus of luminescence thermometry has gradually shifted from the fabrication of more sensitive nanoarchitectures towards the use of the technique as a tool for thermal bioimaging and the unveiling of properties of the thermometers themselves and their local surroundings, as, for instance, the instantaneous ballistic velocity of Brownian nanocrystals suspended in both aqueous and organic solvents [2].

After a general perspective of the work done on luminescence nanothermometry since the explosion of the field one decade ago, the lecture will be focused on examples illustrating the potential of the technology to measure the intracellular temperature [3], including recent results of those measurements during magnetic hyperthermia [4].

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Plasmonic Nanomaterials for Biosensing and Bioimaging

Luis M. Liz-Marzán^{1,2,3}

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Nanoplasmonics can be defined as the science studying the manipulation of light using materials of size much smaller than the radiation wavelength. This technology finds applications in various fields including sensing and diagnostics. An essential component of nanoplasmonics are nanostructured materials which can very efficiently absorb and scatter light by supporting coherent oscillations of free (conduction) electrons. Although the remarkable optical response of "finely divided" metals is well known since more than 150 years ago, the recent development of sophisticated characterization techniques and modeling methods has dramatically reactivated the field. An extremely important pillar supporting the development of nanoplasmonics has been the impressive advancement in synthesis and assembly methods, which provide us with an exquisite control over the composition, morphology and organization of nanostructured metals. Colloid chemistry methods in particular have the advantages of simplicity and large-scale production, while offering a number of parameters that can be used as a handle to direct not only nanoparticle morphology but also surface properties and subsequent processing.

This communication will feature several examples of novel strategies to employ nanostructured materials comprising gold nanoparticles, as substrates for ultrasensitive detection and imaging of biorelevant molecules, based on different plasmonic phenomena such as surface enhanced Raman scattering and plasmonic chirality.

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Luminescent Nanoparticles: A Wonderful Toolbox for Imaging and Assistive Technologies

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Abstract: Lanthanide-doped nanoparticles exhibit unique luminescence properties, including massive Stokes shift, sharp emission bandwidth, high resistance to optical blinking, and photobleaching. They are also unique in converting long-wavelength stimulation into short-wavelength emission. These attributes offer the possibility of developing alternative luminescent labels for organic fluorophores and quantum dots. In recent years, researchers have demonstrated spectral-conversion nanocrystals for many biological applications, such as highly sensitive molecular detection and autofluorescence-free cell imaging. With significant progress over the past decade, we can now design and fabricate nanoparticles that display tailorable optical properties. In particular, by controlling different combinations of dopants and dopant concentrations, we can generate a plethora of colors under excitation with a single wavelength. By incorporating a set of lanthanide ions in defined concentrations into different layers of a core-shell structure, we have expanded the emission spectra of the particles to cover almost the entire visible region, which is not possible with conventional bulk phosphors. This talk will highlight recent advances in the broad utility of lanthanide-based nanocrystals and perovskite nanomaterials for multimodal imaging, biodetection, therapy, X-ray scintillation, and assistive technology.

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PI -9



Nanocrystal Conversion Pathways to Compositionally Complex Nanocrystal Catalysts

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Colloidal syntheses have advanced such that nanocrystals with size- and shape-control can be routinely achieved for many simple compositions. This extraordinary achievement provides eloquent nanocrystal samples for fundamental structure-property studies, revealing fascinating confinement effects that are being leveraged in a diversity of technologies. However, general syntheses for multimetalilc and multicomponent nanocrystals with defined structural features are far less developed. Yet, predictable pathways toward such nanostructures are essential to take advantage of the synergy and multifunctionality that arises from their compositional complexity. This presentation will outline predictable and generalizable syntheses for high-quality multimetallic nanostructures based on nanocrystal conversion pathways, including the thermal conversion of core@shell nanocrystals into high entropy alloy nanocrystals and the transformation of intermetallic nanocrystals into nanocrystal heterostructures with integrated atomic and nanoscale architectures through galvanic replacement. As will be shown, these new nanocrystal compositions, impart durability in corrosive electrocatalytic environments, and reduce reliance on platinum group metals.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Nanomaterials for brain thermometry

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Minimally invasive monitoring of brain activity is essential not only to gain understanding on the working principles of brain, but also for the development of new diagnostic tools. In this talk I will describe how brain thermometry could be an alternative to conventional methods (e.g., magnetic resonance or nuclear medicine) for the acquisition of thermal images of the brain with enough spatial and temperature resolution to track brain activity in minimally perturbed animals. I will focus on the latest advances in transcranial luminescence thermometry introducing a critical discussion on its advantages and shortcomings. I will also show how polymeric nanoparticles and nanoparticles with structural phase transitions in the physiological temperature range can be used for thermal tomography in brain. The talk also includes a critical discussion about the main challenges that the application of optical nanoparticles for brain thermometry will face in next years.

KN-B-1


SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Nanomaterials for magneto-photo thermia to treat cancer

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¹ Fondazione Istituto Italiano di Tecnologia, via Morego 30, 16131, Genoa, ItalyAffiliation (Font : Calibri, 10 pt, Italic)

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Magnetic hyperthermia which uses magnetic nanoparticles as heat transducers and plasmonic photothermia which uses plasmonic and chalcogenide nanoparticles as heat mediators, are emerging as new technological approaches to treat cancer. Both magnetic metallic and semiconductor nanoparticles offer multiple intrinsic features that make them multifunctional materials for therapeutic and imaging purposes.

In this talk, I will review the efforts we have made in the last decade to produce magnetic nanoparticles with optimal performance for magnetic hyperthermia including their synthesis, functionalization, *in vitro* and *in vivo* preclinical studies. I will then introduce the use of semiconductor nanoparticles for radiotherapy and photo-thermia showing also preliminary *in vitro* results and finally I will talk about the latest efforts for the development of inorganic heterostructures to combine magneto and plasmonic nanoparticles and their characterization.

Acknowledgments

This work was partially supported by funding of the AIRC Foundation (AIRC IG-14527) and of the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie HeatnMof grant (No. 860942).

KN-B-2



SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Shining light on life.

Angela B. Seddon

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Today, the 'Gold Standard' for identification of cancer remains histopathology, that is: the visible-light microscopic study of the morphology of excised, dye-stained tissue to diagnose cancer [1]. Histopathology is labour-intensive and highly dependent on the judgement of the pathologist. Excised tissue biopsies are frozen, microtombed, mounted on microscope-slides, and stained with Haematoxylin&Eosin (H&E) dyes. Such dye-staining reveals the cell/tissue morphology for examination by the pathologist using optical-microscopy to inform diagnosis and treatment-planning. Patients must usually wait weeks for their pathology results, which leads to significant patient stress and associated healthcare costs.

Diem [2] was the first to recognise that mid-infrared vibrational spectroscopic information revealed by tissue may revolutionise the way that 21st-Century pathology is performed. Diem highlighted that mid-infrared spectroscopy of tissue can provide immense information on cellular composition/packing, organ/cell architecture, metabolic processes and absence/presence of disease. Vibrational spectral data-processing utilises mathematical procedures (like unsupervised principal component analysis) to analyse subtle spectral differences of the entire spectrum; it has been demonstrated that subtle differences do exist and that normal/diseased areas of tissue can be distinguished spectroscopically [3-5], e.g. Amide I and II and lipid bands. This type of automated pattern recognition of the families of vibrational absorption bands has formed the bedrock of advances in the field and will aid clinicians in future objective diagnosis. The field is both expanding and consolidating

This swell in interest has coincided with growth of the new field of mid-infrared photonics: new bright midinfrared light sources such as interband and quantum cascade lasers and supercontinuum 'rainbow' fibre light sources [6] and fibre lasers [7] as well as low optical loss mid-infrared glass optical fibre conduits to pipe the mid-infrared light to where it is needed [1] are opening the way for more portable and compact systems to shine mid-infrared light on tissue at the point of care. The first proof-of-principle demonstration of mid-infrared spectral tissue imaging using a supercontinuum 'rainbow' fibre source and within the diagnostically-important mid-infrared spectral 'fingerprint' region was reported in [1,8] The Authors point out that to be useful in pathology, the spectroscopic imaging must be able to identify histological regions of tissue based on molecular features, and most importantly epithelial regions directly associated with cancer development.

The paper with review the field and future directions.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

nanoBiomaterials: a shining tool in the field of neurosciences

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Nervous system problems are common and encompass a large spectrum of traumatic injuries, diseases or iatrogenic lesions. The poor regenerative capacity, particularly in the case of the central nervous system (CNS), cannot be attributed to an intrinsic inability of neurons to sprout and re-grow after injury, as axons are able to regenerate in the presence of a permissive growth environment. Nevertheless, for the regenerative program to occur, it is paramount that in a lesion situation, neurons survive.

So far, one of the main challenges facing the neuroscience field is the development of effective therapies that can enhance the regenerative capacity of both, the peripheral nervous system (PNS) and the CNS, based on the advances achieved in basic research.

At the nBTT group we have been using nano-enabled solutions to develop "smart" biomaterials, designed at the nanoscale with controlled architectures and functionalities to provide, in situ and in a targeted manner, the delivery of nucleic acid-based therapeutics to promote nervous tissue repair and restoration of function.

In this talk, these nanobiomaterials will be presented and emphasis will be given to the nanotechnology and bioimaging tools explored and/or developed by us to optimize and holistically assess the biological performance of the developed nanosystems, as well as to contribute to the design of more efficient nucleic acid delivery vectors. Namely, the use of:

- imaging flow cytometry a high-throughput technique with unique features that combines the statistical strength of flow cytometry with image acquisition of every event - to unravel some critical aspects for vector formulation [1];
- atomic force microscopy as a tool to assess the specificity of targeted nanoparticles in biological models of high complexity [2,3];
- microfluidic-based platforms to mimic the in vivo administration of the neurotropic nanoparticles [4].

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Lanthanide upconversion nanoparticles for infrared photodetection and superresolution microscopy

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Abstract

Lanthanide-doped upconversion nanoparticles (UCNPs) can convert low-energy near-infrared (NIR) photons into higher-energy NIR, visible, or even ultraviolet photons through subsequent absorption and accumulation of the energy of two or more excitation photons. Their unique optical properties enable applications in broad areas such as biomedical imaging, nanomedicine, information technology, and energy. In this talk, I will discuss our work on NIR photodetection¹ and super-resolution microscopy² using these nanoparticles.

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KN-B-5



SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Rare Earth Doped Nanoparticles: Manipulating their Architecture for Theranostics

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Light emitting (luminescent) nanoparticles that can be excited with near-infrared (NIR) light are finding use in a number of applications in theranostics (therapy + diagnostics on the same platform). The use of NIR excitation light mitigates the drawbacks associated with commonly used high-energy light (UV or visible) excitation and can penetrate tissues especially when these wavelengths lie within the three biological windows where tissues are optically transparent. At the vanguard are rare earth doped nanoparticles due to the versatility of their luminescence properties. They can be excited with NIR light and can undergo conventional (Stokes) luminescence emitting in the three NIR biological windows. However, unlike other classes of luminescent nanoparticles, they can also undergo a multiphoton process (known as upconversion) where the NIR excitation light is converted to higher energies resulting in anti-Stokes luminescence spanning the UV-visible-NIR regions. Due to the versatility of their optical properties, it now becomes possible to generate upconverted high-energy light in situ to trigger other light activated therapeutic modalities (i.e. drug release, photodynamic therapy), which cannot be directly accessed with high-energy excitation wavelengths since they cannot penetrate tissue. Meanwhile, the NIR emission for can be used for diagnostics (i.e. bioimaging, nanothermometry). Here, we present the synthesis of various NIR excited (and emitting) rare earth doped core/shell (and multishell) nanoparticles and demonstrate how their luminescence properties can be exploited for potential use in nanomedicine.

KN-B-6



Engineering Semiconductor Quantum Dots for Biosensing and Imaging Applications

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Although the unique optoelectronic properties of semiconductor nanoparticle quantum dots (QDs) enable a variety of commercial products including display technology, solid state lighting, and photovoltaics, different design criteria are required for use of these nanoparticles in biomedical devices. We tailor the composition and optical properties of QDs for a variety of biosensing and bioimaging applications with an emphasis on manipulating absorption/excitation properties (e.g., increasing molar extinction coefficient), using wavelengths optimized for tissue depth imaging, and tailoring the degradation and resulting toxicity/biocompatibility of the materials. For example, we use bright red and green emitting QDs in a rapid, instrument-free assay to detect small molecules such as antibiotics in complex water samples (Figure 1) and use near infrared and shortwave infrared emitters to improve the clarity and resolution of in vivo imaging in mice (Figure 2). Finally, biodegradable and biocompatible plasmonic semiconductor nanoparticles could be used to overcome barriers to clinical translation for photoaccoustic imaging and photothermal therapy applications. Notably, the efforts to remove heavy metals from the nanoparticles compositions also reduces the environmental impact of QDs developed for energy applications. By carefully considering material properties and engineering design choices, we develop semiconductor nanoparticles for a wide variety of applications.



Figure 1: Visual sensing with QD-based bead assay for small molecule analytes like the antimicrobial tetracycline (adapted from *Angewandte Chemie*, 2020, 59(48): 21597-21602).



Subcutaneous hock injection (edema) 790 nm **ZnSe/InP/ZnS** imaged on IVIS Imaging lymphatic drainage in **NIR-I** vs. **NIR-II/SWIR**



Subcutaneous tail injection (edema) 1250 nm emitting **PbS/CdS** imaged on Photon, Etc. IR VIVC InGaAs detector for hyperspectral imaging 600-1600 nm integrated emission from 1200-1400 nm

Figure 2: *In vivo* imaging of lymphatic drainage with QDs takes advantage of the NIR-I and NIR-II optical tissue windows. Left: Drainage from the inguinal to axial node is observed with NIR-I imaging following subcutaneous hock injection (from *Nano Letters*, 2021, 21 (7), 3271–3279). Right: Drainage from an edema induced by subcutaneous tail injection shows tortuosity of lymphatic drainage vessels with higher resolution through NIR-II imaging (unpublished data).





TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Selective and efficient conversion of CO to methanol: Towards cascade strategies for CO₂ reduction to liquid fuels

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 CO_2 reduction to fuels is anticipated to play an important role in global efforts to reduce the devastating effects of climate change. Among various approaches being explored, strategies that provide access to solar liquid fuels are particularly important to achieve carbon-neutral cycles. But the underlying chemistry to generate liquid fuels from CO_2 efficiently and selectively has yet to be developed. In this work, a cascade strategy for the generation of methanol efficiently and selectively from CO_2 is presented. It involves initial CO_2 reduction to CO by one catalyst, followed by further reduction to methanol by a transition metal-organic hydride combination. Using NMR, IR, and mass spectrometry, together with labeling studies, chemical synthesis of authentic samples of intermediates and theoretical calculations, selective and efficient conversion of CO to methanol is demonstrated. The key to the high selectivity is the use of organic hydride donors that are inactive towards direct CO_2 reduction and hydrogen generation. These organic hydride donors are inexpensive and renewable and are a promising platform for solar fuels generation from CO_2 .



KN-E-1



SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Development of Efficient and Stable Perovskite Solar Cells and Modules

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Perovskite solar cells (PSC) are a new paradigm in renewable energy because of their high efficiency reaching over 25%. The perovskite solar cells' high efficiency is due to their excellent optoelectronic properties, which were optimized by various cations and anions with different ratios. Another advantage of perovskite solar cells is their simple fabrication through solution-processing methods, either in n-i-p or p-i-n configurations. However, the long-term stability drags down the commercialization of PSCs technology. We have developed strategies to enhance the stability by using functionalized additives and interface engineering by hydrophobic 2-Dimensional perovskite materials, preventing ion migration and protecting the perovskite absorber. As a result, the long-term stability of unencapsulated devices under one sun illumination retains>95% of their original efficiencies after 1000 h ageing. In this talk, we present layer by layer deposition of 3-Dimensional and 2-Dimensional perovskites and compositionally engineered perovskite resulting in over 25.5% certified power conversion efficiency under one sun. Notably, a record efficiency of 22% for the perovskite module with an active area of 26 cm2 was achieved.

KN-E-2



Artificial photosynthesis: state-of-the-art, perspectives and catalysis

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Technical Area: Energy and other Applications

Artificial photosynthesis:¹⁻³ the direct storage of solar energy into chemical bonds (as fuels or chemicals); may be a major pillar for the decarbonization of the energy landscape. Many initiatives worldwide, from purely scientific projects to small size industrial pilot plants are yielding thousands of results in this field, with promising results and open questions. Arguably, the major challenge remains to improve the efficiency of the processes while limiting costs and avoiding the use of critical raw materials. The competition being a centralized alternative where solar power would be transformed into electricity (by photovoltaic or wind farms) and then grid distributed for the production of green fuels or chemicals at industrial hubs.

In this talk, we will discuss some of the most representative achievements in artificial photosynthesis, highlighting their advantages, and addressing their current limitations, if any. We will give special emphasis on the catalysis. Photo-, electro- and/or photo-electro-catalysts are crucial to speed-up the chemical reactions to proceed at industrially relevant conditions.^{4,5} The reduction of the activation energy losses also provides better energy efficiency, avoiding high-energy reaction intermediates. The search for catalysts able to favor both chemical reactions: reduction (chemical bond formation) and oxidation (source of protons and electrons); is a major driving force in the field.

Many successful catalysts are based on noble metals or critical raw materials, far away from practical applications. When discussing artificial photosynthesis as a plausible contribution to decarbonization, energy security and environmental mitigation plans, sustainability and scaling are additional constrains that must be taken into account. There are many hurdles between a promising lab-scale discovery and a technology, many of them involving economic and societal considerations.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Real-time imaging and control of electron currents: towards attochemistry

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Photoinduced electron transfer and charge transfer processes occurring in organic and inorganic materials are the cornerstone of technologies aiming at the conversion of solar energy into electrical energy and at its efficient transport. The early stages of these processes occur in the attosecond time scale (1 attosecond = 10^{-18} seconds), the natural time scale for electronic motion in atoms and molecules. Accessing this time scale requires the use of light pulses with a duration below the femtosecond, which were first produced in the lab at the dawn of this millennium. The first attosecond experiments aiming at the observation of electronic motion in organic molecules date from 2014 [1]. The usual approach in these experiments is to employ an attosecond pulse to generate an electronic wave packet that subsequently evolves under the influence of the nuclear motion and to interrogate the system with a second pulse at a given time delay in order to obtain a picture of the system at that particular time. By varying the delay between the two pulses, one can thus obtain a sequence of frames or the "movie" of the electronic motion.

The experiments usually record photoelectron and/or fragmentation yields as a function of the temporal delay between the two pulses with attosecond resolution. However, in spite of the successful observation of sub- and few-fs dynamics in the recorded yields [1-4], it is not yet clear how the early electron dynamics leaves its signature in molecular fragments that may be created long after those initial steps (usually after going through a series of non adiabatic processes) or why one should expect a reminiscence of such electron dynamics at all. To answer these questions, one must understand i) the electronic excitation or ionization induced by the first pulse, ii) the coupled electron and nuclear dynamics that follows, iii) the interaction of the second pulse with a molecular system in a coherent superposition of states, and iv) the coupled electron and nuclear dynamics that follows, iii) the molecule. Every step is in itself a theoretical and experimental challenge for molecules containing more than two nuclei. In this talk I will review recent experimental and theoretical efforts to account for these four steps and discuss the optimum conditions to visualize electron dynamics in molecules [5], with emphasis on possible applications to systems of optoelectronic interest in the framework of the recently awarded Synergy Grant TOMATTO of the European Research Council [6].

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KN-E-4



SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Quantitative phase imaging using hte WFPI technique with the SEBIQ-phase camera

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Wave Front Phase Imaging by Intensity (WFPI) is a Wooptix proprietary technique that recovers the wavefront phase of an incoming light beam. It uses standard image sensors (color or monochrome) placed at different positions along the axis of light propagation. There are many alternatives to modify the position. For example, placing the image sensor on a translation stage or using a tunable lens like our new SEBI Q-Phase camera.

The main advantage of the technique is the high lateral resolution in the resulting wavefront phase. An appropriate selection of the distance between images produces a result with a lateral resolution equal to the pixel size of the image sensor: the highest resolution on the market. The frame rate is very high, and the accuracy and dynamic range match industry standards (at the highest resolution). We will present our results on this technique applied to Quantitative Phase Imaging.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Spectral image for detecting green mold pathogen on lemon

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Any form of physical forces imposed on the skin of any fruit induces bruises and scars on it. The bruises and scars change directly the skin color of the fruits and the juicy components emitted from the skin can induce various diseases in the fruit. As a consequence, the skin colors and shape change further due to the growing presence of green mold pathogens. The presence of green mold pathogens on lemon surface is detected with hyper-spectral images in the spectral wavelength range of 500 nm to 650 nm. The dominant spectral wavelengths of the fresh lemon and the green mold pathogen are identified as 580nm and 550 nm, respectively, as shown in Fig. 1. The degree of the infection calculated from the spectral intensity ratio of the infected to the fresh lemon in the spectral range of 500 nm to 560 nm increases more as the infection degree increases as shown in Fig. 2. The ratio can be used to effectively estimate the infected degree of lemons by the green mold pathogens. It also shows that the sudden decrease of the spectral intensity corresponding to the dominant spectral wavelength of the fresh lemon, assisted by neighboring spectral wavelengths can be used to classify the fresh and the contaminated lemons. The spectral intensity ratio of discriminating the fresh lemon from the infected is calculated as 1.15.





Fig. 1. lemon surface grafted with a green mold for the spectral range of 500 to 650 nm. The 1^{st} image is without spectral filters.

Fig. 2. Normalized spectral intensity distribution of Fig. 13 in the spectral range of 500 to 560 nm.

Acknowledgments

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Upconverting nanoparticles sensitized by Er^{3+} or Tm^{3+} ions and their applications

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Please indicate preference: __Poster _X_ Oral Specify Technical Area: _X_Biomedical __ Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Upconversion is one of the most studied phenomena in materials sciences. The possibility of conversion near-infrared wavelengths to shorter ones results in many advanced applications. Nanoparticles showing upconversion can be applied in nanomedicine for cancer targeting and treatment, in analytical applications such as pressure or temperature sensors, or anticounterfeiting. These applications benefit from the properties of lanthanide ions, which electronic structure and long-living excited states allow for efficient upconversion.





For several decades, most reports on the upconversion phenomenon concern systems in which Yb³⁺ ions play the role of luminescence sensitizers. This situation is due to the specific properties of the Yb³⁺ ion, i.e., its simple electronic structure and the resulting high absorption of this ion in the range of around 975 nm. In addition to the many advantages of using Yb³⁺ ions, the need to excite with radiation with a wavelength of around 975 nm has its drawbacks. The two most important ones are water absorption in this range and the useful emission range usually narrowed to the visible light.

Excitation by different wavelengths may also result in intense upconversion. Er^{3+} ions are known for efficient absorption at around 1480-1550 nm, whereas

Tm³⁺ ions can absorb 1200-1210 nm wavelengths. Both ions can undergo multiphoton absorption yielding higher excited states and, finally, upconversion emission. Depending on the composition, the emission cover visible to near-infrared range providing excellent possibilities to utilize these bands for temperature sensing or bioimaging.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Wax-based photothermoresponsive switches

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Organic photo- and thermoresponsive switchable fluorescent materials are of interest for several applications. They are normally based on molecules containing the switching unit, whose state induces the variation of the fluorescence of the emitting moiety. Unfortunately, these molecules suffer various drawbacks, especially in the solid state, that are preventing their applications in commercial products: synthetic difficulties to combine the switching and fluorescent units in the same molecules, low tunability of fluorescence colour, transition temperature or excitation wavelength and, for the photoresponsive materials, low fatigue resistance, destructive readout and dependence on the medium.

Herein, we present a novel, general and straightforward synthesis-free strategy to obtain photo thermoresponsive fluorescent materials in the solid state. It is based on readily available fluorescent dyes, whose emission is triggered by the state (solid or liquid) of the phase-change-materials (PCMs) or waxes in which they are embedded, which control the viscosity or the aggregation state of the dye molecules. With this approach we obtained all types of fluorescent switching modes (on/off, on1/on2, off/on) and different colours, by simply selecting the transition mechanism, fluorophore and PCM type. Through the micro/nanostructuration of the fluorophore/PCM mixtures we also demonstrated the preparation of patterned printed labels and transparent fluorescent films, preserving the optical transitions. In this way, upon addition of gold nanoshells, we could make these materials to respond to also near infrared radiation (NIR) through the photothermal heating.^[1-3]



Figure 1. Photo of a polymer film with photo- and thermoswitchable fluorescence, made by solid lipid nanoparticles of PCMs.

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NEW CONCEPTS OF SUBDIFFRACTION IMAGING AND SENSING WITH PHOTON AVALANCHE MATERIALS

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Please indicate preference: Oral (invited)
Specify Technical Area: Biomedical

Photon avalanche (PA) anti-Stokes non-linear emission exhibit very unusual features such as requirement for non-ground state absorption, pump power dependent transmission and luminescence risetime, and most of all, a high non-linearity exceeding S=30 (where S is the power in luminescence intensity vs excitation intensity relationship: ILUM = (IEXC)S) [1]. Since the discovery of PA in 1979 [2] this phenomenon was demonstrated in several materials (bulk monocrystals, glasses or fibers) and successfully applied in lasers or medium IR photon counting [2], however only recently it has been demonstrated in nanocrystals [3], opening the possibility to utilize its extremely nonlinear optical response for novel technique of photon avalanche single beam super-resolution imaging (PASSI) [3,4].

Here we introduce new concepts, materials and experimental demonstrations on using photon avalanche emission for a new types of super-resolution imaging and sensing.

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Polarity Based Nanostructure Design for Near Infrared Luminescence

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Near infrared (NIR) light is known to be transparent to biological tissues. The authors have developed various kinds of luminescent materials for bioimaging involving three dimensional imaging by computer tomography, fluorescence thermometry and multimodal imaging with non-optical imaging such as MRI or SPECT[1]. The basic concept for bright luminescence from a phosphor is simple. An excited system (mostly with light) will relax anyway by emitting light or heat. This understanding will lead us to design the system "not to emit heat" for bright luminescence.

For trivalent rare-earth ions doped in ceramic hosts has long been studied as good candidates for the NIR luminescence. The classical theory for suppressing the heat generation is understood as a phenomenon called multi phonon relaxation (MPR). Originally, the term "phonon" is defined only for crystals but here, we use it just for widely mentioning about "a quantum of heat". The classical theory for the MPR consists of three parameters, phonon energy, $\hbar\omega$, energy separation of an excited level to the next lying level, ΔE , and electron phonon-coupling constant, *C*. The MPR rate is roughly described as

$$W_{\rm MPR} = C \exp\left(-\frac{\Delta E}{\hbar\omega}\right).$$

This simple formular tells us that one should select large ΔE and small $\hbar \omega$ for increasing the number of phonons for the transition for suppressing the phenomenon. Since in the case of the NIR luminescence, ΔE tends to be smaller compared to the visible luminescence system. Therefore, the design for suppressing the heat generation is more severe for designing the NIR phosphors.

On the other hand, the last parameter, electron-phonon coupling constant, C, has not been theoretically well discussed. Recently, the authors have published the theoretical treatment of the constant[2]. We have concluded that the term depends on the polarity of the surrounding of the luminescent center. The stronger the polarity, the smaller the $W_{\rm MPR}$.

Recently, hybrid nanostructures made of the inorganic nano phosphors and organic polymer are often used. In fact, in the case core-shell structure to involve ceramic nanoparitcles in the hydrophobic polymer core, the MPR is suppressed by decreasing the polarity of the core[3].

The basic concept also can be applied for the NIR luminescent organic dyes [4]. One of the intensively studied organic dye by the authors is IR-1061. The dye consists of the organic cation part and inorganic anion, BF_4^- . Once the counter ion, BF_4^- , is replaced to OH^- , the luminescence is quenched by the thermal relaxation. For avoiding the quenching, we dope the dye molecules into hydrophobic core of micelles with hydrophobic core and hydrophilic shell. Here, again, the polarity matters. Since the IR-1061 dye is weakly polarized, if the core is too hydrophobic, it forms dimer go quench the luminescence. For controlling the system, polarity of the core material is important.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Luminescent bioactive nanoglasses and composites

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Various types of nanomaterials play currently important role in different fields of medicine. For example, silica–calcia system is a well-known basic composition of bioactive glass that is used in regenerative medicine. Glass nanostructures might show higher activity in comparison to their well-known microsized counterparts. Moreover, the photoactivity ensured by modified glass composition, makes these materials much more attractive and having broader range of applications.

Hereby, we present studies on nanoparticles of bioactive glass (SiO₂–CaO or SiO₂–CaO-P₂O₅) showing photoluminescence and photoactivity. The sol–gel route was used to fabricate the particles. The composition of the glass matrix was modified among others by addition of lanthanide ions or phthalocyanine complexes with metals. The optical properties (absorption and photoluminescence spectra) of the samples as well as their structural and morphological properties were examined. The results showed that glasses were optically active in different spectral ranges of electromagnetic spectrum – from ultraviolet to near infrared – depending on the activators. Photoactivity was presented as luminescent and photocatalytic properties as well as singlet oxygen generation. The bioactivity tests indicated that when particles were immersed in the simulated body fluid, ions release to the medium appeared and hydroxyapatite formation on the glass surface was observed (glass remineralization). Additional functionalities have been achieved for composites with graphene oxide flakes. Described systems could be used, for example, for monitoring structural changes of the glass immersed in biological fluids, bioimaging, photodynamic therapy, antibacterial treatment, photocatalysis, or dyes adsorption and degradation.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Developing Sensors and Actuators for Biological Environments: Luminescence Thermometry and Plasmonic Heating

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Optical sensing at the nanoscale has been proposed as a strategy to obtain diagnostic information in biomedical applications, which requires de use of light in the near-infrared range, as it is the spectral range in which tissues display a lower extinction coefficient.^[1] This technique has been specifically developed to the measurement of temperature, thus nanomaterials with thermally dependent luminescent properties are proposed as optical sensors.^[2] However, light emission and thermal dependence are not the only requirements of the materials. As the biological environment is heterogeneous in every sense (composition, pH, viscosity, etc), the interaction of the sensors with their environment must be understood to guarantee a reliable thermal read. In the same way, the modifications that emitted light may suffer along its trip to the detector must be considered.^[3]

Optical nanoactuators, i.e. nanoparticles with the ability to modify their surroundings after optical excitation, are subjected to the same requirements. In this case, though, the problem can be circumvented by linking them to sensors that monitor the status of the surrounding tissue, so their action can be controlled. Based on a system that uses lanthanide doped nanoparticles ($CaF_2:Nd^{3+},Y^{3+}$) to measure temperature, and plasmonic nanoparticles (gold nanostars) to activate heating, we aim to discuss the problems and the different ways we found to improve thermal control, including intensity optimization of Nd³⁺ emission and experimental protocols that allow *in situ* calibration of the thermometers.

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Fluorescent Dyes Based On Pyrylium and Azo-compound Structures: Synthesis, PhotoinducedIsomerization, Solvathocromism and Fluorescent Probes For Selective Microenvironment Systems

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Fluorescent environment-sensitive probes are specially designed dyes that change their fluorescenceintensity (fluorogenic dyes) or color (e.g., solvatochromic dyes) in response to change in theirmicroenvironment polarity and molecular order. In this sense, a novel fluorescent dye was synthetized byreaction between pyrylium and azonium ion-structures, forming "PYRYLAZO" type molecules as end-product.

The photophysical and theoretical calculation results show that the excited state of pyrylazo molecule isgoverned by push–pull character of p-p* transition with intramolecular charge transfer.

Electronic absorption spectra of the pyrylazo in different polar solvents indicates that the groundstate(HOMO) of the pyrylazo is highest polarized than the lowest excited state (LUMO), promoting a blueshift in more polar solvents. This absorption spectrum shift was also observed in micelles media, which the position of the absorption band of pyrylazo is dependent of the ionic character of the micelles(cationic, ionic or neutral).

After light excitation at 532 nm, the ns-transient absorption technique show the presence of threedifferent transient species in the visible spectra range (300 – 900 nm). The transient absorption around410 nm was attributed to the Z-isomer of the Pyrylazo, which is only observed after excitation of the E-isomer. The E-isomer transient band is observed around 520 nm as previously observed in theconventional electronic absorption technique. The third species is observed at 800-900 nm and attributed to the triplet-triplet (T-T) absorption of the Z-isomer. Indeed, the T-T absorption band is quenched in thepresence O2, indicating the Z-isomer triplet state may be used to form reactive oxygen species such as102, usually observed in photodynamic therapy (PDT) studies.



Shining a light on biomedical and energy applications

Lifetime-thermometry for real time monitoring of liver inflammation: addressing the "tissue-issue" when measuring temperature in vivo

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Oral

Biomedical

Luminescence nanothermometry aims to provide contactless thermal reading in diverse physical systems. This sensing approach is based on the use of luminescent nanoprobes showing temperature-dependent changes in their spectroscopic properties (i.e. luminescent nanothermometers). In recent years, this technique has led to unimaginable advances, such as the direct measurement of the instantaneous speed of nanoparticles and the monitoring of micro/nano electronic devices. It is in the field of biomedicine, however, where luminescence nanothermometry has provided the most exciting achievements, including thermal monitoring of cell and brain activity, diagnosis of cardiovascular diseases and real-time thermal imaging of tumors during in vivo therapies. Despite the several published works in the field and the advances witnessed as of late, in vivo luminescence nanothermometry is not a sensing technique mature enough to be translated into the clinics. The main problem resides in its reliability when performing measurements in the presence of biological tissues, since erroneous thermal readouts are obtained already at the subcutaneous level. This interference stems from a strong tissue-photon interaction, which hinders the application of luminescence nanothermometry at greater depths. This bottleneck constituted by the interference of biological tissues should therefore be addressed in order to realize the full potential of luminescence nanothermometry in the biomedical field.

In this work, we tackle this hurdle, bringing luminescence nanothermometry one step closer to its reliable implementation in vivo. To do this, we first developed a synthesis route yielding bright nanothermometers with long fluorescence lifetimes, later applying a methodology based on the analysis of lifetime as a thermometric parameter. The differentiators of the showcased thermometric approach are reliability, real-time measurement capabilities, and high accuracy despite the presence of tissue interference. The combination of new materials, new experimental approaches and novel thermal indicator allowed us to measure the temperature of an internal organ (liver) undergoing an inflammation process in an animal model. This is the first demonstration of thermal monitoring of an internal organ via fluorescence lifetime-based thermometry, thus supporting the use of this sensing technique as a reliable diagnostic tool in preclinical research.

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In pursue of a brighter future for silver sulfide nanocrystals in fluorescence imaging and thermal sensing

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Fluorescence imaging affords real-time image s of biological tissues in a safe, non-invasive way thanks to the use of non-ionizing radiation both as the probe and the collected signal. The use of visible/nearinfrared radiation translates also to the need for a relatively inexpensive imaging setup that is easy to operate – being composed, in its simplest form, of a laser source and a photodetector.

Although fluorescence imaging could rely on the autofluorescence of endogenous tissue components, the use of luminescent species as contrast agents greatly improves the performance of this imaging technique. In this vein, luminescent nanoparticles have emerged as ideal candidates to act as fluorescence imaging contrast agents.¹ Among them, silver sulfide nanocrystals have recently emerged as the prime choice, owing to their benign chemical composition and near-infrared emission.² Moreover, their sensitiveness to temperature changes enables gathering information about the thermal state of biological



Bright silver sulfide (Ag₂S) nanocrystals can be used efficiently for imaging and thermal sensing.

systems.³ However, to unleash the full potential of these nanocrystals, their brightness should be enhanced.^{4,5}

In this talk, we will present synthesis strategies and post-synthesis modifications that allow to increase the brightness of these nanocrystals. Their prowess as contrast agents and thermal nanosensors will be showcased with examples of applications at the preclinical level. Challenges lying ahead and promising research directions will also be highlighted.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Hybrid nanoscale materials for light-energy conversion and storage

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Hybrid structures of nanoscale materials can offer exciting opportunities for optoelectronic and energy applications. With the discovery of two dimensional (2D) transition metal dichalcogenides (TMDCs) a new family of semiconducting monolayer structures has emerged. The single layer nature and large surface area brings along interesting opportunities. Tightly bound trions are obsered even at room temperature as a consequence of the greatly enhanced Coulomb interactions and the reduced dielectric screening. The large surface and high interaction area of 2D TMDCs highlights also the option to combine the atomically thin monolayer with other nanoscale structures, such as zero dimensional (0D) solution processed nanocrystals. Such 0D/2D hybrid nanostructures found great attention in recent years due to the ease of fabrication from solution. In fact, 0D nanocrystals offer a variety of different materials properties, ranging from high absorption cross secions, large photoluminescence quantum yield and other light induced properties. In this contribution, I will introduce 0D/2D hybrid systems in which efficient charge transfer was observed even over extended time scales. I will highlight the mechanisms behind the interactions and give prospects for the exploitation of such 0D/2D structures for solar energy applications.^[1-4]

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

From the Cosmos to the Nanoscale: Nanostructured Permanent Magnets for a Green Energy Transition

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Nowadays the lack of sustainable access to several Critical Raw Materials (CRMs) is probably the most serious challenge faced by the European raw materials sector with the permanent magnets to be one of the most vulnerable categories from this condition. Substitution of CRMs (e.g. rare earths and cobalt) in permanent magnets is one of the priority approaches to advance towards a wise diversification of the permanent magnet sector in Europe. An strengthen coexistence of rare earth-based and rare earth-free magnets will play a key role to achieve a green transition. This presentation will start providing an insight on two promising rare earth-free alternatives to contribute to fill the enormous performance gap existing between ferrite and NdFeB, and will end by looking at the cosmos in the search of a future super-magnet.

Mn-Al is a good candidate for substituting bonded Nd-Fe-B magnets. Maximization of the magnetization in the system goes through the synthesis of the only ferromagnetic phase: τ -MnAl. However, an effort focused solely on obtaining this phase will compromise coercivity. Application of "flash-milling" method (record milling times of 30–270s) to gas-atomized MnAlC particles, has resulted in a powder material with a coercivity of 3 kOe (tunable up to 4.5 kOe) and a high remanence, successfully used as precursor in the fabrication of MnAlC magnets [1,2]. As it will be discussed, a combination of efficient nanostructuring and phase transformation processes eases the development of functional magnetic properties in Mn-Al.

In spite of the long history of hard ferrites, the possibility of improving their magnetic performance means an exciting scientific and technological challenge [3]. The trend over recent years has involved the use of CRM additives (e.g. La and Co), which brings again a lack of materials sustainability. It will be shown the possibility of developing a high-coercive (> 6 kOe) Sr-ferrite nanocrystalline powder through the combination of grain size refinement and induced microstrain, sustained on the creation of a nanocomposite system based on resources widely available in Europe.

The EU H2020 project *PASSENGER* will be briefly introduced, as one of the largest international initiatives aiming at the establishment of 8 pilot plants in Europe by 2025 for the industrial fabrication of these two permanent magnet alternatives by 2025 [4].

The presentation will end with an overview on a potential and extremely challenging permanent magnet alternative to the strongest NdFeB magnets existing nowadays, based on findings done on some meteorites.

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SHIFT 2022 - Spectral sHapIng For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Solar Thermal Management Materials

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oral

Since the beginning of civilization, humanity has built houses to sustain comfortable living conditions throughout the seasons. In our modern society, about 50% of the total energy consumption is used for heating and cooling. Growing demands for thermal management in many different sectors, from electronics to housing, inevitably mean increased energy consumption. The primary source of heat is coming from the combustion of fossil, bio or waste-based feedstocks, all contributing to carbon emissions.

In this lecture I will present how we are working on developing materials that capture, store, and release both solar and ambient heat without creating any emissions.

These solar thermal management materials are a unique combination of molecular photo-switches that capture and store solar energy, so-called MOST systems, that together with phase change materials (PCM) can contribute to thermal management. The two classes of materials operate at fundamentally different principles. The input of MOST system is photons, and the output is heat whereas PCM can absorb heat from the environment. By combining the two materials into one, we can harness and upgrade two of the most abundant renewable sources of energy on the planet: ambient heat and sunlight.

The talk will begin with introducing molecular synthesis and design principles, and then transition into materials function demonstrated in lab scale energy capture heat release as well heat to power devices.



Figure 1. (*Left*)) Molecular structure of on NBD/QC photoswitch system. (Centre) Stability test performed at 60 °C through 127 energy storage cycles (right) Illustration of MOST power generation concept.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Novel organic semiconductors as downconverters for photonic applications and low power lighting

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Materials suitable as active components in organic light-emitting diodes (OLEDs) have attracted widespread interest in recent years, as this technology develops towards replacing existing less efficient technologies, e.g., incandescent and fluorescent bulbs, in consumer applications such as solid-state lighting. To this end, both polymers and molecular structures have been exploited. Whilst polymers offer high luminescence and solubility, they can suffer from problems associated with high polydispersity and batch-to-batch reproducibility. Molecular or oligomeric systems offer advantages such as monodispersity, synthetic reproducibility and, depending on structure and device fabrication requirements, they can be processed via vacuum deposition or solution processing techniques. They can be tuned by chemical structure to emit light at any desired wavelength in the visible spectrum (see figure below). At the same time, they can be tailored to absorb at various wavelengths and the absorption/emission characters can be independent of each other. This makes organic materials highly suitable as frequency downconverters for device applications.



Devices emitting white light with higher efficiencies than traditional light bulbs are much sought after. Significant improvements have come through the development of inorganic white light emitting diodes (LEDs) based on gallium nitride and organic versions employing polymers, macromolecules or molecules. This presentation describes a hybrid approach, combining yellow-emitting organic materials with a blueemitting inorganic LED. This approach couples very efficient blue emission with the flexibility, tunability, facile processing and cost effectiveness of the organic colour converter. This presentation will cover a range of organic semiconductor materials designed for colour tunability and facile processing for photonic and optoelectronic applications.



Phosphor-Up-converted white LEDs assisted by 1-D photonic crystals

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Feel free to include figures, tables, acknowledgements and references, but please adjust to ONE PAGE limit. (Font: Calibri, 12pt)

The unique advantages of White Light Generation (WLG) by means of Light Emitting Diodes (LEDs), such as high luminous efficiency, reduced energy consumption and robustness, can be obtained by combining a blue LED with a lanthanide (Ln)-doped phosphor like YAG:Ce3⁺, that has a broad yellow emission which, combined with the complementary blue LED excitation, mimics WLG. However, this phosphor-converted LED (pc-LED) approach, which uses (Stokes) down-conversion light emission, suffers from a red deficiency that increases the Color Temperature towards "cool white light" above 5000 K, together with high LED chip costs.

The pUc-LED concept wishes to overcome these issues by achieving WLG through (anti-Stokes) Upconversion (Uc) photoluminescence, without energy losses due to Stokes shift and excited by a cheaper 980 nm LED in the near IR, using a low cost solution-based sol-gel (SG) technique. The SG process has various advantages in the preparation of the phosphor over other solid state techniques, namely in terms of equipment and energy costs, materials homogeneity and purity. Besides, the SG versatility allows the deposition of high quality one-dimensional multilayer photonic crystal structures in the form of Bragg Mirrors (BMs) or Fabry-Perot Microcavities (MCs), which can be easily integrated with the LED chip.

We have been able to obtain CIE white color coordinates x,y ~ 0.33 by Uc PL in a Ln-doped SG matrix based on the Tm/Yb and Tm/Er/Yb ion combinations and to select Ln-doped matrices (e.g. aluminosilicate glass and titania) with good performance towards WLG, with color temperature (CCT) values below 4000 K. Modifications of CIE parameters brought about by BMs or MCs are also addressed.



SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Searching for renewable energies: the breakthrough of perovskites. <u>I. García-Benito</u>^{*},^{1,2} J. Urieta,¹ A. Molina-Ontoria,¹ M. K. Nazeeruddin,² and N. Martín.¹

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Invited speaker; Technical area: Energy applications

When it comes to meeting our energy requirements, solar energy is regarded as one of the most promising alternatives to fossil fuels. Especially, perovskite solar cells (PSCs) are the most emerging area of research among new generation photovoltaic technologies, owning to their power conversion efficiency (PCE) up to recently certified 25.5%¹. Since the first-time reported all-solid state PSCs in 2012,² significant improvements have been done in deposition methods, chemical compositions, and synthetic techniques, among others. However, the full potential of this technology has recently been questioned by the relatively poor stability of perovskites under operative conditions.³

We have focused our efforts to the design of novel hole transporting materials (HTMs), crucial components to enhance not only the efficiency but also the stability of PCSs. Recently, we synthesized two novel HTMs based on electron-rich spiranic cores (**spiro-POZ** and **spiro-PTZ**) which were implemented in PSCs. In particular, two different PSC architectures were studied: mesoporous and planar, reaching PCEs up to 18.36% for **spiro-PTZ**, comparable with the PCE obtained with spiro-OMeTAD. Notably, the doped-HTMs exhibited excellent long-term stability, the PCE decreases by only 16% after more than 300 days in ambient conditions. Moreover, mesoporous devices retain 94% of their initial PCE after 1200h, under continuous 1 sun illumination.⁴ These impressive results confirm that long-term stability in PCEs can be nicely achieved controlling the interface at the perovskite layer and using doped HTMs by design.



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Seamless integration of photonics within harsh-environment resistant crystals with 3D laser nanolithography: Towards real-world advanced optical sensors

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The integration of optical sensors in environmentally aggressive media is a rarely addressed problem. Standard photonic sensors require from environmental protection and cannot be directly exposed to harsh environments, as either physical erosion, contamination or chemical modification of the sensor external optical surface can modify its functioning. Beyond surface, the mechanical and thermal properties of all involved materials need also to be assessed if the sensor is to be deployed in extreme environments with large temperature changes, high pressures, and vibrations, as thermally induced cracking and/or melting can take place depending on materials and their dissimilarity.

We recently developed a novel 3D nanostructuring process by which industrial hard optical crystals such as sapphire and YAG, which are extremely insensitive to chemicals, resistant to high temperatures and to extreme radiations, can be nanostructured within its volume with feature sizes on the 100 nm level, fabrication fidelity on the 10 nm level, and footprints on the cm-scale [1]. The technique may allow to develop fundamental nanophotonic devices such as photonic crystals, waveguides, gratings, and arbitrary architectures in general, opening up a new avenue of research merging nanophotonics and solid-state optical crystals material sciences.

In this talk we will revise the first principles of this 3D laser nanolithography technique, and the types of photonic and nanophotonic devices that are being devised based on our last experimental findings.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Plasmonic response of nanoparticles arrays and its potential applications

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By employing a spectral representation formalism,^[1] recent results in the study of plasmonic response metal nanoparticles individually and forming arrays. The spectral representation allows us to analyze the optical response by separating the geometry contributions from the dielectric properties of each nanoparticle and its surroundings. Neither numerical nor analytical methods can do this separation. These insights into the physical origin of the optical response are very useful for designing systems with desired properties and potential applications, such as the near-field energy transfer between nanoparticles by considering the coupling between all the thermal electric fields. In this talk, I discuss our results of near-field energy transfer between nanoparticles,^[2] the chiro-optical near-field response of achiral lattices,^[3] the plasmonic response of nanoparticles in non-Bravais,^[4] a honeycomb and vertical-stacked plasmonic lattices,^[5] as well as its influence on shaping and enhancing halide perovskites quantum dots photoluminescence.^[6]

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Lanthanide-doped Glass Light Guides with Bright Luminance in the Green Spectral Range

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The luminance limit in the green-yellow spectral range is still a challenge for modern light sources such as light-emitting diodes (LED), laser diodes, and lasers. This range suffers from a drop in efficiency, the so-called "green gap". Phosphor-converted ultraviolet or blue LEDs represent an interesting alternative to green-emitting LEDs. Here, luminescent borate glasses might be promising candidates as light-converter. They provide a high transparency, a wide glass-forming range, and a good solubility for lanthanide ions. The latter is in particular important for optical activation of the glass with lanthanide ions such as dysprosium (Dy³⁺) and terbium (Tb³⁺). Both ions enable for an intense green-yellowish (Dy³⁺) to green (Tb³⁺) luminescence upon excitation in the ultraviolet spectral range. Though the photoluminescence (PL) quantum efficiency of Dy³⁺ and Tb³⁺ amounts up to 40 % and 60 %, respectively, the luminescence yield is relatively poor. The main reason for this lies in the low optical absorption coefficients of the doped lanthanide ions. Here, luminescent light guides represent a promising way to accumulate the generated light and to enable an increased light output.

In this work, Dy³⁺ and Tb³⁺ single- and double-doped barium borate (BaB) glasses are investigated for their luminescence properties. Their potential as luminescent light guide is evaluated on the basis of ray-tracing simulations. Transmission, photoluminescence, and quantum efficiency measurements serve as input data. The luminous flux at the end of the light guide depends significantly on its length as well as on the surface properties. The best results are obtained for a light guide with the side faces coated with a 100 % reflecting mirror and a rough output face with Lambertian scattering characteristic.



Figure 1. Tb³⁺ single-doped barium borate glass light guide under parallel beam excitation with an ultraviolet laser diode (from the left). The excitation beam is almost completely absorbed over the length of the light guide. A small amount of the luminescence leaves the light guide via the side faces, while the largest part is guided to the end faces due to total internal reflection.



Freedom of spectrum utilization and customization of color and print in solar cell technology

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Now that the cost of PV electricity is approaching 0.01 €/kWh (utility scale) in some places *in Europe* (<u>www.etip-pv.eu</u>), it has become viable to investigate how PV panels can be produced so that they become more attractive in a wider range of applications, as to reach even higher penetration in the electricity mix. More surfaces in the built environment can be rendered into energy generating surfaces as we are now in a position to sacrifice a small fraction of the conversion efficiency to design more aesthetically pleasing PV modules. Colored solar panels can be used to replace conventional façade elements and make buildings more sustainable. Moreover, due to their vertical orientation, using facades for energy production prevents overloading the electricity grid around noon. A new PV manufacturing effort in Europe could address this market, while the more standard panels are mainly produced (for 70%) in China. Production in Europe would also reduce risks and potential bottlenecks in the supply chain.

In the presentation we will discuss the manipulation of incoming as well as outgoing (reflected) light spectra to provide unique features that standard outdoor PV modules do not offer. Several concepts for designing the color of PV modules are of interest. We investigate a 3D-printed external light trap to recycle various broadband sources of reflection on the module level and a design of the module that offers the option to provide simultaneously image displaying and energy harvesting PV modules.



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Flexible photonic systems: from 1D photonic crystals to active planar waveguides

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Invited

Specify Technical Area: Energy and other Applications

Thin-film optics is a key technology for the fabrication of miniaturized photonic devices, wherever the functional role resides in the layered structure of the optical material. Examples span from optical waveguides and photonic-integrated-circuits for optical signal processing, to multilayered resonant structures and cavities for the confinement and spectral selection of the optical field. Active optical waveguides and photonic crystals are among the most versatile examples. Applications range from optical communications and datacom including chip interconnections, to sensors and actuators, to optical filters and mirrors for solar modules. The design of thin-film photonic structures has been refined along decades and extremely sophisticated systems are now available. One further step to add versatility to this kind of systems involves the use of flexible materials, hence flexible photonics field. In fact, by adding mechanical flexibility to the rigid photonic systems, it is possible to greatly expand their application fields. One first example of this is represented by optical fibers and their diverse topology. When coming to more complex patterns and thin-films, design and fabrication must be carefully conceived to produce performant photonic structures. In passing from rigid to flexible substrates suitable fabrication protocols must be developed, to preserve the optical and spectroscopic properties of the systems even in presence of mechanical deformations.

Here, we present the fabrication of 1D photonic crystals and active Er^{3+} planar waveguides via Radio-Frequency sputtering technique on polymer (polyether-ether-ketone) and/or ultrathin flexible glass substrate. The structures deposited on ultrathin flexible glass have very interesting results in terms of both optical and mechanical properties, highlighting the perspectives of RF-sputtering as a promising technique t o fabricate flexible photonic structures also at the industrial scale.

Acknowledgments

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Field optimization for bifacial modules

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Bifacial modules are carving out an increasingly significant space within the photovoltaic market and the strategies of the main manufacturers. The bifacial photovoltaic module is a particular type of panel that manages to generate energy from both sides of the photovoltaic cell, thus increasing energy production compared to a standard photovoltaic module. The increase in production that a bifacial module can guarantee, thanks to the capture of the light reflected from the ground on the rear side, is a much appreciated advantage in large ground-mounted plants, for which payback times are still the most important item today. For this reason it is necessary to install components that can guarantee high production of electricity and better performance.

The Italian project PON Best4U (Bifacial Efficient Solar Cell Technology with 4-Terminal Architecture for Utility Scale) aims to achieve an efficiency of the photovoltaic system under standard conditions 25% higher than the single-side configuration. For this purpose, different approaches have been studied in parallel and will be compared. The most promising solutions will be defined and tested in a demonstrator field. The particular objective of the OR5 is the design of a bifacial photovoltaic field optimized for the exploitation of the albedo of the soil. The purpose is to identify suitable materials, to be deposited on the ground under and around the modules, in order to decrease the part of radiation that is not exploited by the modules, which would therefore be lost. The study is a collaboration between the National Institute of Optics of the CNR of Florence and by the University of Perugia. It was conducted considering the following aspects: identification of suitable materials for the optimization of the collected light, optical simulations of the possible configurations, field measurements on a small scale system.



SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Phase Diagrammes of Complex Materials: From the Katana, Swiss Chocolates to Organic Semiconductors Natalie Stingelin¹

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Specify Technical Area: __Biomedical X Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

In the past decade, significant progress has been made in the fabrication of polymer-based devices, such as organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) and organic photovoltaics (OPVs), predominantly due to important improvements of existing materials and the creation of a wealth of novel compounds. Many challenges, however, still exist: from achieving reliable device fabrication, increasing the device stability and, more fundamentally, gaining a complete understanding how structural features over all length scales affect important optoelectronic and photophysical processes in such polymers, including charge transport, charge generation, and general photovoltaic processes. Here we demonstrate how classical polymer science tools can be used to elucidate the structure development of semiconducting polymers from the liquid phase, how such knowledge can be exploited to manipulate their phase transformations and solid-state order and, in turn, their electronic features and device performances. More specifically, we will illustrate how rules that explain the mechanical properties of the Katana and distinguishes good from lesser tasty chocolates, can be applied to organic semiconductors to manipulate their properties and, hence, and their consequent performance when used as active layers in organic optoelectronic devices, with focus on organic organic photovoltaic cells. Moreover, we discuss how the relatively new fast-calorimetry technique, that can measure with rates of up to 5,000 °C/s can be used for the identification of thermodynamic transitions of donor polymers (PCDTBT) and acceptor molecules (fullerene derivatives) commonly used in the organic solar cell area. Examples are provided how the change in glass transition temperature of PCDTBT can be used to track polymer degradation upon light exposure. In short, we will demonstrate how thermal analysis can be exploited to obtain important structural information of organic solar cell materials (and beyond!), and processing guidelines can, in turn, be established towards materials of specific optical or electrical characteristics, and improved materials design for organic photovoltaic blends.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Nanostructure strategies towards performance-enhanced perovskite solar cells

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Organic-inorganic hybrid perovskite solar cells have attracted much attention due to their high power conversion efficiency (\geq 23%) and low-cost fabrication. Directions to further improve these solar cells include strategies to enhance their stability and their efficiency by modifying either the perovskite absorber layer or the electron/hole transport layer. For example, the transparent electron transport layer (ETL) can be an important tuning knob influencing the charge extraction, [1] light harvesting, [2] and stability [3] in these solar cells, or the use of up-conversion nanoparticles to get better performance in the near IR part of the visible spectrum. [4] Here we present two strategies based on nanostructuration, first a fundamental study of upconversion fluorescence enhancement effects near Au nanodisks by scanning near-field optical microscopy and second the effects of a nanocolumnar TiO2 layer on the performance and the stability of Cs0.05(FA0.83MA0.17)0.95Pb(I0.83Br0.17)3 perovskite solar cells. For the first case, the enhancement and localization of light near the metallic structures are directly visualized by using a single Er/Yb-codoped fluorescent nanocrystal glued at the end of a sharp scanning tip. [5] For the second we find that, compared to devices with planar TiO2 ETLs, the TiO2 nanocolumns can significantly enhance the power conversion efficiency of the perovskite solar cells by 17 % and prolong their shelf life. By analyzing the optical properties, solar cells characteristics, as well as transport/recombination properties by impedance spectroscopy, we observed light-trapping and reduced carrier recombination in solar cells associated with the use of TiO2 nanocolumn arrays. [6]

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Colloidal Quantum Dot Heterostructures for Photon Upconversion

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Please indicate preference: __Poster _X_Oral Specify Technical Area: __Biomedical _X_Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Photon upconversion is a process by which two or more low-energy photons are absorbed and one higherenergy photon is emitted by a material. Upconverters based on semiconductor quantum dot (QD) nanostructures are advantageous for solar energy applications because their optical properties are highly tunable with structure and composition. We previously showed that a QD-based upconversion layer can improve the efficiency of a single junction solar cell beyond the Shockley-Queisser limit by converting lower energy light into above bandgap illumination [1]. We have demonstrated NIR-to-visible upconversion in CdSe(Te)/CdS/CdSe core/rod/emitter nanostructures under continuous wave (CW) excitation. We also found that bandgap engineering through alloying resulted in a 10x improvement in upconversion efficiency and a 100x improvement in the upconversion PL/total PL ratio [2]. However, the upconversion efficiency remains limited by nonradiative recombination due to surface and interface defects. The performance of these heterostructures can be significantly improved through higher quality material interfaces and finer control over their morphology and composition. An advanced level of synthesis-structure-property control will also enable us to further investigate the effects of specific structural changes on upconversion efficiency. However, reliable fabrication of multi-component nanostructures presents a major challenge across the field, as complex structures introduce additional variables where controlled studies are lacking. We have synthesized analogous spherical CdTe/CdS/CdSe core/shell/shell structures to achieve better structural quality and passivate defect states that limit optical performance [3]. We systematically isolated and probed the effects of synthesis parameters such as particle concentration, precursor concentrations, and ligand ratios to determine their roles in the nanocrystal growth. We present a systematic study of synthetic conditions needed to realize the structural features we have found to facilitate efficient photon upconversion. This investigation of synthesisstructure-property relationships will help create a framework for rational design and synthesis of efficient nanostructures tailored for solar energy harvesting and conversion.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Bioleaching critical minerals from end-of-life feedstocks

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Please indicate preference: __Poster _X Oral Specify Technical Area: __Biomedical X_Energy and other Applications __SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Minerals such as rare earth elements, cobalt, lithium, nickel, and others are essential for computers, smart phones, electric vehicles, and other modern and future technologies but are often not readily available in the United States. These technologies are critical for communication, medicine, security, and green energy and transportation. Lack of a stable domestic supply of critical minerals can leave the U.S. vulnerable to dynamic markets, catastrophic events, and political or other global disruptions. To help bolster a sustainable manufacturing capability and mitigate future supply chain risks, we developed a bioprocess to recover critical minerals from end-of-life (EOL) products or waste streams. We have researched the effectiveness of biorecovery of critical minerals from industrial wastes such as petroleum fluid catalytic cracking catalyst, fluorescent phosphor powder, and phosphogypsum (fertilizer & phosphoric acid waste). Additionally, we determined the economic benefit and environmental impact of our biorecovery process. To further reduce the carbon footprint and improve the economics, we found that agricultural and municipal wastes can be used to produce the bioleaching solutions for recovery of these minerals. Recent efforts to bioleach and separate critical minerals from EOL materials such as magnets and lithium-ion batteries (LIB) have also proven successful. For example, using design of experiment modeling and laboratory testing, we identified optimal leaching conditions for improved economics of a LIB bioleaching process and anticipate a \$39M NPV and improved environmental sustainability as compared to other leaching technologies. This presentation will provide a summary of our bioprocess and recent research results.



SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Responsible rare earths: circular economy approaches including life cycle assessment

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Many of us buy fairtrade coffee, tea or bananas but how many of us think about the origin of the raw materials in our complex manufactured goods? Responsible sourcing is fast becoming an important issue in manufacturing, accelerated by public attention to a few high profile stories, such as conflict minerals ('blood diamonds and 'coltan') or child labour (cobalt) that are are driving change. Rare earth elements (REE), despite all their wonderful properties, have a poor reputation in regard to responsible sourcing. Years of bad environmental performance by many of the Chinese producers, the common association with radioactive thorium and uranium and the high energy demand to manufacture ores to alloys all lead to a view of rare earths as rather undesirable raw materials. In energy applications, we need REE more now than ever before, and in larger quantities, for example, to produce the direct drive motors and generators in electric vehicles and wind turbines. Responsible sourcing is needed quickly to aid the energy transition.

Geologists sit right at the beginning of REE supply chains and there is much that we can do to be involved in the responsible sourcing agenda. We need to understand the formation and nature of REE deposits. There are plenty of them to choose from as future sources. These range from mineral sands to igneous rocks, to weathered rocks with REE adsorbed on clays, to by-products of other mineral production. We need to integrate environmental and social Issues into our new geomodels, as in the EU H2020-funded HiTech AlkCarb project, which created new geomodels for rare earths in alkaline rocks and carbonatites.

We need to make quantitative comparison of the environmental impacts of mineral production from different deposit types via life cycle assessment (LCA) techniques that speak the same language as manufacturers. These techniques can forecast and lower a mine environmental footprint throughout its lifetime.

We need to join up with colleagues across the full value chain to instigate circular economy approaches. This includes better communication with researchers creating new REE materials; thinking about which REE and other element combinations are most environmentally efficient. It also includes better integration of 'Mining' and 'Recycling' that are often separated at either end of the linear value chain. But both are raw materials suppliers in a circular economy and there are many geological skills can be applied equally well to the anthropogenic stocks of minerals as to the original raw materials.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Materials for banknotes security

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

Banknotes, specially euro banknotes, stand out for being a very technological product, not only for the production processes they must follow until their issuance, but also for the myriad of technologies and materials they incorporate that guarantee the banknote security and authenticity.

The anti-counterfeiting measures run from eye-catching security features that ease banknote recognition by citizens to readable security elements that facilitate the automatic machine banknote processing and authentication.

In order to keep counterfeiters away, the Eurosystem endeavours to continuously run and fund R&D projects. However, security is not the unique commitment the Eurosystem is involved in. Sustainability and durability are also principal driving forces that encourage the Eurosystem to keep updating euro banknotes. In this sense, all materials employed in banknote production have to accomplish with high health and safety standards and to facilitate the reduction of the banknote environmental footprint from a cradle to grave perspective.

In the presentation, we will review the current technologies employed for the euro security and show the processes and categories of R&D projects. Should you wish to help us achieve a more secure, durable and environmentally friendly euro banknote, please contact us.



Fig 1: Banknote glow under standard (left) and special (right) UV light. Source: European Central Bank



SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Halide perovskites for next generation optoelectronic devices

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Invited speaker Specify Technical Area: Energy and other Applications

Halide perovskites are generating enormous excitement for their use in high-performance yet inexpensive optoelectronic applications. Nevertheless, , these solution processed materials have a plethora of microand nano-scale heterogeneities and their impact on performance and stability need to be understood.

Here, we will describe a series of multimodal microscopy measurements to determine the relationship between material structure, chemistry and photophysical properties. We will show how synchrotron nanoprobe and optical spectroscopic methods correlated at the nanoscale explain why this emerging family of semiconductors is remarkably tolerant to defects. These observations reflect that the quest of highly pristineness in traditional semiconductors such as c-Si or GaN is not necessarily a condition for low temperature, solution processed halide perovskites to perform well when integrated into devices. We will comment on the implications these findings have for the fabrication of highly efficient solar cells, LEDs and high-energy detectors.



SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Molecular Solar Cells. From Dyes to Hybrid Semiconductors)

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During my lecture I will present our latest results^{1,2} on the characterization of different type of solar cells from DSSC and OPV to MAPI using advanced photo-induced time resolved techniques. Using PICE (Photoinduced charge extraction), PIT-PV (Photo-induced Transient PhotoVoltage) and other techniques, we have been able to distinguish between capacitive electronic charge, and a larger amount of charge due to the intrinsic properties of the perovskite material. Moreover, the results allow us to compare different materials, used as hole transport materials (HTM), and the relationship between their HOMO and LUMO energy levels, the solar cell efficiency and the charge losses due to interfacial charge recombination processes occurring at the device under illumination. These techniques and the measurements carried out are key to understand the device function and improve further the efficiency and stability on perovskite MAPI based solar cells (Figure 1).



Figure 1. Use of self-assembled molecules as selective contacts in methyl ammonium lead iodide (MAPI) perovskite solar cells.

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SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Porphyrinoid-Based Charge and Photon Management Dirk M. Guldi

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At the heart of much of our research is the application of porphyrinoid molecules for **Solar Energy Conversion** schemes in terms of novel electron donor-acceptor ensembles and interfaces. Our expertise in time-resolved laser spectroscopic methods (i.e., femtosecond transient absorption spectroscopy, nanosecond transient absorption spectroscopy, flash-photolysis, time-correlated single photon counting), photochemistry, electrochemistry (i.e., spectroelectrochemistry and photoelectrochemistry) and photovoltaic device characterization gives assists in providing insight into fundamental aspects of **Photon**and **Charge-Management**. I will elude on how we leverage our ability to develop basic knowledge about processes that govern modular assemblies of nanoscale interfaces to reach macroscopic scales. To this end, I will highlight our interwoven work, which implements microscopic and ultrafast time-resolved spectroscopic investigations, and, which are perfectly complemented by device performance measurements and catalytic production of $H_2/O_2 -$ all of them as analytical tools needed to analyze systems that convert solar energy into useful sources of power.



SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Hydrogen: present and Future

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Hydrogen is one of the key technological solutions for decarbonization and electrification, but it is not the only one. There are electrical options such as batteries, intermediate transitions such as biogas, and other options that will surely be developed in the coming years allowing to define the future energy mix to reach the 2050 zero emissions goal. It is true that for some applications hydrogen is the best solution and so far the only one to decarbonize it, such as heavy transport or the railway sector, for example.

This keynote aims to review the European and National plans to develop and deploy the hydrogen economy, based on the objectives defined for 2030 and 2050 to be net zero emissions. Spain, as a key country in this development and deployment of renewable hydrogen, shows its great renewable capacity and integration, in addition to its privileged geographical location.

Real applications of the use of renewable hydrogen in different industrial sectors are mentioned to show the wide potential that hydrogen can provide towards decarbonization, both as an energy vector and as an industrial raw material.

Likewise, the main ongoing and future European and National projects are also reviewed. It can be observed how the entire hydrogen value chain is covered, from the production, based on renewable sources and their storage, to its transformation into energy again based on fuel cells, or its final application.

Finally, the future European and National challenges are mentioned, with the aim of being able to meet the fixed objectives to achieve the complete decarbonization of the economy to reach a net zero emissions by 2050.

Key words: Hydrogen, green hydrogen, renewable energies, decarbonization, Zero emissions, electrolysis, fuel cells, applications, strategy, roadmap, Europe, Spain, challenges.



Shining a light on biomedical and energy applications

Upconversion emission properties in transition metal, lanthanide co-doped systems: a spectral selective, time-resolved investigation

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

We investigate the upconversion (UPC) emission properties in transition metal (TM), lanthanide (Ln) based systems in spectral and temporal domains. The questions we address are the following: How the low solubility and heterovalency of transition metals impact on the local structure, and hence the f-f absorption/emission transitions of Ln? How the spectral selective and time-resolved excitation impact on the Ln emission colour, intensity and dynamics compared to fixed, cw excitation? To what extent the complex picture of UPC processes includes the Yb -TM dimer sensitization? We seek answers to all these questions using a battery of spectral and temporal resolved luminescence approaches monitoring several Ln absorption/emission transitions, emission decays and energy density dependencies.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Synthesis of MnAIC / Hydrogel Inks for Fabricating Alternative Permanent Magnets by Bonding and 3D-printing

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

High-tech sectors are increasing their interest on 3D-printing as it allows for fabricating complex and highperformance objects with tailored properties and a minimal waste generation [1]. The manufacturing of permanent magnets (PMs) by 3D-printing requires high filling factors and preserving the PM properties. On the other hand, an important research and technological effort is dedicated on finding alternative rare earthfree PMs. MnAl-based alloys are promising alternative candidates due to the high availability of constituent elements and diminished environmental impact [2]. The potential that MnAlC shows for developing alternative PMs by 3D-printing using Fused Filament Fabrication (FFF) has been demonstrated recently [3].

This work is focused on developing magnetic composites, using a hydrogel as matrix material and gasatomized τ -MnAlC particles (mean particle size of 50 µm) as filler. The hydrogel matrix was synthesized using alginate (ALG) and methylcellulose (MC) as thickener additive. It was found that 2.5:1 ALG:MC ratio allows for an adequate viscosity of the resulting composite to be loaded in syringes (Fig. 1a) for 3D-printing by direct ink writing technology.

Figures 1b and 1c show Scanning Electron Microscopy (SEM) images of the resulting cured composites, where it is observed a smooth surface with the MnAIC particles well dispersed along the hydrogel. The hysteresis loops (Fig. 1d) of the composites with different MnAIC load were measured by Vibrating Sample Magnetometry (VSM), showing that the magnetization scales with the MnAIC content, while the coercive field remains constant. This shows that the magnetic properties of the MnAIC particles are not deteriorated along the ink synthesis. The composites have shown suitable and promising properties for their application in the development of a new generation of alternative PMs by bonding and 3D-printing technologies.

Figure 1. (a) Syringes loaded with hydrogel and inks with different MnAIC particles load; SEM images of the composites with (b) 35 wt% and (c) 50 wt% content of MnAIC particles; (d) Room temperature hysteresis loops for the composites with 35 wt% and 50 wt% MnAIC content compared to the measured for the starting MnAIC powders.



Applied Field (kOe)

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Effect of Chalcogen Substitution Atom on the Performance Parameters of PM6:Y6-based Ternary Solar Cells

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

Ternary organic solar cells (TOSCs) are a promising strategy to improve the power conversion efficiency in organic solar cells¹. The combination of fullerene and non-fullerene acceptors works to optimize the light absorption and phase separation for better charge dissociation and collection². Currently, it has been reported that PCBM61 and PCBM71 as third component allows to improve the efficiency of PM6:Y6 binary system. The main role of the fullerenes lies on the enhancement of the V_{OC} and morphology. The effects on the morphology result in the reduction of recombination, and improvement of FF ^{3,4}. This work describes the synthesis and characterization of three chalcogens substituted PCBM derivatives with a 5-membered aromatic ring linked to the methyl ester position with the objective to study the relationship between interphase separation and power conversion efficiency. Therefore, the effect of furan, thiophene and selenophene in the PCBM derivatives (PCBFu, PCBTh and PCBSe, respectively) are investigated on the photovoltaic performance of ternary organic solar cells based on PM6:Y6. We observed that the addition of the PCBTh and PCBSe derivatives increase the short circuit current density and the fill factor pointing to the suppression of charge recombination. In addition, surface analysis confirms that the morphology is optimized in both cases, which implies that organized thin film nanomorphology is key for suppression of carrier losses.



Figure 1. a) Devices structure; b) Current-density vs. voltage characteristics under AM 1.5G illumination; c) EQE spectra of binary and ternaries devices.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Self-Assembled Molecules as Selective Contacts in CsPbBr₃ Nanocrystal Light Emitting Diodes

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

Metal halide perovskite nanocrystals (PerNCs) have demonstrated their potential as light sources when forming part of efficient light emitting diodes (LEDs). However, despite these promising results, PerLEDs still face two main challenges to approach commercial market counterparts, which are long-term stability and efficiency. The nanometer-sized PerNCs semiconductors exhibit narrow full-width at half maximum photoluminescence, hence high color purity, and high PL quantum yield, both features strongly required for LED application. Furthermore, the density of surface defects of PerNCs can be reduced by proper surface passivation. Yet, the presence of defects at the interface between the NCs and the carrier transport layers also affects charge transport and injection and, consequently, the stability of the device. In this direction, molecular passivation of the perovskite interfaces has demonstrated its potential to reduce non-radiative recombination and increase the stability of the devices.

In this work, we report the application of two carbazole-based self-assembled molecules (SAMs), **EADR03**, and **EADR04**, (see Figure 1a), to enhance the hole injection in CsPbBr₃ PerLEDs (Figure 1b). Such devices (measured in controlled atmosphere without encapsulation) featured an increase in the luminance compared to the devices prepared with the widely used polymer PTAA amine or without hole transport material (HTM) (Figure 1c). Moreover, despite **EADR03** and **EADR04** structure differs in one phenyl ring in the bridge, the extra ring provides more stability to the devices, even surpassing the one obtained with PTAA. Through the analysis of the data obtained by structural and optoelectronic characterization, we will describe the contribution of the SAMs and the influence of their structure to the performance of the devices.



Figure 1. a) Chemical structure of the SAMs used in this work, b) scheme of the prepared devices, and c) luminance vs applied bias of the devices prepared with SAMs, PTAA or without HTM.



Understanding the Role of Particle Size in the Development of Flexible Permanent Magnet-Polymer Filaments for Additive Manufacturing

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Additive manufacturing (AM) of composites is attracting much interest in high-tech sectors for fabricating complex high-performance objects with tailored properties [1]. For permanent magnets (PMs), the challenge is to develop magnets by AM with no geometrical restrictions, high filling factor (FF), and non-deteriorated PM properties [2], together with finding alternatives to rare earth-based magnets [3].

Composites (PM particles/polymer) based on τ -MnAlC, Sr-ferrite, NdFeB, and hybrid (Sr-ferrite/NdFeB) powders (mean particle size: 5-50 μ m) were analyzed. The different composites (FF>80%) allowed for obtaining filaments (length > 10 m) with coercivity ranging between 1.5-10 kOe [4]. Particle size was crucial for extruding flexible filaments, being the extrusion effectiveness and FF enhanced by optimizing the fine-to-coarse particles ratio. MnAlC-based objects were 3D-printed under controlled temperature, proving that alternative materials can be efficiently synthesized and processed to develop novel PMs by AM (Fig. 1) [4].



Figure 1. (a) Images of gas-atomized MnAIC particles, polymer, MnAIC/polymer composite, filament and 3D-printed objects; and (b) 3D-printed MnAIC-based disc together with the 3D plot and 2D maps of the magnetic flux density measured at the disc surface.

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Shining a light on biomedical and energy applications

Novel Carbazole-Based Conjugated Molecules as Self-Assembled Hole Transporting Monolayers for Inverted Perovskite Solar Cells

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Renewable solar energy is considered the main candidate to provide clean and green energy for the upcoming years. Among the different types of photovoltaic technologies available, inverted perovskite solar cell (IPSC) is a promising approach due to their easy fabrication and low manufacturing cost with minimum environmental impact. Inverted structure (p-i-n configuration) consists basically in a light-absorbing perovskite layer which is sandwiched between a hole transport material (HTM) and an electron transport material (ETM) (**Fig 1a**).[1]

The use of organic self-assembled monolayers (SAMs), as a HTM materials in the interface of IPSC devices, have recently attracted the attention because of their easy preparation, low costs, good solution deposition and the ability to tune the properties of these materials by modifying their chemical structure.[2] This work aims to design and synthesize new carbazole-based conjugated molecules, featuring special functional groups, to study and understand the effects and interactions at the SAM/perovskite interface, improving the performance of IPSCs devices. Thus, setting the carboxylic acid function (-COOH) as an anchoring group and the biphenyl moiety as a conjugated spacer linker, different functional groups, were included in the carbazole core of the prepared SAMs (**Fig. 1b**).



Figure 1. a) Inverted perovskite solar cell device architecture, b) chemical structure and constituents of SAMs synthesized in this study.

All the new compounds were well characterized by spectroscopy and spectrometric techniques and the stability, performance, changes in the surface work function (WF) and surface dipoles additions in the SAM/perovskite interface were study in the fabricated IPSCs devices.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Upconversion luminescence of novel FeS₂@NaYF₄: Yb³⁺, Er³⁺ nanocomposites

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Two world common elements, Fe and S, are elements that build all types of iron sulfides with different chemical compositions, crystal structures, and photophysical properties, i.e., troilite (FeS), pyrrhotite (Fe($_{1-x}$)S, x=0-0,2), pyrite (FeS₂), marcasite (FeS₂), or greigite (Fe₃S₄). Those types of materials can be synthesized via the hydrothermal method. Iron sulfides are semiconducting materials that absorb radiation in a broad spectrum range; nanosized particles can exhibit weak plasmonic and magnetic properties [1].

UC is an energy conversion process where one photon of high-energy radiation is emitted after excitation with two or more low-energy photons. The hexagonal sodium yttrium fluoride (β -NaYF₄) is a well-known matrix material for upconversion luminescence (UC). Due to its low phonon energy and high chemical stability, it has been confirmed as one of the most efficient UC host. The material doped with Yb³⁺/Er³⁺ ions shows exceptional UC properties. Here, after excitation with Yb³⁺ ions with λ = 975 nm laser, characteristic emission bands of the Er³⁺ ions can be observed. The emission of Er³⁺ ions from thermally coupled levels ($\lambda \approx 525$ nm) changes the intensity with temperature alteration in the system [2].

Nanocomposites are nanomaterials consisting of two or more phases of solid materials with at least one dimension in the nanoscale (≤ 100 nm). Here, the NaYF₄: Yb³⁺/Er³⁺ nanocrystals and FS₂@NaYF₄:Yb³⁺/Er³⁺ nanocomposite were synthesized. The physicochemical and photophysical properties of both materials were compared. The FeS₂ absorption properties and UC luminescence of NaYF₄: Yb³⁺/Er³⁺ were combined. Both materials, i.e., FeS₂@NaYF₄:Yb³⁺/Er³⁺ and NaYF₄:Yb³⁺/Er³⁺ exhibit visible-green up-conversion luminescence. The different ratio between emission bands (color tuning) was observed due to interaction between the materials core and shell. The influence of temperature on the UC luminescence properties for both materials was investigated. These innovative materials can be used in optoelectronics, detection and security systems, and as novel sensors.

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Machine learning and the improvement of readouts provided by luminescent thermometers

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Figure 1. Advantages of computational methods in luminescence thermometry.

As highlighted in recent developments of luminescence thermometry ^{1,2}, the future of the field heavily depends on the synthesis of luminescent probes capable of providing highly precise and accurate thermal readouts. As a consequence, much weight has been placed by the scientific community on the production of stable and highly luminescent thermometers. While such an approach has justifiably its place and merit, the fact is that there are hardly any researchers searching for other routes of improvement. In particular, the maximization of profit from the calibration data provided by their probes is almost completely neglected. In fact, most of the time the selection of the thermometric parameter to be used is only based on a visual inspection of the luminescence spectrum of the sample. While some progress has been made in that sense with, for instance, the work of Maturi et al.³ in which a multiple linear regression is applied to many parameters, the exploitation of computational methods to build better regression models is still in its infancy in the field of luminescence thermometry. In this work, we contribute to that regard by showing how the use of dimensionality reduction (i.e., the transformation of data from a high-dimensional space into a lower dimension one) algorithms or neural networks are very powerful to provide more reliable thermal readouts than the ones provided by the commonly selected thermometric parameters.

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Designing all-photonic molecular analogues of electrical components: a molecular filter based on Ln³⁺

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The increasing demand for computing power and downscaling is reaching the limits of incompatibility with the lithographic methods limitations, precluding further the shrinkage of the electronic components using state-of-the-art top-down approaches.^[1,2] In addition, the current chip shortage exposes the excessive world dependence on silicon, stressing the need for silicon-free active and passive components. Among the diverse strategies followed so far, molecules that can replace the active electronic components is emerging as a promising alternative, combining the reduced dimensions with a new paradigm of interaction using photons instead of electrons.^[3,4] In this presentation, we will address a Eu³⁺/Tb³⁺ co-doped di-ureasil organic- hybrid material as an illustrative example of an all-photonic device based on the emission temporal dynamics of Eu³⁺ and Tb³⁺ ions. The all-photonic active device presents temperature-reprogrammable changes from a low pass filter to a high pass one, being studied in solid state, which constitutes a firm step forward towards the rational design and development of molecular analogues for conventional electrical circuit passive components.



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Simulating the emission of co-doped Yb³⁺/Er³⁺ upconverting nanoparticles

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Lanthanide-doped nanoparticles (NPs) have great potential for energy conversion applications, as their optical properties could be manipulated by changing the doping amount, the NP size, the surface coating, and through the plasmonic coupling effect in the presence of metallic nanoparticles.^[1,2] Concerning the well-known Yb³⁺/Er³⁺ upconversion NPs (*e.g.*, NaYF₄:Yb³⁺:Er³⁺), the Yb³⁺–Er³⁺ energy transfer plays an important role in the red (Er^{3+ 4}F_{9/2}→⁴I_{15/2}) and green (Er^{3+ 2}H_{11/2}→⁴I_{15/2} and ⁴S_{3/2}→⁴I_{15/2}) emissions upon excitation at 980 nm (Yb^{3+ 2}F_{7/2}→²F_{5/2}) (Fig. 1). However, the determination of the distances (distribution) between donor and acceptor Ln³⁺ ions inside an upconversion NP is still a challenging task.^[3]







Fig. 2. Example of a doping process simulation with Yb^{3+} (18%) and Er^{3+} (2%) in a NaYF₄ spherical NP with 6 nm of diameter.

Despite advances in the calculation of Lnenergy transfer rates,^[4–6] the Ln distribution of the Ln³⁺ inside a real-size NP was not addressed due to a lack of a computational code that can simultaneously simulate a doping process and extract Ln-Ln distances in one NP containing dozens of thousands of host atoms. In this sense, we developed a code (written in C) that can simulate the doping process and extract the Ln-Ln distances distribution in an entire spherical NP in a few seconds (Fig. 2).

Once the Ln–Ln distance distribution is obtained, the Ln-Ln energy transfer rates are estimated and applied in a system of rate equation model describing all interactions between the $|N\rangle$ states (Fig. 1). The solution of a rate equation model

provides the population of each level, including the $Er^{3+4}F_{9/2}$, ${}^{4}S_{3/2}$, and ${}^{2}H_{11/2}$, responsible for the emissions in the green and red spectral ranges. Therefore, this work implements, for the first time, simulations of the emission of real-sized upconverting NPs, opening perspectives on the modeling of the dependence of the red and green emissions with temperature and with the excitation power density.

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Upconverting luminescent material as an all-photonic platform for molecular logic: from basic to more complex logic operations

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications ____ SHIFT-DBL (Satellite Meeting "Light beyond energy")



The ongoing evolution of the internet of things, digitalization, and networking are increasing the need for additional computing power, which is a major technological challenge. The future paradigm of computing requires logic elements constituted of nanomaterials with a rational design that can be obtained by employing bottom-up nanotechnology. In the early 90's, the pioneering work of Prasanna da Silva *et al.* inspired the first general and practical approach to information processing and computing based on molecules able to perform logic operations [1,2]. Since then, the research field grows to study systems based on organic molecules and exploiting chemical inputs [3]. Despite recognizing that nowadays trivalent lanthanide ions (Ln³⁺) can improve the state-of-the-art of Molecular logic devices, only a few works have been reported so far, and most of them respond to chemical inputs, operating in wet conditions. Nevertheless, physical inputs have several advantages as input-output homogeneity, reconfiguration, integration, remote control, and dry conditions, allowing the system to perform computing cycles of diverse logic operations [4].

Herein, we present an inorganic upconverting material based on Sr₂YF₇ crystal co-doped with Yb³⁺ and Er³⁺, to demonstrate the potential of these rationally designed platforms to implement different logic operations, through the unique photophysical properties of the Ln³⁺ ions. The optical response of the Sr₂YF₇:Ln³⁺ system can be fine-tuned by employing the features of the 980 nm pulsed excitation source delivering a fully controllable color tuning in the green-red spectral range that was exploited for defining innovative approaches to design diverse logic gates triggered exclusively by physical logic inputs.

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Understanding the anomalous behavior of liquid water through upconversion nanothermometry

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Water is the most important liquid of all, playing a fundamental role in many industrial and biological processes.^[1] However, despite being the most used solvent, water is the least understood because it presents anomalous properties when compared to the behavior of other common liquids. In the past decades, several researchers have shown that there are two distinct organizations of the molecules of water in the supercooled regime: a low-density liquid (LDL), with a more organized tetrahedral hydrogenbonding network, and a high-density liquid (HDL), with a distorted tetrahedral configuration.^[2] Therefore, if these different motifs remain coexisting under ambient conditions, the anomalous properties of water can be explained by their mixed properties. In this sense, we have developed a novel experimental approach to investigating the instantaneous Brownian velocity of upconverting nanoparticles (UCNPs) suspended in water.^[3] Once the Brownian velocity corresponds to the thermal motion arising from the particle-solvent interactions, the trends in the temperature-dependent Brownian velocity can give us powerful information regarding the temperature dependence of the hydrogen-bond network in the vicinity of the UCNPs.

In this work, we have been able to demonstrate that the crossover temperature (T_c) arising from the bilinear trend of the instantaneous Brownian velocity of the water suspended UCNPs at ambient conditions is related to the LDL-to-HDL conversion. Moreover, the variations in T_c resulting from changes in the size of the UCNPs or the pH of the aqueous media resemble the effect of changing the temperature and pressure in the phase diagram of pure liquid water, respectively. These results are indeed related to the anomalies of water because UCNPs suspended in other solvents containing hydrogen bonds, such as ethanol and heavy water, do not present such behavior in their temperature-dependent Brownian velocity trend. These findings are extremely relevant because they provide experimental evidence of the existence of two distinct organizations of water molecules under ambient conditions, paving the way for revolutionizing the understanding of biochemistry since the anomalous properties of water may be fundamental for the existence of life as we know.

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Shining a light on biomedical and energy applications

Enhancement of single nanoparticle luminescence and trapping force by surface plasmon polaritons

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The lanthanide-doped upconverting nanoparticles (UCNPs) are promising single-particle imaging probes thanks to their unique luminescence properties.¹ The plasmonic traps provide the potential to enhance the emission of trapped particles, break diffraction-limit, and stabilize traps. However, conventional excitation of surface plasmon polaritons (SPPs) by direct laser radiation causes thermal effect.² Herein, we demonstrated the excitation of SPPs by single UCNP to enhance the luminescence intensity of the same single UCNP and the trapping force acting on it. A 980 nm laser serves both to optically trap and to excite luminescence. A colloidal dispersion of NaYF₄: 2%Er³⁺, 20%Yb³⁺ UCNPs with bright visible emission (540-560 nm) was used to excite the SPPs. An Au-patterned substrate with a strong absorption at this wavelength was used to generate SPPs. Experimental results indicate that the luminescence intensity of a single UCNP is enhanced while using the Au-patterned substrate (Figure 1a). The laser power dependence of the optical trapping force shows a linear trend in both cases. The trapping force acting on a UCNP above the Au-patterned substrate shows a significant increase (Figure 1b). Such enhancement of luminescence and trapping force has a great potential in bio-photonic applications and stable nanoscale manipulation.



Figure 1. (a) Luminescence intensity of a trapped single UCNP: on glass substrate (top panel) and on Au-patterned substrate (bottom panel). (b) Laser power dependent optical trapping force acting on the single UCNP on glass and Au-patterned substrate.

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Down-shifting layers for silicon-based PV module applications

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Please indicate preference: __Poster _X_Oral Specify Technical Area: __Biomedical _X_Energy and other Applications ___SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

The silicon-based photovoltaic (PV) technology is under continuous improvement and nowadays plays an essential role in the decarbonisation of electrical systems mainly due to its feasibility, competitive costs and high efficiencies. The PV share is dominated by silicon technologies, representing around 95% of the market. mc-Si technology leads with approximately 60% of the share, in contraposition to c-Si technology, representing around 35% of the share. However, mc-Si technology is cheaper but exhibits a relatively poor response in the short-wavelength photons of the solar spectrum, mainly due to the thermalisation losses from the absorption of high-energy photons. Among the different available techniques to improve the short-wavelength response, one promising approach consists of using luminescent down-shifting (DS) layers, which convert the not harvested UV radiation into highly efficient visible light.

As a continuation of our work searching for efficient down-shifters for photovoltaic applications, in this work, we study the synthesis, the structure, and the photoluminescence of six new compounds with the general formula $[M1M2(bz)_4(phen)_2(tta)_2]$ where M1 and M2 can be Eu^{3+} , Gd^{3+} , Tb^{3+} and we study the effect of M1 and M2 on the photoluminescence. Moreover, we have encapsulated the compounds dispersed in an EVA film on a photovoltaic mini-module and studied the increase in the external quantum efficiency (EQE) and the evolution of the intensity-voltage (I-V) curves to quantify the improvement of the energy conversion in the photovoltaic process. [1]



Fig. 1. View of the mini-module under natural (a) and 340nm (b) radiation.

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Composites with lanthanide doped fluorescent particles for flying, seed-like soft robots that monitor environmental temperature

Shining a light on biomedical and energy applications

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Addressing environmental challenges requires sustainable strategies for accessing and monitoring environmental parameters. Current methods lack spatio-temporal resolution of data, have limited availability, and are based on active electronic components, which lead to high costs and *e*-waste.

We develop small, biodegradable flying objects composed of fluorescent sensing materials ("i-Seeds") that can act as self-deployable and biodegradable robots inspired by natural plant seeds. The seeds contain fluorescent and responsive materials that enable them to sense environmental parameters. Sensing is based on physical mechanisms or chemical transduction with fluorescence-based readout. Environmental parameters can thus be read *via* drones equipped with fluorescent LiDAR technology and geo-referenced with software in real time.

Here, we present fluorescent i-Seeds inspired from *Acer campestre* and *Tragopogon pratensis* natural seeds that monitor temperature as an environmental parameter. The artificial seeds are produced via 3D printing technologies using polylactic acid (PLA) polymer. This polymer was selected due to its biodegradability. The artificial seeds contain particles of upconverting lanthanide doped materials, which can absorb low energy excitation sources and convert it to emissions at visible wavelengths that are easy to detect by the drones. The concentration of these materials within the polymer host was optimized by investigating the optical and mechanical properties. They provide two functionalities: (i) they allow for fluorescent labelling for the detection of i-Seeds in the field, and (ii) their optical properties are temperature dependent, which allows us to quantify the local temperature. Using band-shape thermometry, we can reconstruct the temperature from the photoluminescence spectra, based on emission located with the RGB (red-green-blue) regions.

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Shining a light on biomedical and energy applications

Multi-material and multi-colour 3D printing enabled by upconversion and metallic catalyst

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Please indicate preference: 1st: Oral; 2nd: Poster

Specify Technical Area: Energy and other Applications

Near infrared (NIR) to ultraviolet (UV)/visible light upconversion (UC) has been demonstrated to have potential for 3D printing [1]–[3]. However, this method is limited in terms of throughput. Our approach utilizes the synergistic effect of Ag(I) ions to enhance the crosslinking of photopolymer via NIR to UV/visible UC, as shown in Figure 1 (a-b). This allows for faster fabrication than when using a traditional UV absorbing photoinitator. Furthermore, photopolymer 3D printing is limited in terms of multi-material integration. In our approach, after the 3D printing process, the Ag(I) ions embedded into the photopolymer serve as seeding sites for electroless copper plating (Cu), allowing integration of metallized parts, as shown in Figure 1 (c-d) [4]. Finally, selective plating enables the manufacture of objects with metal and plastic surfaces, all whilst simultaneously having the high resolution and low cost of stereolithography (SLA). Moreover, thanks to the enhanced penetration depth [3], this technique can be used to extend the capability of SLA for multi-material and multi-colour fabrication, as shown in the flexible-rigid (elastomer/acrylate) demonstrator of Figure 1 (e).



Figure 1: NIR to UV/visible UC-assisted laser patterning of photopolymer (a) without and (b) with Ag(I) ions; (c) schematics UC-assisted multimaterial manufacturing; 3D printed (d) dielectric/metal and (e) flexible/rigid demonstrators.

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Acknowledgments

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

New Frontiers for High-sensitivity Luminescence Manometry

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

Optical (luminescence) pressure sensing offers promising opportunities to investigate and monitor the variation of physicochemical and spectroscopic properties of materials under extreme conditions, by monitoring the selected manometric parameters (e.g. band intensity ratio, line shift, emission lifetime, FWHM). However, a limiting bottleneck for pressure readouts is the usually occurring quenching of the emission signal of the luminescent sensor material upon its high-pressure compression. Whereas, in the case of low-pressure sensing, the limitations are related to the fundamental concept of remote pressure sensing, i.e., measurements of physical parameters directly related to the material structure and affected by its compression, e.g. emission line shift, sound velocity, unit cell volume, etc.

Here we give a new look on the high-sensitivity high-pressure sensing, also showing how to significantly increase the luminescence signal intensity of the lanthanide-based sensor materials [1-3]. These goals can be realized by taking the benefits of the inter-ionic energy transfer and temperature/pressure-induced configurational crossover processes, the luminescence signal of the developed sensor materials can be enhanced by 2-3 orders of magnitude, with marginal quenching under extreme conditions. Moreover, we show how to overcome the limitations of monitoring the low-pressure range (i.e. vacuum), by changing the sensing concept from the materials compression to the light-induced heating-cooling of the active compounds, governed by the internal pressure of the system [4-6].

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From Polymer Films to Self Assembling Molecular Electrodes for Efficient and Stable Inverted Perovskite Solar Cells

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PTAA (polymer poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine]) and **Spiro-OMeTAD** (2,20,7,70-tetrakis[N,N-di(4-methoxyphenyl)amino]-9,90-spirobifluorene) are two widely used commercially available hole selective contacts (HSCs). In particular, **PTAA** shows high efficiencies in inverted (p-i-n type) perovskite solar cells (iPSCs), which are comparable with the record efficiencies of **Spiro-OMeTAD** in regular PSCs. However, using the relatively low-cost **Spiro-OMeTAD** as a HSC is meaningful for the cost-effective iPSCs compared to **PTAA**. This work modifies **Spiro-OMeTAD** by introducing a carboxylic acid anchoring group allowing it to form self-assembled monolayers (SAMs) as HSCs for iPSCs. The resulting devices showed comparable efficiencies with **PTAA** based devices, and excellent long-term illumination stability. Charge transfer and charge carrier dynamics are studied by using advanced characterization techniques to better understand the interfacial kinetics. Our results demonstrate that this **Spiro-OMeTAD** derivative as a HSC has a great potential in producing low-cost iPSCs devices with good long-term stability and high performance.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

OE-19

Hybrid nanosystems for new solar-based technology solutions

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Technological progress relies on solar conversion as one of the most promising alternatives for the clean and sustainable energy supply. But given the source intermittency and the fluctuations in the energy demand, another crucial aspect is the energy storage. Nowadays solutions make use of separated systems for the energy conversion and conservation, implying energetic losses and bulky structures while an interesting new approach consists in a synergistic and compact solution combining light absorption, charge separation and accumulation. Such idea will need strong support from the material science with new materials and structures or new systems exploring combinations of properties and functionalities. In this work I want to present very attractive nanomaterials like transparent conductive oxides as candidates for next generation of light driven optoelectronic with an eye on green solutions like carbon based materials as for the case of GQDs. Discussion will be also extended to the possible exploitation of multi charge transfers in order to enhance for example the efficiency of energy conversion. Regarding the first class of materials we analyzed in particular the case of Indium Tin Oxide in the form of nanocrystals and their optical and electronic response upon light intervention. From what concern the GQDs here we present the spectroscopic characterization of some derivatives for the potential use as host capable of delocalize new charges.





Outdoor performance of nanocrystal luminescent solar concentrators

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Please indicate preference: _X_ Oral Specify Technical Area: __Biomedical _X_ Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Deployment of photovoltaics (PV) in the urban environment is usually done by installing PV modules on rooftops. Making PV components an integral part of the building envelope is growing fast and is referred to as Building Integrated Photovoltaics (BIPV). BIPV solutions exist in opaque and transparent form, and both are designed to be part of building facades. The latter solution requires optimization of transparency in relation to efficiency as the PV-window has two functions. While transparent PV already is used, the Luminescent Solar Concentrator (LSC) in combination with side-mounted solar cells has been identified as a solution due to its ability to absorb only certain wavelengths allowing for tuning the apparent window color and transparency, and its low costs. The LSC has been a topic of research since the mid 1970s. In the past decade, alternative luminophores used in the LSC have been developed that are tunable and more stable than organic dyes, i.e., semiconductor quantum dots/rods, or, more generally, nanocrystals. LSC device efficiencies, however, are still low. Moreover, outdoor performance tests are rarely reported.

In this paper, we compare the outdoor performance of LSC devices for three different nanocrystal materials (InP, CdSe, CuInS₂), an organic dye (Lumogen Red), and a reference LSC, without luminophores. The nanocrystals are synthesized in sufficiently large quantities for use in coating a 50x45 cm² sized PMMA plate.

--2

The coating is laminated between two PMMA plates. On the four sides, strips of CIS cells are mounted (see figure pages). The five LSC devices are mounted vertically in North-South direction. I-V measurements are performed every 2 minutes for all four strips individually. The LSC devices have been monitored since mid-January 2020.



Results of show monthly average power outputs for all four cell strips combined in Watt (see figure for CuInS₂ nanocrystals) for a full year. Seasonal effects with higher power outputs in the summer months are observed, while degradation is absent. We will present data combined with average visible transmission (AVT) and indoor I-V measurements taken at standard testing conditions (STC), and show validation through ray trace and system modelling efforts.





10-14TH OCTOBER, 2022

hift²²

Shining a light on biomedical and energy applications

Lanthanide-based logic: a venture for the future of molecular computing

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications _____SHIFT-DBL (Satellite Meeting "Light beyond energy")

Managing the continuous and fast-growing volume of information, the progress of the Internet-of-Things, evolution from digitalization to networking, are huge technological chores. These are highly demanding challenges to Si-based integrated chips that are getting closer to the miniaturization limit with the current top-down approach, opening the gates to a new generation of efficient computing systems that constitute an unsettling step forward. [1] Information processing and computing based on molecules that perform logic operations may play a decisive role in the future of the computer industry.

Molecular logic gates are molecular counterparts of electronic devices [2,3] that, instead of exclusively electrical signals, can be stimulated by diverse chemical or physical input signals producing, many often, optical outputs according to a well-



defined logical transfer function. Among the distinct materials reported so far for molecular logics, the Ln³⁺based ones appear as a commendable choice, as they can respond to both chemical and physical stimuli, presenting the unique photophysical properties that them quite popular for photonics applications.

In this presentation, we will frame the main of contributions Ln³⁺-based materials in molecular logic, discussing their potential to integrate future molecular photonic-electronic hybrid logic computing systems. Examples of molecular logic devices using Ln³⁺ and exclusively physical stimuli, developed in the *Phantom-g* research group [4] will be revised together with a perspective on the major challenges faced by this field in the years to come.

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OE-21

For more information



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Shining a light on biomedical and energy applications

Upconversion for photovoltaics: can it ever really work?

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Oral – Energy and other Applications

This paper presents the highlights of our recent critical review regarding the opportunities for enhancing solar energy harvesting using photon upconversion (UC) ^[1]. The main focus is on UC for silicon photovoltaics (PV), given that this is by far the dominant technology. In particular, with bifacial PV technology (**Figure 1a**) it is relatively simple to attach a UC layer to the rear of the module. This work considers a lanthanide-based UC layer based on trivalent erbium (Er^{3+}) that after absorption of two 1400 – 1650 nm photons results in the emission of a single ~980 nm photon from the ${}^{4}I_{11/2}$ level of the Er^{3+} ion via energy transfer UC (**Figure 1b**). Theory indicates that the available photocurrent in the 1400 – 1650 nm region of the terrestrial solar spectrum could yield an enhancement of 2.77 mA/cm² (6% relative) for an ideal (50% efficient) UC system (**Figure 1c**).

However, our analysis demonstrates that many challenges remain before UC could significantly enhance the performance of silicon PV operating under terrestrial (non-concentrated) sunlight. Our photophysical model indicates that at least two orders-of-magnitude increase – in either, equivalently, i) the intermediate state lifetime, ii) the energy transfer rate, or iii) the generation rate – are required before such UC-PV can start to become efficient.

We discuss possible methods for increasing the generation rate, G, including the use of:

- geometrical optics for concentrating sunlight;
- ii) co-sensitizers to expand the near-infrared absorption range;
- iii) enhancing generation via plasmonic structures; and
- iv) enhancing generation via photonic structures.

The opportunities and challenges for each of these approaches to achieve efficient solar UC are discussed when applied to bifacial silicon PV, while financial considerations are also taken into account. Other pathways to success (*e.g.* via organic UC) as well as applications to luminescent solar concentrators (LSCs) and photocatalysis will also be briefly presented, time permitting.

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Figure 1(a) A bifacial silicon PV module harvests above-bandgap (280–1200nm) light from front side, while **(b)** a rear UC layer based on Er^{3+} can harvest sub-bandgap photons. **(c)** The terrestrial solar photon flux indicates that harvesting all 1400–1650nm photons with a UC efficiency of 50% could theoretically enhance the photocurrent density by 6% ^{[1].}





The study of three types of materials for "green" hydrogen production by water splitting: TiO₂, ZnO and CdS.

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Green hydrogen production represents a very promising contribution to a clean, sustainable, and renewable energy source. These photocatalytic materials play a key role in H_2 production, and it has proven that they are corrosion resistant, chemically stable, and highly efficient photocatalysts. In this work three main groups of photocatalysts are studied, namely titanium oxide, zinc oxide and $Zn_{1-x}Cd_xS$. Crystallinity and particle size, which can be controlled by the synthesis methods and conditions, have a significant impact on the photocatalytic water-splitting performance of a photocatalyst [1]. Therefore, several preparation methods, such as sol-gel, hydrothermal and simple precipitation methods, were addressed to achieve lower particle size and nanostructured materials with high surface area. Co-catalysts are believed to separate photogenerated electrons and holes by forming a Schottky barrier at the metal-semiconductor interface, at which O_2 and H_2 evolution reaction occur. Copper or nickel metals were used as a replacement for noble metal co-catalyst, the last ones are scarce in the Nature and expensive compared with the formers. The hydrogen production performance was measured by home-built photocatalytic set-up consisting of source of light and hydrogen production reactor located at the focuses of an elliptic cylinder reflector. The response on UV or VIS light could be registered independently with a mass spectrometer. The hydrogen production obtained by UV irradiation with the catalyst $Zn_{0.6}Cd_{0.4}S$ is 14110 µmol·h⁻¹·g_{cat}⁻¹. This value, using non-noble metals, is comparable to results obtained with Pt-TiO₂ (16500 μ mol·h⁻¹·g_{cat}⁻¹) [2].

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Free carrier generation via photo-induced energy transfer in Perovskite-TMDC (0D-2D) Hybrid System

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Transition metal dichalcogenide (TMDC) semiconductors show an indirect to direct bandgap transition from bulk to monolayer with improved light-matter interaction and carrier mobility. This makes them an excellent component in optoelectronic devices. The atomically thin nature of these materials results in a weak (<1%) light absorption and consequently show low photocurrents. Integration of strong light absorbing, wider bandgap 0D materials such as CdSe, CdS, perovskite nanocrystals with TMDC monolayers can improve the overall absorption of the heterostructure due to exciton energy transfer between the two materials.

In this contribution, we present an efficient photo-induced energy transfer in a OD-2D heterostructure of CsPbBr₃ (di-dodecyl, dimethyl ammonium as ligand) and MoSe₂ monolayer. MoSe₂ and CsPbBr₃ heterostructure form a type I structure with MoSe₂ being the lower bandgap material. We use steady-state, time-resolved µ-PL spectroscopy and photocurrent measurement techniques to probe the photo-induced energy transfer between a set of different CsPbBr₃ NCs and MoSe₂. The results show that the energy transfer mainly results in the generation of free carrier in MoSe₂ monolayers which is imperative in the realization of efficient optoelectronic devices. Our results are important for optoelectronic devices that rely on the efficient dissociation of high binding energy excitons in 2D materials.

DE-24



SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

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Shining a light on biomedical and energy applications

SPECTROELECTROCHEMICAL INVESTIGATIONS FOR PHOTODOPING OF COLLOIDALTIN DOPED INDIUM OXIDE NANOCRYSTALS

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Solar power is a potential alternative solution for the global sustainable energy crisis The exploitation of solar energy can be done effectively by combining light energy conversion and storage functions into one single component by taking advantage of a novel approach which helps to avoid the losses associated with the compartmentalization of these two functions [1]. Photodoping of metal oxide nanocrystals can be considered as one of the most interesting strategies for realising this task. This photo-induced n-type doping allows multiple charge accumulation of electrons induced by absorption of high-energy photons above the band gap of the material[1, 2]. In fact, it has been reported that the capacitance values exhibited by doped metal oxide nanocrystals after photodoping may rival those of the best supercapacitors used in commercial energy-storage devices, exposing these systems as extremely promising materials for future light-driven energy storage solutions [3]. To understand and optimize the charge accumulation process of metal oxide nanocrystals during the light driven charging, a spectroelectrochemical approach capable of relating the optical response to the electrochemical signatures is necessary [4]. We have charged the metal oxide NCs with a light source in a controlled atmosphere, simultaneously monitoring the changes in the open circuit voltage by extending the instrumental set up for photodoping with a Potentiostat. A long-term impact on the development of solar chargeable devices can be envisaged by the fruitful implementation of photodoping in solar energy storage applications which will advance the alternative sustainable solutions for energy production to facilitate the carbon neutrality strategy.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Upconversion for security tags and future applications

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Please indicate preference: Oral Specify Technical Area: Energy and other Applications

NIR-excitable lanthanide nanocrystals (LnNC) show multi-color emission pattern composed of a multitude of narrow bands of varying intensity in the ultraviolet, visible, near-infrared, and short-wave infrared detectable with miniaturized optical instruments and simple color (RGB) cameras in complex environments. This makes these chemically inert luminescent materials ideal candidates for anticounterfeiting and authentication applications as well as for modules in optical sensors in which the LnNCs can be used as nanolamps in combination with analyte-sensitive fluorophores or the temperature sensitivity of defined emission bands can be utilized.

Therefore, we are building up and exploring a platform of LnNC with application-specifically tuned size, composition, and surface chemistry to enable i.) luminescence tagging of relevant materials, ii.) fabrication of security inks for printable QR codes, iv.) temperature sensing, and v.) the design of self-referenced sensor beads for (micro)biologically relevant analytes. This research involves the synthesis of multi-color Ln-NC with defined sizes, their spectroscopic characterization, and the assessment of their suitability for the aimed applications. Furthermore, we are developing a miniaturized and portable optical scanner device for the accurate detection and read-out of the emerging LnNC-based security tags and optical sensors.



Figure 1: Color codes easily assessable by co-doping the same nanocrystal host with different lanthanides as emissive centers.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Fabrication of Anti-counterfeiting Nanocomposites with Multiple Security Features via Integration of a Photoresponsive Polymer and Upconverting Nanoparticles

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Anti-counterfeiting materials are used to distinguish real banknotes, products, and documents from counterfeits, fakes, or unauthorized replicas. However, conventional anti-counterfeiting materials generally exhibit a single anti-counterfeiting function, resulting in a low level of security. Herein, we demonstrate a novel anti-counterfeiting nanocomposite with numerous prominent security features.^[1] The nanocomposite was fabricated by doping upconverting nanoparticles (UCNPs) in a photoresponsive azobenzene-containing polymer (azopolymer). Because of the *cis-trans* photoisomerization of the azopolymer, the nanocomposite exhibited photoinduced reversible color changes suitable for anti-counterfeiting applications. Additionally, imprinted microstructures were fabricated on the photo-softened nanocomposite wi photoinduced orientation for encryption. Importantly, UCNPs in the nanocomposite emit visible light upon excitation by near-infrared light, enabling the observation of various anti-counterfeiting structures with high contrast. The nanocomposite can be conveniently processed and applied to banknotes, medicines, wines, and other products (**Figure 1**). The results of this study open a new avenue for the development of high-end anti-counterfeiting materials.



Figure 1. Schematic of the anti-counterfeiting nanocomposite comprising of the azopolymer (PAzo) and UCNPs for different applications.

Reference 1. Liu, Y. et al., Adv. Funct. Mater. 2021, 31, 2103908.



CNH2's recent advances in reversible solid oxide devices using scalable and cost-effective manufacturing processes

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The current energy demand together with the regulations that establish the need to be climate neutral by 2050 make hydrogen technologies emerge as one of the best solutions to be integrated in sectors where electrification and renewable energies are difficult to be implemented. Within hydrogen technologies, solid oxide devices are the most promising systems because their high operating temperature offers high efficiencies for both hydrogen to electricity transformation and hydrogen generation from renewable energies. However, the commercialization of these systems depends to a large extent on increasing the durability and reducing the manufacturing costs of the devices, where the processing methods are of great relevance.

This work presents the most recent advances of the Hydrogen National Center in the development of solid oxide systems capable of operating in reversible mode, as a fuel cell and as an electrolyzer. The fabrication of electrolyte-supported SOFCs has been carried out using industrially scalable and cost-effective methods. Yttria stabilized zirconium oxide electrolyte supports (YSZ) have been fabricated by tape casting, and subsequently, by airbrush deposition, layers with thicknesses of 20-30 µm of Nickel and Yttria stabilized zirconium oxide fuel electrode (NiO-YSZ), 2-4 µm gadolinium doped ceria barrier (Gd0. 2Ce0.8O1.9, GDC) and 20-30 µm lanthanum strontium manganite air electrode (La0.8Sr0.2MnO3, LSM). The fabricated cells were characterized using a scanning electron microscope (SEM) equipped with an energy dispersive X-ray detector (EDX). The electrochemical studies have been performed through polarization curve measurements (I-V-P), electrochemical impedance spectroscopy (EIS) and degradation tests under constant current with a multichannel Potentiostat/Galvanostat VMP3 (Biologic), using different fuel compositions at temperatures between 750 and 900°C.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications

Shining a light on biomedical and energy applications

Unprecedented atomic-scale details of the interface in lanthanide-based core@shell nanocrystals: when the interface controls the "device".

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Core-shell architectures have played a pivotal role in the developm ent of lanthanide (Ln)-based nanocrystals (NCs), which have risen a s an important class of luminescent nanomaterials due to their upc onverting/downshifting capabilities for various technological applic ations. Advances in controlling energy migration pathways in such nanostructures recently attracted considerable attention to proper ly adjust their optical characteristics to specific requirements for va rious energy and biomedical applications.

In this presentation, we will demonstrate that the outcome of the s ynthesis of core-shell Ln-based NCs can easily and significantly devi ates from the initially anticipated organization of the core and shell domains. Such deviations can be identified and characterized by ST EM-based methods (ADF-STEM images and spatially resolved EDXS /STEM) with unprecedented atomic-scale details (Figure 1). The int erface pattern (which reflects the chemical and structural organizat ion of the boundary/discontinuity region between the core and she Il sub-domains) appears to be an important and useful notion to pr operly describe the atomic-scale organization of core-shell Ln-base d NCs. The experimental results will show that the interface patter n can be engineered from abrupt to diffuse, with the possibility to modulate the magnitude of the latter. Although the size of the star ting core particles is important, such a parameter is not reliable, on its own, to predict which type of interface pattern will be formed. I ndeed, interface patterns ranging from segregated to partial and to tal alloying will be presented. Finally, it will be shown that importa nt photoluminescence properties such as the emission spectrum, t he absolute upconversion or downshifting photoluminescence qua ntum yields can be significantly modified without changing the ove rall architecture and/or chemical composition. Because of the mass ive utilization of core-shell Ln-based NCs in the biomedical and ene rgy fields, the presentation will be of major interest to the whole c ommunity. This new field of research is of critical interest to prevent uncontrolled structural/ chemical ran



Figure 1. Refined high-resolution annular dark-field scanning transmission electron microscopy images overlaid by chemical maps (green dots) reflecting the probability of finding at least one heavy lanthanide element (Er or Yb) within individual atomic columns of β -*NaErF*₄:*Yb@NaYF*₄ core-shell nanocrystals with diffuse (top) and abrupt (bottom) interfaces. Purple circles indicate the initial size of the starting core particles.

domness and deviations from the initially designed structures, which might seriously compromise the succ essful translation of core-shell Ln-based NCs from bench to market.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Application of Upconversion and Downshifting Luminescence of Lanthanide-based Phosphors in Plastic Recycling

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Oral - Energy and other Applications

In 2018, the EU agreed on ambitious targets: to increase the reuse and recycling of plastic waste to 50% by 2025, to 55% by 2030, whereas in 2020 only 35% was recycled. In the total volume of plastic waste collected in Europe, multilayer flexible plastic (MFP) for food packaging accounts for about 49%. However, with the state-of-the-art near-infrared (NIR) sorting technology, packaging waste can only be sorted according to main polymers (polyolefins, polyethylenterephthalat (PET), polystyrene, polyvinylchloride) and colours. It leads to a large amount of MFP containing waste that cannot be recovered by any existing industrial recycling technology.

Selective tracer-based sorting (TBS) of food packaging items from bulk end-of-life plastics of industrial and municipal waste can help to keep those packaging items to be recyclable, thus assisting a realization of a circular economy. Different sorting codes based on luminescent tracers with specific excitation/emission spectral lines and high quantum yield of luminescence must be developed for the TBS technology. Unique features of lanthanide (Ln³⁺) luminescence, such as large Stokes and anti-Stokes shift, high signal to noise ratio, high resistance to photo- and photochemical degradation, availability of cheap NIR laser diodes for excitation, sharp emission lines make them promising as photonic markers for plastics recycling [1]. The TBS is based on optical signatures emitted from luminescent tracer materials doped into the polymer or applied *via* printed labels [2]. In this presentation we provide an example of the Ln³⁺ luminescent tracers used in the TBS process, which explains a possibility to distinguish between two specifications (for instance, food and non-food) or the reliable recognition of multilayer packaging. Within TBS, both upconversion luminescence and downshifting short-wave inferred (SWIR) luminescence of markers, excited at 980 nm, can be used as



Figure 1. Application of up-conversionbased fluorescent markers on labels (left bottle) as well as in the packaging material (right bottle) [2]. specific signatures for different materials.

In addition, we discuss measurements of luminescence quantum yield (PLQY) as a figure of merit of TBS markers with upconversion and downshifting SWIR luminescence. For example, we have implemented PLQY measurements not only by an absolute method (using an integrating sphere) but also by a relative method (using a comparison with a reference luminescence). The latter approach may also be of interest for the characterization of upconversion nanomaterials widely used in imaging and biological applications.

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OE-30



Novel and high-sensitive primary and self-referencing thermometers based on the excitation spectra of lanthanide ions

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Remote sensing through ratiometric luminescence thermometry based on trivalent lanthanide ions (Ln(III)) has lately become a promising technique due to its numerous applications.¹ Most available Ln(III)based luminescent thermometers require a calibration process with a reference thermal probe (secondary thermometers) and recurrent calibrations are mandatory, particularly when the thermometers are used in different media.² This is sometimes impractical, and a medium-independent calibration relation is postulated, which is potentially inaccurate. Thus, the determination of the temperature based on wellgrounded physical principles by primary thermometers is the only way to overcome these challenges. Despite being considered one of the most important developments in luminescence thermometry, primary luminescent thermometers are scarce. We proposed, implemented, and validated primary thermometers requiring calibration at one known temperature (primary-T), which are also self-referencing, employing ratiometric data from the excitation spectrum of Ln(III). By combining with the emission spectrum, thermometers not requiring calibration (primary-S) were devised. A Eu(III)-β-diketonate complex was used as a proof-of-concept, but the approach is universal and other Ln(III)-based materials can be explored. Because many thermometric parameters are employed for temperature prediction an unprecedented very high accuracy of 0.2% in the physiological range is obtained.

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Synthesis and Characterization of Persistent Blue Light Luminescence Nanoparticles for Photodynamic Therapy (PDT)

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Specify Technical Area: Biomedical, SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

The antimicrobial resistance is becoming a worldwide threat, being the cause of morbidity and mortality in patients with chronic lung infections. The European project Light4Lungs (L4L) aims to develop a novel therapeutic treatment by using inhalable luminescent particles to kill the lungs bacteria. These multidrug-resistant bacteria such as *P. aeruginosa* and *S. aureus* contain endogenous photosensitizers (porphyrins) which can be excited by light and create cytotoxic reactive oxygen species and consequently eliminating the pathogenic bacteria. The particles responsible to excite the porphyrins must be excited in the inhaler (by using a UV LED), emit with a preference wavelength of 400 nm (1) and the emission must last enough time to reach the patient lungs.

In this current scenario, we have synthesized different biocompatible particles with persistent luminescence in the blue part of the spectrum and characterized them by using different techniques (**Fig. 1**). The main materials prepared for the photodynamic treatment are titanium doped zirconium oxide (ZrO₂:Ti⁴⁺), magnesium doped barium zirconium oxide (BaZrO₃:Mg²⁺) and europium, neodymium co-doped calcium aluminum oxide (CaAl₂O₄:Eu²⁺:Nd³⁺). Different optimization strategies such as doping amount and annealing temperature have been used to increase both luminescence intensity and persistent luminescence lifetime. Finally, we have also investigated the dispersion of these materials in order to prepare a stable colloidal solution and facilitate their use in the inhaler.



Figure 1. (a) TEM image of ZrO₂:Ti⁴⁺ nanoparticles, **(b)** persistent luminescence decay of different particles synthesized in this work and **(c)** photo of the of persistent luminescence after exciting the particles for 2 minutes at 280 nm.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Luminescence of different up-converting nanoparticles in blood

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Up-converting nanoparticles (UCNPs) doped with lanthanide ions (Ln³⁺) show unique spectroscopic properties and are promising candidates for advanced biomedical applications [1]. Many research groups are trying to obtain highly luminescent UCNPs under excitation wavelengths from the biological windows [2]. The main goal of our research was to determine the whole human blood penetration depth based on the luminescence of multi-mode NIR laser-excited UCNPs. The high-quality core/shell materials with hexagonal phases were obtained using precipitation in high-boiling-point solvents and then transferred to the water by acid treatment [3,4]. The different rare earth ions were used as light sensitizers: Yb³⁺ ions for 975 nm, Er³⁺ for 808, 975, and 1532 nm, or Tm³⁺ for 1208 nm covering the optical transparency windows, important for medicine. We registered the emissions of ligand-free UCNPs in the water and whole human blood at different sample depths. The effect of light absorption and scattering of blood components (mainly by hemoglobin) was observed. The research allowed us to estimate the depth to which the excitation radiation penetrates the sample and how thick a layer of blood allows to observe the emission. The presented results are important for developing UCNPs' applications in biomedicine.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Handling of single multicellular spheroids: a 3D tumor model

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Preference: Oral Specify Technical Area: Biomedical

During last decades, numerous researchers are employing 3D cell culture techniques to prepare multicellular spheroids¹, whose cellular metabolism is closer to the one of tissues than monolayer cultures. In particular, spheroids resemble tissues better regarding thermal shock. Furthermore, their high reproducibility and significant size and shape control, are helping spheroids to fill the gap between biological assays in monolayer and *in vivo* experiments. In this work, we propose to explore the response of tumour spheroids to light, following the different handling methods used in photothermia assays.

The growth of the spheroid was performed by forced-floating method, resulting in \approx 200 μ m spheroid diameter. In order to study their different mechanical properties, these spheroids were developed from two different cell lines: MCF-7, from breast human cancer epithelial tissue (adenocarcinoma) and U-87mg, also epithelial tissue, but from a brain human cancer (glioblastoma astrocytoma). Both cell lines present a differentiated way which cells join together. On the one hand, MCF-7 cells, form side-by-side junctions that give rise to compact spheroids. On the other hand, U-87mg are elongated-shape and have branches (pseudopods) through which they join together, leading to a less dense spheroid (Figure 1).



Figure 1: (a) MCF-7 cells (b) MCF-7 spheroid (c) U-87mg cells (d) U-87mg spheroid. Scale: 80µm

We have researched the biological response of spheroids to near-infrared laser irradiation, depending on wavelength and laser power. The properties of the spheroid have been also studied by handling with optical manipulation techniques. As light may increase the temperature of the sample, the study is completed with the synthesis and internalization of rare earth doped nanoparticles in the spheroid, to work as thermal sensors.

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Straight-forward synthesis of upconversion nanoparticles for biosensing applications using a polymer-assisted open-air modest-temperature method: control of shape and emission.

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Please indicate preference: Oral Specify Technical Area: Biomedical

Upconversion nanoparticles (UCNPs) are uniquely suited to biomedical and biosensing applications, but their synthesis demands either oxygen-free high-temperature reactions or expensive solvothermal synthesis equipment. These synthesis demands present a considerable barrier-to-entry to new and interdisciplinary researchers interested in the field.

This talk will describe a straight-forward method to synthesize polyvinylpyrrolidone (PVP)-coated UCNPs using readily available and low-cost laboratory equipment (i.e. a hot-plate, oil bath, and round-bottom flask). We will describe how the advantageous red emission of UCNPs can be enhanced dramatically by using Mn²⁺ as a co-dopant, via a confirmed three-photon upconversion mechanism, and via a potential size-dependent quantum yield enhancement, inferred after recent reports by others.[1,2] Further, we will describe yet-to-be published results which show that rhombus shaped/bipyramidal shaped UCNPs can be produced by altering the relative amount of molecular weight of PVP polymer used in the reaction scheme.

Ultimately, we hope that the techniques and methods discussed will enable wider participation in the fascinating and useful field of UCNP research.



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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Optical molecular detection trough fluorescence quenching

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Fluorescent sensors are appealing in biology and medicine fields, for which examples of fluorescent supramolecular sensing of relevant biomarkers in water or biofluids have proven their importance. In particular, a turn-off fluorescent sensor sensitive to a target biomarker can be used to detect it. In this communication, we show the results based on the quenching of the fluorescence of a new developed macromolecule cage designed to detect 3-Nitrotyrosine (NT) [1]. NT is a relevant biomarker of kidney disease. When kidneys are damaged, NT concentration in blood is considerably high.

Fluorescence quenching has been analyzed using the Stern-Volmer theory and a limit of detection within the reported physiological concentrations of NT in chronic kidney disease has been established.



Figure 1: Scheme of Chronic Kidney Disease, inducing NT production in blood. NT selectively enters the macromolecule cage and quenches it fluorescence.

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Effect of Al₂O₃ on the crystallization of NaYF₄ in oxyfluoride silicate glassceramics for optical thermometer

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Temperature (T) is a fundamental parameter that must be measured precisely in many scientific and engineering fields. The limitations of the traditional contact devices make it essential for the development of low-cost, portable, dependable, and safe temperature sensors for a wide range of applications¹. In this context, optical thermometry based on fluorescence intensity ratio (FIR) has received a lot of attention in the last decades because of its quick response, electromagnetic passivity, self-reference, and high sensitivity². The approach that utilizes two emission bands from thermally coupled levels (TCLs) of rare earth (RE³⁺) ions has been used to develop the FIR technique, which has been improved significantly in the past few decades. However, limitations such as rapid electrons exchange between the two monitoring TCLs energy levels limit the thermometer's upper limit of relative sensitivity ³. Also, a narrow energy difference between TCLs would result in spectral overlap of the two monitoring peaks, which would be unfavorable to signal recognition. These drawbacks limit the further improvement of thermometer sensitivity.

To overcome these limitations, it is necessary to propose a new approach based on the intensity ratio of non-thermally coupled (NTCLs) energy levels in the same and/or different luminescent centers⁴ related to the high efficiency of the luminescence of the RE³⁺ ions in a crystalline phase within the glass-ceramics (GCs). In particular, sodium yttrium fluoride phase (NaYF₄) in glass-ceramics became one of the most efficient host materials for UC among investigated fluoride GCs, with the incorporation of Er^{3+} for green emission⁵. However, the role of the network modifier like Al₂O₃ on the structural and luminescence properties is still in discussion. In fact, there is not enough data on the effect of the Al₂O₃ content in the base glass composition on the precipitation of NaYF₄ phase and its phase transition (cubic \rightarrow hexagonal or hexagonal \rightarrow cubic) in oxyfluoride silicate GCs.

In this work, Transparent oxyfluoride GCs with embedded β -Na_{1.5}Y_{1.5}F₆ crystals doped with Er³⁺ ions were fabricated by a melt-quenching method with subsequent heat treatment. The structural and spectroscopic characterizations were performed to verify the precipitation of β -Na_{1.5}Y_{1.5}F₆ crystals and the partition of the Er³⁺ dopant into the crystals. The effect of the Al₂O₃ content (5, 10, and 20 mol%) on the properties were also discussed. Bright green up-conversion (UC) emission was achieved in Er³⁺-doped GCs. Furthermore, the temperature-dependent visible UC behavior based on thermally coupled energy levels (TCLs) and non-thermally coupled energy levels (NTCLs) was also examined in the temperature range 298 K to 823 K showing a maximum relative sensitivity (Sr) of 1.1% K⁻¹ at 298 K for TCLs in Er-G and Er-GC samples.

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FLTX2: The novel ALL-IN-ONE Tamoxifen Derivative: Antiestrogen, Fluorescent and Photosensitizer

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Tamoxifen is the most widely used selective modulator of estrogen receptors (SERM) and the first strategy as coadjuvant therapy for the treatment of estrogen-receptor positive (ER+) breast cancer. However, long-term tamoxifen treatment is not devoid of undesirable effects, being the most life-threatening the increased risk of uterine cancers. Current knowledge indicates that side effects are related to the affinity of tamoxifen for ER but also to other non-canonical cellular targets. These drawbacks have encouraged the development of novel tamoxifen derivatives with antiestrogen properties but lacking agonistic uterine tropism. One of this is FLTX1 [1], formed by the covalent binding of tamoxifen and 7-nitrobenzofurazan (NBD), which has proven to have excellent pharmacological properties (pure antiestrogen in breast cells and lack of agonistic effect in uterus) and also an emergent behavior as highly efficient laser dye [2,3,4].

In this communication we describe the newest derivative, FLTX2, designed to couple the laser properties of FLTX1 to a photosensitization mechanism [5,6]. FLTX2 incorporates a Rose Bengal (RB) group, which is a known photosensitizer for Reactive Oxygen Species (ROS) generation. Our analyses demonstrate (1) FLTX2 is endowed with similar antiestrogen potency as tamoxifen and its predecessor FLTX1, (2) shows a strong absorption in the blue spectral range, associated to the NBD moiety, which efficiently transfers the excitation energy to RB through intramolecular FRET mechanism, (3) generates superoxide anions in a concentration- and irradiation time-dependent process, and (4) Induces concentration- and time-dependent MCF7 apoptotic cell death. These properties make FLTX2 a promising candidate to lead a novel generation of SERMs with the endogenous capacity to bind ER+ breast cancer cells and to promote cell death *in situ* by photosensitization.

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The influence of experimental parameters on the luminescent properties of red-emitting hybrids for bioimaging

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Europium β -diketone complexes (Eu-complexes) have excellent photophysical properties for bioimaging applications, nevertheless, they often present low water-solubility and questionable photostability [1]. The strategy of binding these complexes on the surface of silica nanoparticles (NPS) has been used to diminish photodegradation and solve solubility issues. The challenge, however, is to improve the luminescent properties of these hybrid materials [2]. Therefore, in this study, we show how the silica nanoparticle size, the type of functionalization, and the synthesis approach to anchoring Eu-complexes using HTTA (3thenoyltrifluoroacetone) and HDBM (dibenzoylmethane) ligands influence on photophysical properties of luminescent hybrids. For this, 50 and 170 nm-NPS were synthesized and functionalized with carboxylic acid groups (NPS-COOH) and phenanthroline derivatives (NPS-Phen). The complexes were anchored by two approaches. In approach 1, Eu³⁺ ions were first coordinated by COOH or Phen groups with subsequent coordination of deprotonated β -diketones TTA⁻ and DBM⁻. In approach 2, *tris*- β -diketonate complexes were synthesized and coordinated by the same chelating groups grafted on the NPS. By anchoring the Eucomplexes on the surface of NPS resulted in better luminescent properties, such as higher excited state lifetime (τ) and intrinsic quantum emission yields (\emptyset_{Ln}^{Ln}), compared to the isolated complexes. Hybrids synthesized by approach 1 with 50 nm-NPS-Phen, showed the highest ϕ_{Ln}^{Ln} due to greater sensitization of Eu³⁺ ions by the Phen ligand. The NPS size barely changed the photophysical properties. Finally, the hybrids synthesized by approach 1, in general, resulted in higher values of \emptyset_{Ln}^{Ln} and τ showing that this approach might be a more interesting strategy for anchoring complexes on the NPS surface. The cytotoxicity of these hybrids was evaluated by MTT assays in Huh 7.5 cells, and it was observed that the hybrids presented IC₅₀ values around 10 μ g/mL. However, the toxicity can be reduced by making the surface charge of the nanoparticles more positive. In general, the hybrids showed interesting luminescent properties to be applied in bioimaging, being possible to modulate the toxicity of the nanoparticles by the surface charge.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Dual magnetic field and temperature optical probes based on lanthanidedoped NaREF₄ nanoparticles containing hierarchically structured heterogeneous crystalline phases

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The engineering of core@multishell nanoparticles containing heterogeneous crystalline phases in different layers constitutes an important strategy for obtaining optical probes. The possibility of obtaining an optomagnetic core@multishell nanoparticle capable of emitting in the visible and near-infrared ranges by upconversion and downshifting processes is highly desirable, especially when its optical responses are dependent on temperature and magnetic field variations. This work proposes synthesizing hierarchically structured core@multishell nanoparticles of heterogeneous crystalline phases: a cubic core containing Dy^{III} ion responsible for magnetic properties and optical active hexagonal shells where Er^{III}, Yb^{III}, and Nd^{III} ions were allocated. The synthesis strategy was efficient in obtaining spheroidal nanoparticles of approximately 13 nm of heterogeneous crystalline phases, formed by a cubic phase core and hexagonal phase-shells, confirmed by XRD, TEM, and luminescence measurements. The hierarchy was obtained satisfactorily and can be confirmed by EDS mapping and HAADAF images, optimizing and arrange the optical or magnetic properties of interest in different regions of the nanoparticle. Optically active shells, in the hexagonal phase, emit in the visible region and the NIR range after excitation at 980, 808, and 1550 nm, covering two different biological windows. The nanoparticle emissions are affected by temperature, where the emissions of Er emissions in 528 and 540nm can be taken to propose a temperature probe based on upconversion emissions in a temperature range of 77 to 427K. Emissions in the NIR cover higher temperatures ranging from 427 to 633K. The core@multishell nanoparticle can also have its luminescence modulated by the application of an external magnetic field, where at 15K the increase in the intensity of the magnetic field improves the emission intensities and promotes the unfolding of Zeeman's doublets, for the transition ⁴S_{3/2} of the Er^{III} ion. However, at 150K the increase of magnetic field decreases the intensities of the upconversion emission. The magneto-optical properties of nanoparticle reveal its versatile nature and its applicability as magnetic field and optical temperature probes in which the parameters, temperature, and field, can be measured simultaneously.



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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Improving stability and thermal sensitivity of an optically trapped upconversion nanoparticle by coating with a thermo-sensitive polymer

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Lanthanide-based upconverting nanoparticles (UCNPs) are trustworthy workhorses in luminescent nanothermometry. The use of UCNPs-based nanothermometers has enabled the determination of the thermal properties of cell membranes and monitoring of in vivo thermal therapies in real time. However, UCNPs boast low thermal sensitivity and brightness, which, along with the difficulty in controlling individual UCNP remotely, make them less than ideal nanothermometers at the single-particle level. In this work, we show how these problems can be elegantly solved using a thermoresponsive polymeric coating. Upon decorating the surface of NaYF₄: Er^{3+} ,Yb³⁺ UCNPs with poly(N-isopropylacrylamide) (PNIPAM), a >10 fold enhancement in optical forces is observed, allowing stable trapping and manipulation of a single UCNP in the physiological temperature range (20-45 °C). This optical force improvement is accompanied by a significant enhancement of the thermal sensitivity — reaching a maximum value of 8% °C⁻¹ at 32 °C caused by the temperature-induced collapse of PNIPAM. Numerical simulations reveal that the enhancement in thermal sensitivity mainly stems from the interaction of trapping and re-emitted radiations with the highrefractive-index polymeric coating that behaves as a nanolens of high numerical aperture. The results included in this work demonstrates how UCNP nanothermometers can be further improved by an adequate surface decoration and open a new avenue towards highly sensitive single-particle nanothermometry.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Rare-earth-doped microspinner for non-invasive sensing

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The precise and non-invasive control over single particles is key for an array of physical and bio-medical applications, such as microfluidics and biophysics. In particular, the three-dimensional manipulation of single rare-earth-doped luminescent particles is of great interest due to their biocompatibility and the sensitivity of their luminescent properties to environmental conditions, which stand out among other dielectric luminescent particles. [1] The analysis of the damped rotation dynamics of an optically trapped microparticle is a novel and powerful tool that allows not only the controlled and remote manipulation of the sensor, but also an improved characterization of the medium and fast recording of its content. [2]

Here, an optically trapped and rotated rare-earth-doped β -NaYF₄:RE³⁺ microparticle is presented as a novel sensor to characterize the properties of a liquid medium at the microscale (temperature, viscosity and detection of bio-objects). [3,4]



Figure. Schematic representation of the different applications of a single rare-earth-doped β -NaYF₄ microparticle optically trapped and rotated in a liquid medium.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Polymeric Surfaces based on Template Replica for Cell Culture

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Cell culture plays a key role in cell biology research. Allowing the growth and the proliferation of cells in an artificial environment provide a better understanding of cell behavior which is influenced by surface properties of the material^{1,2}. Polydimethylsiloxane (PDMS) is a material used in biomedical devices because of its biocompatibility, low toxicity and high oxidative and thermal stability. PDMS is elastic, optically transparent, inert material and cheap. It is a polymer that has a combination of properties due to the presence of an inorganic siloxane backbone and organic methyl groups attached to silicon. It is fluid a room temperature and this property makes the polymer suitable for the fabrication of replica from a stamp.

The aim of this work is to design and fabricate polymeric surfaces prepared by template technique from macroporous silicon substrates in order to use them as supports for cell cultures³⁻⁵. Negative replicas on PDMS as well as positive ones and, a biocompatible and biodegradable (poly(lactide-co-glycolide) (PGLA) polymer have been reproduced. PDMS microstructures have been obtained as a result of the negative replica from the MacroPSi template. Through the PDMS negative substrate, PDMS and PGLA porous surfaces have been obtained (Figure 1). Wettability properties of the polymer substrates were analyzed to study the effect of the texture surface and the properties of the material. Because the hydrophobicity of the PDMS and PGLA, cell culture on these surfaces is unfavorable. Because that the surfaces have been chemically modified with proteins. The efficiency of these polymeric surfaces to support adhesion and viability cells was analyzed.



PGLA Replicate

Figure 1. ESEM images of polymeric replicas procedure from macroporous silicon template.

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Nanocomposite films of α -synuclein with inorganic nanoparticles

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Investigation on organic-inorganic hybrid nanocomposites has been recently boosted for interesting applications in biomedicine, such as in diagnosis and therapy, also due to the possibility of finely tuning their physicochemical properties as well as their functionality. Moreover, the chemical interactions between biomolecules and nanoparticles are of considerable interest, from a basic science to an applied point of view.

 α -synuclein is a prototypical intrinsically disordered protein, well known in the field of neuropathology for its association with some neurodegenerative conditions such as the Parkinson's disease. Due to their common hallmark, these pathologies are also known as α -synucleinopathies. Under particular conditions which perturb its disordered native structure, such as changes in the chemical environment, α -synuclein predominantly assumes a β -sheet conformation, leading to the formation of fibrils. This behavior makes α synuclein suitable for the development of nano-biocomposite nanomaterials such as nanofilms and filaments. Moreover, the use of a protein as the structural component of a nanocomposite, together with the use of biocompatible nanoparticles, guarantees the biocompatibility of the material, essential feature for possible use in biomedical applications.

The present research has been focused on the preparation of free-standing films composed of inorganic nanoparticles and α -synuclein, obtained by means of a special chemical procedure. Several films have been prepared by using various types of inorganic nanoparticles to obtain materials with tailored properties, such as luminescence (e.g. upconversion) or magnetic susceptibility. Combination of different kinds of nanoparticles were also considered to obtain multifunctional films with a broad range of features and possible applications as bio-sensors in bio-devices components. The luminescence properties of the obtained nanocomposite films were measured and compared with those obtained for the isolated nanoparticles.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Hybrid polymer-ceramic mechanosensors for near-IR induced, color responsive pressure sensing in vivo

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Mechanical stresses at the cell-matrix interface and within hollow neuromuscular organs regulate many important biological processes, including stem cell differentiation, axon guidance, cardiogenesis and digestion. Existing mechanosensitive techniques, including traction force microscopy (TFM) and atomic force microscopy (AFM) are ill equipped to quantify these stresses because of their large size, while Forster resonance energy transfer based fluorescent protein tethers (FRET tethers) are limited in their dynamic range (<100 pN), propensity for photobleaching and sensitivity to autofluorescence. Hybrid organic-inorganic fluorescent nanomaterials have the potential to shrink the mechanosensing capabilities of devices like AFM down to the nano to micro scale without sacrificing photostability or introducing toxic compounds into the system. Here, we introduce a hybrid polymer-ceramic platform based on the mechanosensitive upconversion luminescence of lanthanide doped nanoparticles (UCNP) embedded uniformly within a biocompatible polystyrene microsphere that can be interrogated with near-IR excitation to maximize tissue penetration and minimize autofluorescence background. We show that stress induced spectral shifts (+12 cm-1 per GPA) of the aliphatic (2900, 2950 cm-1) and aromatic (3050 cm-1) C-H stretching modes of the polystyrene host matrix couple to quenching modes of the red ($4S3/2 \rightarrow 4F9/2$) and green ($4F9/2 \rightarrow 4I9/2$) emitting states of trivalent Erbium dopants in the 20 nm core@shell NaY0.8Yb0.18Er0.02F4@NaYF4 UCNP. This results in a decrease in 540 nm (green) emission relative to 660 nm (red) emission within the elastic regime of polystyrene (<50 MPa). Mechano-optical calibration of this stress response was performed on individual microbeads using a home built confocal-AFM under the assumption of Hertzian contact mechanics. Under anisotropic compressive loading, we observe a linear percentage change in the ratio of integrated red to green emission (%ΔIR:IG) of ~2% per 10 MPa which is consistent with the ~4% per 100 MPa sensitivity observed for identical UCNP within a Diamond Anvil Cell (DAC) with a different organic host matrix (Silicone oil) under hydrostatic loading. Moreover, we demonstrate the biocompatibility of the platform by deploying it to probe pharyngeal pumping dynamics of live, C. elegans nematode worms. Microbead consumption produces no measurable effect on worm fecundity or pumping efficacy. Moreover, the microbeads are bright enough to image at 12.5 Hertz (980 nm, 2 kW/cm2), making them an attractive platform for non-invasive real time stress sensing within the lumen of neuromuscular organs.



Er³⁺-doped nanoparticles as primary thermometers and NIR radiation sensors

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The real-time temperature monitoring during laser-supported thermal therapies is pivotal to guaranteeing an efficient and safe application since it prevents the surrounding tissue from overheating. The simultaneous measurement of incident P_D would be an additional asset providing real-time feedback and enabling parameter adjustments for optimized therapy ^[1].

In this work, we use the Er³⁺ emission of the NaGdF₄/NaGdF₄:Yb³⁺,Er³⁺/NaGdF₄ upconverting nanoparticles upon 980 nm laser excitation to determine both the absolute temperature and the excitation power density. The Er³⁺:²H_{11/2}→⁴I_{15/2} and ⁴S_{3/2}→⁴I_{15/2} emission bands, which are commonly used for thermometric purposes, overlap with the ²H_{9/2} →⁴I_{13/2} emission band. This interference can lead to temperature miscalculations^[2]. Applying a procedure based on the methodology of a luminescent primary thermometer to successfully resolve the overlapping Er³⁺ transitions, we are able to show that this system work as a primary thermometer, granting reliable temperature measurements, and to employ ²H_{9/2} →⁴I_{13/2} emission to quantify the excitation NIR power density.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Ultrafast decay alkaline-earth rare-earth fluoride nanoparticles for novel X-ray and γ -ray scintillators

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Please indicate preference: ___Poster ___Oral

Specify Technical Area: Biomedical Energy and other Applications SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Alkaline-earth rare-earth fluoride (MLnF) nanoparticles have been extensively studied over the past decade for a plethora of applications ranging from energy storage to biolabeling and bioimaging. Here, we investigate MLnF core-shell nanoparticles doped with lanthanide ions with a fast spontaneous emission rate as promising building blocks for scintillators. Scintillators are materials that can efficiently convert high energy photons into low-energy photons in UV-Vis regime. Scintillators are a major component in high energy radiation detection (X-rays, γ -rays) including positron emission tomography (PET). To tune the emission to the UV-Vis regime and understand the decay dynamics of excited states, we investigate the MLnF nanoparticles and the impact of various compositional factors including host lattice, dopant type and dopant concentration.

To fulfill the criteria for an ideal scintillator (high Z, short rise and decay time), here we propose to make solution processable nanoscintillators based on SrLuF host lattice (effective Z:54.5) with an FCC close packed structure in which some of the Lu sites are exchanged with high Z trivalent lanthanides (Pr^{3+,} Ce³⁺). To reduce surface quenching, we form an epitaxial shell of undoped SrLuF around the core nanoparticles via dropwise hot injection approach. The Pr^{3+,} Ce³⁺ doped nanoscintillators offer dipole allowed transitions (interconfigurational transitions) between 4f and 5d states for fast scintillation with short radiative decay lifetime.

We employ a range of structural, optical and X-ray characterization techniques on the colloidally synthesized nanoscintillators to identify the compositional dependence of emission wavelength and emission decay dynamics. To understand the scintillation properties, we have looked at both steady state and time resolved X-ray luminescence response from the nanoparticles. A broad band corresponding to 4f-5d transition has been consistently observed for all samples with peaks between 325-350nm and decay lifetime varying between ~18-24ns.

Finally, we incorporate the nanoscintillators into a flexible elastomer of PDMS to form an optically clear scintillator film and investigate the scintillation response of the PDMS and nanoparticles composite film. This understanding is a key step to develop next-generation ultrafast, low-cost and flexible scintillator materials.



Shining a light on biomedical and energy applications

Seeing the Force: Single Avalanching Upconverting Nanoparticles as

Ultrasensitive Local Force Transducers

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It has lately been shown that ensembles of lanthanide-doped upconverting nanoparticles (UCNPs) exhibit changes in their emission spectra due to applied forces in the nano-Newton regime and beyond [1-3]. Avalanching UCNPs (ANPs) [4], possessing steeply nonlinear optical responses, are ideally suited for sensing minute changes in their environments, as small perturbations are expected to usher large changes in signal. Because ANPs absorb and emit tissue-penetrating near-infrared (NIR) light, they are uniquely positioned for sensing within biological cells and fluids. In order to characterize and understand the response of these ANPs to local stress and hence determine their functionality as mechano-sensors, it is important to study their mechano-opto-physics on a *single particle level*. Utilizing a custom designed combined AFM and inverted optical microscope system (Fig. 1a), we correlate *sub-nano-Newton*-range applied forces and observable changes in hyperspectral optical signals (Fig. 1b-c) for isolated optimally-designed single ANPs, demonstrating their attractiveness as physiologically-relevant ultrasensitive local force sensors.



Fig. 1. a) Sub-nano-Newton force is applied to a single ANP with an AFM tip while excited with NIR light from below. The ANP Tm³⁺-doped hexagonal NaYF₄ unit cell is shown. b) Force-dependent *increasing intensity* emission spectra, attained for a single ANP while excited at 1064 nm. c) Duo-wavelength force-dependent ratio-metric change emission spectra, attained for a single, differently designed, ANP while excited at the same conditions as in b).

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Influence of cell incubation parameters on molecular imaging of atherosclerosis with functionalized gold nanoshells

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Please indicate preference: ___Poster X Oral

Specify Technical Area: X Biomedical ____ Energy and other Applications

There is an urgent need for contrast agents to detect the first stage of atherosclerosis, which is characterized by endothelium inflammation and subsequent overexpression of ICAM-1 molecules and other cell adhesion molecules [1]. Cardiovascular Optical Coherence Tomography (CV-OCT) is the imaging technique with the highest spatial resolution and sensitivity of those used for clinical diagnosis of this disease. Among the available commercial nanoparticles, core/shell gold nanoparticles (gold nanoshells, GNSs) provide the strongest signal in CV-OCT [2].

We have previously reported that it is possible to target endothelial inflammation in vitro using GNSs functionalized with a peptide that binds specifically to the ICAM-1 molecules. This targeting was demonstrated both under static and dynamic conditions [3], as schematized in **Figure 1(A)**.

In this work, we studied the adhesion phenomena in detail, and determined which are the optimal incubation parameters (such as GNSs concentration, incubation time and solution temperature) to obtain the highest adhesion efficiency to endothelial cells under inflammation conditions as assessed by CV-OCT, dark field microscopy and dynamic light scattering. Our results demonstrated that these parameters are of paramount importance (**Figure 1(B)**) and must be taken into consideration for further experiments before testing their potential as clinical molecular contrast agents of atherosclerosis.



Figure 1. (A) Schematic representation of the functionalized GNSs' adhesion to inflamed endothelial cells. (B) Evolution of the adhesion efficiency of GNSs to inflamed endothelial cells with the concentration of GNSs.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Expanding the Library of Photon Avalanching Nanoparticles

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Please indicate preference: __Oral __ Specify Technical Area: __Biomedical Applications__

Lanthanide-doped photon avalanching nanoparticles (ANPs) represent a unique and highly-nonlinear class of upconverting nanoparticles (UCNPs), which under lower-energy near-infrared (NIR) excitation emit higher-energy visible light. Different from classical UCNPs, in ANPs a small increase in the laser excitation power (e.g. by 1%) can lead to a dramatic enhancement of the emission intensity (e.g. 100%). Such a behavior is typically manifested by the nonlinearity factor, *s*, reaching values of 30 and higher for photon avalanching process vs. 2-5 for the conventional upconversion emission. Although avalanche-like UCNPs have been shown before,^[1] true photon ANPs, operating at room temperature conditions, were discovered only recently.^[2] Due to the highly nonlinear excitation-emission characteristic of these ANPs, they were showcased as super-resolution optical probes, allowing to resolve structures below 100 nm with a conventional laser scanning microscope.

In view of this finding, further development and optimization of ANPs offers new advancements in biomedical applications of super-resolution imaging, ultra-sensitive analyte detection, and precision drug delivery. Thus, current research efforts are directed in developing ANPs of varied compositions and architectures that would be well-tailored for these tasks. Particular improvements are being sought in creating libraries of ANPs for multiplexing applications, in reducing excitation power threshold to initiate photon avalanching process, and in improving imaging speeds in laser scanning microscopy. These features can be obtained by creating heterostructured core/shell ANPs where photon avalanching property of ion can be borrowed by another one rationally engineered energy transfer network. Here, we explore questions associated with ANP usage and present novel ANPs that could be fit for undertaking challenges beyond the reach of conventional UCNPs.

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Imaging the nanoscale structure of the cell with correlative super resolution light and electron microscopy

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SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

The plasma membrane separates the cell's interior from the outside world. The exchange of signals and materials across this barrier is regulated by a multitude of channels, transporters, receptors, and trafficking organelles. Mapping the molecular structure and dynamics of the plasma membrane is key to understanding how human cells function in health and malfunction in disease. Electron microscopy can produce high resolution images of the membrane. Historically, it has been challenging to locate and identify proteins within these images. Recently-developed fluorescent super-resolution localization microscopy, however, can visualize fluorophore-labeled molecules with better than 20 nm precision. We developed a correlative super-resolution light and EM method (CLEM) that couples these complementary methods to produce images where identified proteins are mapped within the dense native structural environment of the cell. This correlative method is uniquely suited to determine the nanometer-scale organization of the plasma membrane and associated organelles.

Clathrin-mediated endocytosis is the primary mechanism human cells use to internalize receptors, nutrients, hormones, and other cargo. It is fundamental to the function of cells and tissues. Using our CLEM method, we studied 19 key proteins involved in clathrin-mediated endocytosis. Our data provides a comprehensive molecular architecture of endocytic vesicles in human cells. We discovered that key regulatory and cargo proteins distribute into distinct nanoscale spatial zones; inside, outside, and at the edge of the clathrin coat in human cells. The presence and amount of many factors within these zones change during vesicle growth. From these data we present a model that the formation and curvature of single endocytic vesicles is driven by the recruitment, re-organization, and loss of proteins within these distinct nanoscale zones.

We next used large-scale transmission electron microscopy to study clathrin-mediated endocytosis across many types of cells. We created and analyzed ultra-high precision platinum replica TEM images of over 33,000 endocytic structures from nearly two hundred cells and eight different cell types. We also developed a new cryo-EM tomography method that allows us to image lattice organization within single clathrin structures in the native environment of a plasma membrane in the frozen state. This lets us directly study clathrin at molecular resolutions inside cells. Our primary finding is that flat clathrin lattices are loosely assembled and spontaneously curve into domes without energy-dependent clathrin exchange or recruited proteins in a living cell membrane. This is a new but central concept in understanding how clathrin-mediated endocytosis works in human cells to regulate traffic across the plasma membrane and cellular signaling.

KN-DBL-1



TENERIFE, CANARY ISLANDS

Shining a light on biomedical and energy applications

High-speed 3D microscopy for life-science applications

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Please indicate preference: __Poster _X_Oral Specify Technical Area: _X_Biomedical __ Energy and other Applications _X_SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Living things change over time and are usually 3-dimensional (3D), yet most high-speed microscopes image a single 2D plane, and are often limited by phototoxicity. High-speed 3D microscopy can permit interrogation of cellular function and signaling, in-vivo movements, blood flow changes and physiological responses to perturbations. We developed swept confocally aligned planar excitation (SCAPE) microscopy to meet this need. SCAPE microscopy is a single-objective light-sheet approach that can image living samples in 3D at cellular resolution at up to 300 volumes per second, with high signal to noise and minimal photodamage. The single-objective geometry of SCAPE also permits imaging of diverse, unmounted, freely moving, large or intact samples.

We have applied SCAPE microscopy to imaging small organisms such as C. elegans, zebrafish larvae and fruit flies, as well as intact mouse olfactory epithelium and in-vivo mouse brain. In these systems, we have leveraged the power of genetically encoded fluorescent indicators of cellular activity, as well as tracking and extracting 4D movements and tissue deformations to uncover new physiological processes.

We have also developed a clinical version of SCAPE microscopy, for high-speed in-situ histopathology, as well as systems capable of high-throughput and high-content imaging of fresh, fixed, cleared and expanded samples. I will describe the fundamentals of single objective light sheet microscopy and demonstrate the wide range of applications for this approach.

KN-DBL-2



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Holographic manipulation of neuronal circuits

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SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Genetic targeting of neuronal cells with activity reporters (calcium or voltage indicators) has initiated the paradigmatic transition whereby photons have replaced electrons for reading large-scale brain activities at cellular resolution. In parallel, optogenetics has demonstrated that targeting neuronal cells with photosensitive microbial opsins, enables the transduction of photons into electrical currents of opposite polarities thus writing, through activation or inhibition, neuronal signals in a non-invasive way. These progresses have in turn stimulated the development of sophisticated optical methods to enable "all optical" in depth brain circuits interrogation with high spatial and temporal resolution on large volumes.

Here, we will review the most significant breakthroughs of the past years, which enable reading and writing neuronal activity at the relevant spatiotemporal scale for brain circuits manipulation, with particular emphasis on the most recent advances in what we named circuit optogenetics [1,2]: a combination of approaches including holographic light illumination, temporal focusing, opsins engineering and laser development enabling the control of single or multiple targets independently in space and time with single-neuron and single-spike precision, at large depths.

Finally, we will show few examples of all-optical manipulation of neuronal circuits on different experimental paradigms including the demonstration of the presence hub cell in developing mouse brain, the investigation of interlayer signal propagation in mouse retina circuits [3] and the high throughput investigation of neuronal connectivity.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

The nanodomain basis of synaptic function

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Please indicate preference: __Poster _X_ Oral Specify Technical Area: __Biomedical __Energy and other Applications _X_SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Optical, chemical, and computational methods to improve the resolution of light microscopy have powered dramatic new insight to cellular molecular complexes. These advances have been particularly important for understanding the molecular events underlying our thoughts and actions, most notably in the synapses of the brain. At synapses, organization of key proteins over nanometer scales governs nearly all aspects of neuronal information transmission: activity-release coupling in the presynaptic terminal, the net strength of postsynaptic receptor activation, and the nature and time course of intracellular signaling. Exploiting high-resolution live-cell and single-molecule localization microscopy, we have identified several elements of synaptic protein nanoarchitecture which subserve these functions. An emerging principle of this architecture is the accumulation of key proteins within nanometer-scale domains, where they localize function to discrete synaptic subregions. One critical example is the subsynaptic architecture of NMDA receptors. These neurotransmitter receptors that gate calcium entry to control initiation of numerous forms of neural plasticity throughout our lives, and they are indeed known to be found in subsynaptic nanodomains. However, the relevance of this organization for synaptic function has remained unclear because the spatial relationships of these receptor nanoclusters to other functional regions of the synapse is unknown. I will discuss our recent work using DNA-Exchange PAINT to elucidate the functionally relevant nanoarchitecture of NMDARs within single synapses.

KN-DBL-4



MORPHOLOGY, TOPOLOGY AND FUNCTION OF ENDOSOME-MITOCHONDRIA INTERACTIONS IN BREAST CANCER CELLS

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Please indicate preference: __Poster _x_ Oral Specify Technical Area: __Biomedical __Energy and other Applications _x_ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Recently, interactions between early endosomes and mitochondria have been shown to facilitate the translocation of iron into mitochondria. However, little is known about how endosome-mitochondria interactions are regulated and how they affect iron translocation to mitochondria in breast cancer cells. Interestingly, there are clear differences in the mitochondrial and endosomal morphology as well as endosome-mitochondria interactions among different breast cancer cell lines. To address this issue, we have engaged in a comprehensive analysis of the organelle network morphology and distribution in breast cancer vs. non-cancerous cells using machine learning classification approaches. Organelle Topology-based Cell Classification Pipeline (OTCCP) was introduced as a novel approach that quantifies, for the first time, the topological features of subcellular organelles, removing the bias of visual interpretation, to classify different breast cancer cell lines using machine learning methodology. We propose that the spatial context of organelles (topology), specifically their subcellular location and inter-organelle relationships, can be used to inform breast cancer cell classification. In particular, we showed that interactions between early endosomes and mitochondria provide an increased accuracy to discriminate between breast cancer cells grown in 2D culture vs. 3D multicellular tumor spheroids. Furthermore, we have shown that Divalent Metal Transporter 1 (DMT1) modulates iron exit from endosomes and transport into mitochondria via regulation of endosome-mitochondria interactions. We evaluated the role of DMT1 in two distinct breast cancer cell lines: estrogen receptor positive T47D and triple-negative MDA-MB-231. In both cell lines, we demonstrate colocalization between DMT1 and early endosomes and/or mitochondria, but only in MDA-MB-231, DMT1 acts as a bridge between early endosomes and mitochondria. Moreover, we have shown that DMT1 regulates mitochondria iron translocation and labile iron levels via modulation of endosomemitochondria interactions in MDA-MB-231 cells. These results are in agreement with MDA-MB-231 cells' displaying a delay in iron release in comparison to T47D, making them more sensitive to disruptions in mitochondria iron translocation. In summary, we have shown that DMT1 regulates early endosomes dynamics as well as endosome-mitochondria interactions to support higher mitochondria iron translocation/lower labile iron pool levels, which are necessary for sustaining mitochondrial bioenergetics and invasive cell migration. These results suggest a complex cross-talk between iron uptake and transport and organelle morphology and intracellular distribution. Unravelling this intricate relationship between iron, endosomes, mitochondria, oxidative stress, and cancer progression will provide new tools for cancer therapy and diagnosis.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Super-resolution imaging of chromatin structure and dynamics in health and disease

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__ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Super-resolution microscopy has been playing an instrumental role in providing new insights into how the genome is folded and packaged inside intact nuclei in single cells. I will present our work on using super-resolution microscopy to visualize and quantify the spatial organization of chromatin with nanoscale spatial resolution in single cells. Our work has revealed that at the nucleosomal level chromatin is a disordered fiber composed of groups of nucleosomes packaged at varying densities, which we named nucleosome clutches. Despite the heterogeneity of nucleosome clutch organization, the size and packing density of nucleosome clutches is cell-type specific and correlates with cell fate. Our recent results also show that nucleosome clutches and chromatin nano-structure can be remodeled via chemo-mechanical cues. In particular degenerative chemo-mechanical cues during disease lead to aberrant chromatin nano-structure and loss of mechano-epigenetic memory, potentially leading to alterations in cell phenotype.



Role of membrane environment on binding allostery in pacemaker ion channels at single molecule resolution

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Please indicate preference: ___Poster X Oral Specify Technical Area: __Biomedical __ Energy and other Applications X SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Pacemaker ion channels are involved in maintaining electrical activity in oscillatory circuits found in the brain and heart¹. The activity of these channels is also directly regulated by second messengers such as cAMP which bind to the cyclic nucleotide binding domain in the C-terminus. Previous work² has uncovered evidence for both positive and negative cooperativity in cAMP binding but this has been controversial since bulk measurements suffer from limited parameter resolution. Efforts to eliminate this ambiguity using single-molecule techniques have been hampered by the inability to directly monitor binding of individual ligand molecules to membrane receptors at physiological concentrations. Here we overcome these challenges using nanophotonic zero-mode waveguides to directly resolve binding dynamics of individual ligands to multimeric HCN1 and HCN2 ion channels³. To determine the impact of membrane environment on channel gating and allostery, we have reconstituted purified ion channels in various membrane environments and measured their single molecule binding dynamics. We find that ligand binding allostery is profoundly influenced by both membrane environment and electrochemical potential. This approach for observing stepwise binding in multimeric proteins under well-defined conditions can be utilized to quantitatively probe ligand-binding allostery at single-molecule resolution in other intact membrane proteins and receptors.

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Engineering fluorescence emission for enhanced super-resolution microscopy

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The advent of super-resolution microscopy techniques, and in particular single molecule localization (SMLM) approaches, has made it possible to revisit the understanding of biological systems in terms of both structure and dynamics. However, many efforts are still needed to make SMLM approaches more precise, quantitative and reproducible. We propose various instrumental developments that allow the extraction of axial information with alternative approaches such as supercritical angle fluorescence (SAF) which intrinsically revealed the molecules' positions[1-2]. We will also discuss solutions that allow access to a uniform field of view increased by a factor of 16 and that facilitate the observation of several targets simultaneously by ratiometric measurements up to 200 µmx200 µm field of view [3]. These developments will be illustrated on different biological problems such as adhesion process or neurobiology (cf fig. 1).

SMLM imaging is often limited to the first micron of the biological sample. I will present Modloc [4], a new single molecule localization strategy based on a time signature. By shifting a structured excitation pattern, it induces a time modulated emission of the fluorophores where the phase holds its position. An efficient demodulation optical assembly compatible with short emitters On-time has been designed. Performances of ModLoc, will be discussed, in particular its 2 fold lateral precision improvement or its unique uniform axial precision of 6.8 nm. By applying the modulation in a tilted direction, an almost isotropic 3D localization is obtained over the whole capture range up to 40 μ m in depth and inside complex sample such as organoids.



2D single molecule imaging STORM imaging of beta2 spectrin (AF647) over e field of view of 160 µm x 30 µm²

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Super-Resolution and Machine-Learning enabled Live-Cell BioImaging Ricardo Henriques*¹⁻²

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Computational analysis has become an essential part of microscopy, enabling and enhancing quantitative imaging approaches. Several cutting-edge microscopy methods now depend on an analytical step to process large volumes of recorded data, extract analytical information, and produce a final rendered image. Single-molecule localization-based super-resolution microscopy is a notorious example. In recent years, our team and collaborators have built an opensource ecosystem of combined computational and optical approaches particularly dedicated to improving livecell microscopy, super-resolution imaging and helping researchers retrieve high-fidelity quantitative data from their images. This talk will present some of the recent technologies we have recently developed. First, I will introduce **ZeroCostDL4Mic**¹, an entry-level platform simplifying the application of **Deep-Learning** (DL) analysis to biological microscopy images, by exploiting free openly-accessible cloud-based computational resources. ZeroCostDL4Mic allows researchers with no coding expertise to train and apply key DL tasks to perform segmentation, object detection, denoising, super-resolution microscopy, and microscopy modality image-to-image translation. We'll demonstrate the application of the platform to study multiple biological processes, including in eucaryotic¹ and procaryotic cells². Next, I will cover recent development we have created for superresolution microscopy through the **NanoJ**³ platform, highlighting the Super-Resolution Radial Fluctuations (SRRF)⁴ approach and its combination with real-time controlled microfluidics live-to-fix cell imaging, dubbed NanoJ-Fluidics⁵, and real-time quality control on the predicted super-resolution images via the SQUIRREL⁶.

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Deciphering location of ligand-induced conformational changes and ligandbinding sites in an ion channel

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Ion channels are a diverse class of membrane proteins that are involved in cellular excitability in numerous tissues. An example are acid-sensing ion channels (ASICs), which are trimeric membrane that open a cation-selective pore in response to proton binding to their extracellular domain. The resulting cellular depolarization modulates synaptic activity and has been suggested to contribute to learning and memory, as well as fear conditioning. However, excessive stimulation of ASICs can contribute to the initiation or propagation of pain or cell death during ischemic events like stroke. Therefore, recent efforts have focused on identifying compounds that potently and selectively inhibit ASICs, including small molecules, venom-derived peptide toxins and endogenous neuropeptides. Here, we present examples of where we used fluorescent non-canonical amino acids or Cys-conjugated dyes to probe ligand-induced conformational changes in the extracellular, transmembrane and intracellular domains of ASICs. Additionally, we show how light-sensitive non-canonical amino acids can help identify binding sites of peptide ligands via UV-induced crosslinking. Together, this showcases a broad and complementary tool kit that enables detailed interrogation of the molecular function of an ion channel using light.

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SHIFT 2022 - Spectral sHapIng For biomedical and energy applicaTions TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Tracing electrical circuits in neural networks and in proteins

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Genetically Encoded Voltage Indicators (GEVI) are fluorescent proteins that optically report changes in membrane potential. In an effort to develop retinal prosthetics, we have expressed the GEVI, Bongwoori-R3 in retinal ganglion cells enabling the discovery of electrical synapse. In order to improve the optical signal from neural networks, we have also explored how charge moves through a protein to alter its fluorescent output. External surface chemistry orients internal side chains making them more susceptible to environmental conditions revealing new insights into how proteins handle charge.



TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Designing Brighter Dyes for Advanced Fluorescence Microscopy

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Specific labeling of biomolecules with bright, photostable fluorophores is the keystone of fluorescence microscopy. An expanding method to label cellular components utilizes genetically encoded self-labeling tags, which enable the attachment of chemical fluorophores to specific proteins inside living cells. This strategy combines the genetic specificity of fluorescent proteins with the favorable photophysics of synthetic dyes. However, intracellular labeling using these techniques requires small, cell-permeable fluorophores, thereby limiting utility to a small number of classic, unoptimized dyes. We discovered a simple structural modification to standard fluorophores that improves brightness and photostability while preserving other spectral properties and cell permeability. Inspired by computational experiments, we replaced the *N*,*N*-dimethylamino substituents in tetramethylrhodamine with a four-membered azetidine ring. This net addition of two carbon atoms doubles the quantum efficiency and improves the photon yield in living cells. The novel substitution is generalizable to fluorophores from different structural classes, yielding a palette of synthetically tractable chemical dyes with improved quantum efficiency and enabling multicolor single-molecule imaging experiments. These brighter versions of classic fluorophores can be further modified to fine-tune spectral and chemical properties for advanced imaging experiments in increasingly complex biological samples.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

The power of LOV

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Seeing is believing. Who would deny it? Biology relied on observations as its main methodology for centuries. After all, isn't nature what we aim to unravel? We simply need to observe what naturally occurs, make hypotheses, test and refine them to finally understand how nature works. While this view still holds true in cell biology, in recent decades, a novel methodology has emerged, one that prompts us to take action. Surely the concept of perturbing a biological process to understand the mechanism(s) behind it is relatively old, with gene knock-out and overexpression, for instance, dating back to the late 80s. Nonetheless, nowadays we recognize that temporal changes in the localization, interactome and activation status of biomolecules (proteins, RNAs, lipids, etc.) greatly contribute to their function. Therefore, modern cell biologists apply perturbations of a more sophisticated kind than gene knock-out or overexpression: reversible, highly spatially-confinable, rapid, and tunable perturbations that are made possible using light as the external trigger. Optogenetics is the state-of-the-art technology that uses genetically-encoded lightsensitive proteins to steer biological processes in a highly spatio-temporal way. In this talk, I will present some optogenetic tools developed by us in the past few years based on the light oxygen voltage (LOV) domain of Avena sativa phototrophin 1. LINuS and LEXY are tools to control with blue light nuclear protein import and export, respectively. BLADE is a blue light-inducible gene expression system for Escherichia coli. These tools showcase the power of the LOV domain as a photoreceptor to use to engineer optogenetic tools for cell biology.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

The smallest vertebrate brain knows how to sing

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Understanding how distributed neuronal circuits integrate sensory information and generate behavior is a central goal of neuroscience. However, it has been difficult to study neuronal networks at single-cell resolution across the entire adult brain in vertebrates because of their size and opacity. We address this challenge by introducing the fish Danionella cerebrum (formerly D. translucida) as a model organism. This teleost remains small and transparent even in adulthood, when neural circuits and behavior have matured. Despite having the smallest known adult vertebrate brain, Danionella displays a rich set of behaviors, including courtship, shoaling, schooling and acoustic communication.



TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Fluorescent Nd³⁺-based nanoparticles for NIR nanothermometry

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Determining temperature at the nanometric scale is a challenge. Being able to do so, will help us to improve our basic knowledge about nanosystems and their behavior. Applications can be found in a wide number of fields, including temperature variations at nanoscale resolution in hyperthermia or in molecular or cell biology [1]. Among a variety of possibilities, fluorescent nanothermometers (FNTs) are based on the temperature dependence of photoluminescence (PL). Several studies have been carried out [2] to help selecting the most suitable system and advising about how the measurements should be performed.



Figure 1: PL spectra of LaOCI: Nd³⁺ under 808 nm excitation. The inset shows a simplified Dieke diagram with the assigned transitions displayed on the spectra.

For biological systems, FNTs in the IR are preferred over those with visible PL, so that visible autofluorescence can be avoided and phototoxicity drops down when IR radiation is used as a probe. We propose the LaOCI: Nd³⁺ [3] for their use as nanothermometer investigating the ratiometric behavior between its intra and inter band transition dependence with temperature.

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Holographic optical tweezers for dynamic control of erythrocyte flickering

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Preference: Poster or Oral Technical Area: SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Red blood cells (erythrocytes) exhibit membrane fluctuations that give rise to flickering motion as dynamic reporters of spectrin skeleton activity under ATP consumption^{1–3}.

By mapping the membrane flickering using a fast imaging up to 1000 Hz, here we prove this biological activity as mechanically controllable under optical traps spatially extended along the membrane. We implemented a holographic tweezers⁴ that sculptures a coherent laser beam giving rise to a tightly focused force-field along the equatorial cell-contour, whose oscillations can be controlled in space and time. Such optical cell manipulator induces trapping landscapes without using force-transducing microparticles nor altering cell membrane properties, thus allowing an accurate and reversible mechanical feedback manipulation of living cells.

Our work paves the way for moulding optical forces on living cell membranes, defining new touchless strategies to achieve mechanobiological control on different kinds of cellular shapes.

Figure. Upper panel: spatial fluctuation maps for a free-standing and trapped cell, reported as mean standard deviation of membrane deformations $\delta h(\theta, t)$. The black line is the mean position of the membrane contour. Bottom panel: normalized probability density function (PDF) of δh for free-standing (red dots) and trapped cells (blue diamonds). Long (non-Gaussian) tails correspond to active kickers in the free-standing population, as highlighted by the distribution Kurtosis.



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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Neural engineering with photons as neurotransmitters

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Cell communication is basic for the development of multicellular living organisms as well as for their correct homeostasis. Miscommunication is the cause of many diseases and can even lead to cell death. Neural cells are not an exception and failure in neuronal signal transmission leads to diseases of different nature, from depression to schizophrenia or Parkinson. In this work, we describe a powerful and versatile cell communication system based on light, which we have named PhAST for Photon-Assisted Synaptic Transmission. PhAST relies on the expression of a calcium sensitive luciferase that emits light upon intracellular increase of calcium. The coupling of this NanoLantern (NL) ligth to a postsynaptic light sensitive ion channel allows depolarization and signal transmission to the downstream neuron. We followed the flow of information in a neuronal circuit, and have designed microfluidic devices to apply physiologically relevant stimuli to sensory cells while reading out calcium imaging in downstream interneurons. We also conceived new deep learning microscopy pipelines to visualize volumetric calcium recordings with bioluminescent reporters in freely moving animals (1). To show case the versatility of such an all-optical transmitter system, we have successfully installed this system in the nose touch pathway of C. elegans, overcoming a cell specific glutamate defect in ASH, the main nose touch effector, using a blue NL coupled to extremely sensitive CHR2 variant (2). In addition, the expression of PhAST in this sexually dimorphic pathway increases the nose touch sensitivity of wild type males almost to the levels of hermaphrodites. Lastly, coupling a green NL to the ACR1 anion chanelrhodopsin in this same circuit caused a change in polarity, overwriting the endogenous reversal signal and completely abolishing the response to nose touch.

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TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

oral-DBL-4

Seeing AMPA receptor complexes in a new light

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AMPARs (α -amino-3-hydroxyl-5-methyl-4-isoxazole-propionic acid receptors) are ubiquitous in the vertebrate brain and mediate the majority of the fast excitatory synaptic transmission. To allow efficient signal transmission AMPARs have to be positioned in the proximity of presynaptic release sites. The localization at the postsynaptic density and trafficking of AMPARs is mediated by Stargazin (Stg), also called y2, amongst other auxiliary proteins.

Current models suggest that Stg and the AMPAR form a complex already in the endoplasmic reticulum. Although dissociation of the complex has been proposed, the AMPA receptor also regarded as a stable unit consisting of the tetrameric receptor and additional auxiliary subunits for its entire trafficking cycle. We performed multi-color super-resolution and live cell imaging to reconcile these ideas, revealing organization and interaction of these AMPAR constituents. Control experiments showed that our labelled subunits form normal functional complexes but also colocalize poorly in heterologous cells, suggesting two overlapping modes of operation. Confocal live-cell imaging in neurons showed directed motion of single clusters of GluA2 (a subunit of the AMPAR) and Stg. The movements happen independently and suggest that after the proteins are synthesized, at least some fraction are transported separately.

In order to study the organization of the proteins in the subcellular space, STED images of fixed dissociated neurons were recorded. Stg is found in confined clusters within the postsynaptic membrane, whereas for the AMPAR additionally a diffuse signal at the soma can be seen, which points to a fraction of AMPARs that is retained in an intracellular pool without Stg.

Within the mature synapse, co-localized clusters of GluA2 and Stg are predominant. These stable complexes at the postsynaptic density have been reported previously. They maintain the basal activity of the synapse. A comparison with labelling of native subunits showed that the majority of GluA2 is clustered, and co-localized with postsynaptic proteins (like PSD95) and interacting with Stg, single Stg clusters without GluA2 are prevalent. These excess Stg clusters might be present to rapidly form complexes with trafficked GluA2 subunits, when new receptors are added to the postsynapse.





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Shining a light on biomedical and energy applications

Autofluorescence-free *in vivo* imaging in the time domain: Tailoring nanoparticles towards their application as contrast agents in the infrared

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The advancements made in optics working in the infrared have brought interest in optical bioimaging back to the forefront of research investigating *in vivo* biomedical imaging. The paradigm of the near-infrared transparency windows (NIR-I: 680 – 950 nm, NIR-IIa: 1000 – 1350 nm, NIR-IIb: 1500 – 1700 nm) allowed to turn optical imaging into more than just a method for topical imaging applications and enabled researchers to look under the skin or through a small animal. Nevertheless, new

challenges emerged, especially the predominance of autofluorescence of biological tissues (e.g., due to melanin), which hamper the application of classical optical imaging techniques.¹

We present a strategy to avoid this problem by employing firstly luminescent nanomaterials emitting in the NIR-II and secondly by applying nanoparticles whose fluorescence lifetimes are orders of magnitudes longer than those of the fluorophores responsible for tissue autofluorescence. In this presentation we identify potential sources of tissue fluorescence in the NIR and describe approaches for successful biomedical imaging in the time-domain taking advantage not only of the synthesis of rare-earth-doped but also semiconductor nanoparticles with tailored life times in the NIR transparency windows. These studies are based on dopant engineering and optimization of morphological characteristics like shells that in combination with time-gating imaging techniques enable multiplexing and temperature measurements. The use of nanoparticles with different lifetimes but otherwise similar properties allowed therefore a signal analysis in the time domain and their *in vivo* differentiation in a mouse model.

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Seeing inside the cell using LIVE-PAINT: A new way to image proteins in live cells using super-resolution microscopy

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Super-resolution techniques have enabled scientists to view structures within cells with a much higher resolution than conventional microscopy. Despite the number of super-resolution microscopy techniques available, live cell super-resolution microscopy remains challenging. Photo-activated localization microscopy (PALM) can be used in vivo but requires a direct fusion of a fluorophore to the protein of interest (Betzig et al., 2006). This approach can be problematic because a direct fusion to a fluorescent protein can disrupt the normal function and localization of the protein being studied. Moreover, once the fluorescent protein is photobleached no more data can be collected from that molecule.

To overcome these problems, we developed LIVE-PAINT, a novel live-cell super-resolution microscopy technique that is easy to implement and minimally perturbing (Oi et al., 2020). In LIVE-PAINT, a peptide-protein pair, one fused to the protein of interest and the other to a fluorescent protein, reversibly interact (Figure 1A). When the peptide-protein pair bind, a blink is observed, and the precise location can be determined (Figure 1B). In a few minutes, enough binding events occur to generate an image of the protein of interest with a resolution of around 20 nm (Figure 1C).

We have used LIVE-PAINT to image proteins inside live budding yeast; including proteins that are not amenable to direct fusions to a fluorescent protein. Furthermore, we have demonstrated that LIVE-PAINT can be used to track moving proteins. Lastly, we have demonstrated that we can multiplex LIVE-PAINT using orthogonal peptide-protein pairs. We anticipate that LIVE-PAINT will have a wide range of applications and we are currently adapting LIVE-PAINT to be compatible with mammalian cells.



Figure 1: An overview of LIVE-PAINT. A) A schematic of LIVE-PAINT. B) Montage of frames, 0.2 s apart, taken from the boxed region of a fluorescence microscopy of the video of a budding yeast with Cdc12p labelled using LIVE-PAINT. C) Super-resolution image of Cdc12 generated using LIVE-PAINT. Scale bars are 2 µm.

oral-DBL-6



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

NIR to UV up-converting nanoparticles for PDT applications

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Up-converting nanoparticles (UCNPs) have been intensively investigated in recent years because of their unique biomedical applications, e.g., in biophotonics, biomedical sensors, and photodynamic therapy (PDT) [1]. Currently, available PDTs base on irradiating the tissue with a laser or LED, most commonly from the visible light range. Unfortunately, due to the high absorption of VIS radiation by the human body, the usage of PDT is limited to the surface tissues [2]. However, combining classical PDT with UCNPs enables deeptissue treatment, as high-energy radiation is generated in the treated tissue *via* NIR irradiation that can penetrate deeper than visible light [3].

The most commonly used matrix for UCNPs with biological applications is NaYF₄. However, when applied in NIR to UV UCNPs (e.g., doped with Yb³⁺ and Tm³⁺ ions), the material shows most UC emissions in the visible range [4]. The alternatives are lithium-based nanoparticles of LiYF₄ doped with Yb³⁺ or LiYbF₄ doped with activator ions. These structures show intense UV emission under NIR irradiation due to the more effective absorption of NIR radiation and energy transfer processes populating higher excited states of activator (Tm³⁺) ions [5,6].

LiYbF₄ nanoparticles doped with Tm³⁺ ions and covered with a LiYF₄ shell were synthesized using the thermal decomposition method. All of the obtained UCNPs were characterized using XRD (X-ray powder diffraction), DLS (dynamic light scattering), and transmission electron microscopy (TEM, HRTEM). To prove core@shell structure, EDX (energy dispersive x-ray spectroscopy) mapping was performed. Finally, the emission spectra of UCNPs were collected under NIR laser irradiation (λ_{ex} = 975 nm), and the UC mechanism was determined *via* laser power-dependent emission measurements.

Acknowledgements

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Photo-Switchable Polymer Nano-Assemblies <u>Alexander Zika^{*1}</u>, Franziska Gröhn¹

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Inspired by natural systems, self-assembling building blocks forming functional supramolecular units are highly promising. Especially smart systems independently responsive to external triggers are of particular interest.^[1] In this contribution we will present a novel type of photo-switchable self-assembled nano-object in aqueous solution. The supramolecular assemblies consist of polyelectrolytes and multivalent ionic connector molecules, in particular photoacids and azo compounds.^[2]

Basis is the electrostatic self-assembly of polyelectrolytes and stiff multivalent ions in aqueous solution yielding well-defined assemblies of a few hundred nanometers in size. We will reveal how the charge ratio and molecular building block structure direct the supramolecular nanoscale structure and the behavior upon irradiation.^[3] The supramolecular polymer assemblies are characterized by static and dynamic light scattering, isothermic titration calorimetry, ζ -potential measurements and optical steady-state spectroscopy. Assembly thermodynamics and the interplay of interaction forces will be key to a fundamental discussion and understanding.^[4]

With regard to the world's decreasing energy resources, developing novel and sustainable strategies to exploit solar energy becomes more and more important. Thus, the concept shown here also represents a complementary approach towards a system for the conversion of energy upon irradiation; that is from light energy into nanoscale size and shape changes. While our focus lies on the fundamental introduction and understanding of a concept to form triggerable supramolecular nanoscale structures in solution, this route is further promising for applications in drug delivery or as nanosensors.



Figure 1. Light-switchable nanoparticle shape by electrostatic self-assembly: SANS for assemblies of a linear polyelectrolyte with lightresponsive ionic dye molecules as connectors (Ay38) before (blue) and after (red) irradiation.^[5] Here, classical trans-cis isomerization is used as trigger, while in this talk we will focus on the newer concept of using photoacids as nanostructure-switch.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Wheat seedlings' bioimaging and dependence of phytotoxicity on size and functionalization of upconverting NaYF₄:Yb,Er@NaYF₄ nanoparticles

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Poster SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Nanoparticles (NPs) have become widely used around the world. Accordingly, monitoring and detecting them inside the living organisms is important. One of the main problems with visualizing NPs in biological materials is distinguishing the NPs' emission from the autofluorescence of the surrounding tissues or cells. Upconverting lanthanide-doped NPs (UCNPs) may help solve this problem because these structures exhibit anti-Stokes emission (up-conversion) and covert NIR or IR radiation into visible light. Thanks to that, the autofluorescence of the background is negligible.

Therefore, in the presented research, the distribution of UCNPs (NaYF₄:Yb,Er@NaYF₄, 22 and 63 nm) that are non-functionalized or functionalized with PAA or PEG in wheat seedlings was investigated. The whole plants were imaged using an up-conversion laser scanner. All of the tested UCNPs were successfully detected in the plants.



Fig. 1. Wheat seedlings in daylight (left) and under NIR radiation (right).

Furthermore, the effect of UCNPs on the growth of the seedlings was tested. The obtained results revealed that the impact of the NPs depended on their type, size, and concentration. Among the non-functionalized NPs, the smaller ones (22 nm) had a stronger negative impact on the growth rate, whereas the bigger ones (63 nm) caused higher disruption in the germination rate. Among the functionalized NPs, only the NaYF₄:Yb,Er@NaYF₄@PAA (22 nm) at the highest concentration (100 μ g/mL) significantly influenced the number and mass of roots. In addition, bare NaYF₄:Yb,Er@NaYF₄ (22 nm) NPs interrupted the cell membranes of the tested plants.

This research was funded by the National Science Centre, Poland, grant number UMO-2016/23/D/NZ8/01112.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

From Thermometry to Bioimaging: Lanthanide Activated Nanoparticles as Multifunctional Tools for Biomedical Applications

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Lanthanide-activated fluoride-based nanostructures can be extremely interesting versatile tools, paving the way for many modern applications in nanomedicine, e.g. bioimaging, sensing, drug delivery and photodynamic therapy, as well as useful sensors for environmental uses.

Environmental-friendly preparations using a green chemistry approach, as hydrothermal synthesis, are nowadays highly desirable to obtain nanoparticles-based colloids, directly dispersible in hydrophilic media, as physiological or saline solutions.

In this communication we investigated KY_3F_{10} citrate-capped nanocrystals activated with several lanthanide ions, namely Er^{3+} , Yb^{3+} , Nd^{3+} , Gd^{3+} , synthesized by means of a facile microwave-assisted method, which significantly shortens reaction times and permits a fine control of the size of the nanomaterials.

Core@shell multifunctional architectures have been studied in colloidal water dispersion. Thermometric features in the optical spectrum have been considered, by exploiting some thermosensitive lanthanide emissions. Particularly, the lanthanide emissions in the Near Infrared range have been investigated for application as diagnostic tools in Optical Imaging (OI) techniques.

Furthermore, due to the strong paramagnetic properties of lanthanides (e.g. Gd³⁺) and X-rays absorption cross sections of both Yttrium and lanthanides, the nanostructures under investigation are extremely useful for simultaneous MRI and CT imaging for *in vivo* imaging applications.

Biocompatibility studies of the nanomaterials revealed very low cytotoxicity in different human cell lines, probably due to very high stability and low chemical dissolution of KY₃F₁₀ host. All these features point to a successful use of these fluoride-based core@shell nanoarchitectures for simultaneous diagnostics and temperature sensing tools.





TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

DEVELOPMENT AND OPTIMIZATION OF CALCIUM FLUORESCENT SENSORS BASED ON BK ION CHANNELS

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Please indicate preference: _X_Poster __ Oral Specify Technical Area: __Biomedical __ Energy and other Applications _X_ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Large-conductance calcium activated K⁺ channels (BK) play a crucial role in the control of neuronal excitability. At the presynaptic terminals, BK channels interact with voltage-gated Ca²⁺ channels (VGCCs), in spatially restricted domains called "Ca²⁺ nanodomains", providing a negative feedback mechanism for Ca²⁺ influx and regulating neurotransmitter release. These properties make BK channels ideal candidates to develop new genetically encoded calcium indicators to report changes in [Ca²⁺] restricted to nanodomains.

Based on FRETable BK channels previously developed in our laboratory (1), we have generated a potential Ca²⁺ sensor (BK-860cpGFP) by inserting a circularly permutated green fluorescent protein (cpGFP) into the BK amino acid position 860. Here we show that BK function is not altered by the cpGFP insertion. Addition of ionomycin to BK-860cpGFP-transfected HEK293 cells induced an increase in cpGFP fluorescence, which was associated to Ca²⁺ binding to specific sites in the BK channel. Simultaneous imaging and electrophysiology experiments in excised membrane patches allowed us to characterize the Ca²⁺ and voltage-sensitivity of the fluorescent signal. By using the superresolution microscopy technique STORM, we have also demonstrated that BK-860cpGFP forms complexes with VGCCs similar to those formed with wild-type BK channels.

Despite these promising results, we have found a high variability in the sensor calcium responses and different outcomes among the distinct preparations used. We checked if other parameters could be involved in the sensor response, and we found that BK-860cpGFP responses in ionomycin experiments were largely due to pH changes detected by the cpGFP. Therefore, the possible application of the sensor could be hindered by this unwanted behavior. For that reason, optimized BK sensor versions obtained using a different strategy (i. e., employing the GCaMP calcium-sensing features) are being tested.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

TRACKING THE DEVELOPMENT OF CHOLESTASIS RAT MODEL WITH AUTOFLUORESCENCE AND EMITTING Ag₂S NPS

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Please indicate preference: Oral Poster

Specify Technical Area: Biomedical Energy and other Applications

The fast-moving advances of optics and nanotechnology working in the near-infrared (NIR) biological windows have brought *in vivo* optical imaging back to the forefront of research. Liver diseases are among the ten most frequent causes of death in the Western World and are characterized by an increase of both total and direct bilirubin in bloodstream ^[1]. Bilirubin is also an endogenous fluorophore that was proposed to be a principal molecular agent responsible of autofluorescence emissions in the NIR-I (680-950 nm) ^[2]. Therefore, the aim of this study was to evaluate the autofluorescence signal of bilirubin in the NIR in order to detect cholestasis. For this purpose, we used a rat model with liver cholestasis by ligation of bile ducts causing the inflammatory response and biliary proliferation. We demonstrated bilirubin deposition in the rat organs by increment of autofluorescence intensity which also could be correlated with organs status from the bilirubin concentration in them. In addition, we investigated breaking of the blood brain barrier (BBB) as side effects of cholestasis which results in hepatic encephalopathy. Towards this goal we employed Ag₂S nanoparticles as contrast agents intravenously which accumulated in the disease model but not in the control in the brain, demonstrating permeability and damage to the BBB. This work will improve the understanding of cholestasis with the help of a noninvasive technic, developing bilirubin as a future endogenous fluorophore for diagnosis of hepatic diseases.



Figure 1. NIR-fluorescence in a rat model with hepatic failure (A) Autofluorescence at 930 nm of different organs with cholestasis excited at 800 nm (St=Stomach, C=Cecum, K=Kidney, E=Epididymis, S=Spleen, LI=Large intestine, SI=Small intestine, H=Heart. Principal organs with emissions are kidneys, liver, stomach, and large intestines. (B) Brain of a rat with cholestasis showing accumulation of Ag₂S nanoparticles.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Every particle with a crown: protein corona guided accumulation of upconverting nanoparticles in cancer cells

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Poster Biomedical Applications

Upconverting nanoparticles (UCNPs) stand out as multifunctional agents that can be used in bioimaging, drug delivery and therapy. In order to use UCNPs as nanomedicines the challenge remains to attain longlasting blood-circulation, for UCNPs to arrive at the target location. UCNPs present in biological medium are exposed to a mixture of biomolecules and proteins, forming "protein corona". It is detrimental that UCNPprotein complexes would not be eliminated by phagocytic cells. Accordingly, coating the surface of UCNPs with negatively charged molecules (i.e. carboxyl group, silica) allows to create compounds that are easily uptaken and retained by cells.

Little is known about protein corona formation and structure depending on the surface coating of UCNPs and how it affects the cellular uptake. In addition, any surface modification of UCNP will alter size and protein composition of protein corona around the UCNP. For this reason, studies on protein corona formed around differently coated UCNPs are crucial to find the most suitable surface modifications for biomedical application.

The aim of this work was to investigate the protein corona composition and size around citrate, SiO_2 and phospholipid coated $LiYF_4:Yb^{3+}$, Tm^{3+} UCNPs as well as corona's impact on cellular internalization. Physical characteristics of UCNPs in medium containing serum proteins were studied together with UCNPs' interaction with proteins and biologically active molecules. All in all, the surface coating of UCNPs plays a significant role in UCNP protein corona composition, formation and cellular internalization.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Diffractive microlenses inside laser crystals by 3D fs-laser nanolithography

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Nowadays there is a growing demand for ultra-small optical lenses, as well as for an enhancement of their focusing efficiency. Diffractive microlenses exploit the fundamental phenomenon of diffraction to focus light and reduce the thickness of the lens to the wavelength scale. Diffractive microlenses are composed of spatially arranged zones which impart an appropriate phase shift to achieve constructive interference of the transmitted waves at the focus [1].

In this work, diffractive microlenses are designed to function in the interior (i.e. within the volume) of laser crystals, following a 3D design criteria that mimics with high fidelity the feature sizes achievable in nanofabrication by means of recently developed technique of 3D femtosecond laser nanolithography of YAG and sapphire crystals [2]. This technique allows to reliably fabricate hollow (air) nanostructures within the volume of a crystal with a characteristic feature size of 100 nm, without the appearance of fractures, and with lengths on the mm to cm scale across the lens plane. The focusing capabilities of the designed structure were simulated using both the Finite-Difference Time-Domain (FDTD) and the Beam Propagation Methods (BPM). Once the design of diverse microlenses for focusing in air, in dielectric, or in water, and with medium to high numerical apertures, was successfully achieved, key experimental constraints related to achieving a good fidelity between design and fabrication were analyzed in detailed and new fabrication parameters were developed. In order to fabricate the designed diffractive microlenses, basic parameters such as the laser writing speed, laser power, pulse repetition rate, and pulse time sequence (i.e. single or multi-pulse bursts) were studied to see their effects on the cross-section area, aspect ratio, and etching rate of the nanopores. All these results will be reported for the first time to our knowledge, in this presentation.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Degradation analysis of highly UV-resistant down-shifting layers for applications on photovoltaics devices

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Nowadays, the silicon-based photovoltaic (PV) technology plays an essential role in the decarbonization transition in electrical systems due to its practicability, competitive costs, and the achievement of high efficiencies. 95% of the photovoltaic market is dominated by this technology with multi-crystalline silicon (mc-Si) technology leading with approximately 60% of the share. However, mc-Si technology exhibits a relatively poor response in the UV region of the solar spectrum, mainly due to the thermalization losses from the absorption of high-energy photons [1]. Among the different available techniques to improve the short-wavelength response, the most promising approaches are the use of luminescent down-shifting (DS) layers. In addition, luminescent DS layers placed outside of the solar cell have the potential ability to



Fig 1. Evolution of the EQE during the accelerated degradation inside the climatic chamber of the PV mini-module with encapsulated DS layer.

reduce the solar cell operating temperature and, therefore, increase its electrical power in outdoor applications. Our group has worked for several years in highly luminescent rare-earth-based DS compounds, which benefit from large Stokes shifts [2,3]. The durability of DS layers is a key issue to incorporate this technology into the PV installations because the polymers and encapsulants experiment degradation when exposed to outdoor conditions and UV radiation. In this work we analys the performance and durability of DS layers formed by [Eu(bta)₃mephen], taken as a reference compound, embedded into EVA, and aged under UV radiation for long exposure times.

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Understanding of light-driven chemical reactions using in situ Raman spectroscopy

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Please indicate preference: _x_Poster __ Oral Specify Technical Area: __Biomedical _x_Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

A high percent of the energy supply of the world is based on fossil fuels, and humankind is expected to face a crisis due to the fast depletion of fossil fuels and increasing levels of CO₂ in the atmosphere. Nowadays has become imperative for scientists to find ways of transforming undesirable CO₂ to useful chemicals, and among emerging technologies that enables a wide variety of applications in this context, it can be find the photocatalysis processes. Numerous materials have been explored as photocatalysts, and the versatility of these materials and reactions has been expanded in recent years. Understanding the relationship between the physicochemical properties of photocatalytic materials and their performances as well as the fundamentals in catalytic processes is important to synthesize photocatalytic materials. The objective, in this context, concerns the research and study of materials that are able to support the mechanisms behind the aforementioned processes, performing light-driven chemical reactions, such as CO₂ reduction, looking for trigger multi-electron transfer reactions. Based on this, *in-situ* Raman spectroscopy is especially useful for investigations of heterogeneous catalytic systems, because it is able to provide fingerprinting-type information about the molecular structures of the catalysts as well as reaction intermediates under reactive conditions. In this work we explore through *in-situ* Raman Spectroscopy the photocalityc reaction of materials like indium tin oxide (ITO).



The strategy for enhancement the thermometric performance of Ln³⁺ based luminescence thermometry

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Lanthanide ions (Ln^{3+}) have long been found in a wide range of applications. More recently, their optical properties such as narrow emission lines, have favored their use in luminescence thermometry (LT). However, a factor that may limits the use of Ln^{3+} ions doped materials as temperature sensors is their low absorption cross-section, which results in limited emission brightness. Indeed, if the emission brightness is insufficient then the signal-to-noise ratio is reduced to the point where the accuracy of the temperature readout is affected, making measurement unavailable. Therefore, in LT application, particular attention should be paid to temperature resolution, reliability and relative sensitivity on a par with brightness. One possibility to obtain luminescent-enhanced Ln^{3+} ions emission is to excite them through the energy transfer from transition metal (TM^{3+}) ions. In this process, an enhanced luminescence of the Ln^{3+} ion is obtained due to the much larger absorption cross-section of TM comparing to Ln^{3+} . In addition, due to the $TM^{3+} \rightarrow Ln^{3+}$ energy transfer, the LT thus obtained is characterized by greater susceptibility to temperature changes due leading to an enhancement of its relative sensitivity.

Therefore, the present study [1] was undertaken to analyze the effect of Cr^{3+} ions concentration on the thermometric properties of a GdScO₃:Er³⁺,Nd³⁺ ratiometric luminescence thermometer based on the intensity ratio of Nd³⁺ to Er³⁺ ions. Up to a 25-fold increase in the emission intensity of Nd³⁺-Er³⁺ ions was observed in the presence of Cr³⁺ ions due to the high absorption cross section and efficient Cr³⁺ \rightarrow Ln³⁺ energy transfer. Furthermore, the co-doping of Cr³⁺ ions enabled a significant extension spectral range of optical excitation at which Nd³⁺ to Er³⁺ ions emission can be generated. As mentioned, the energy transfer from Cr³⁺ ions to Ln³⁺ will favorably influence the thermometric properties and, as expected, the experimental results confirmed a strong susceptibility to temperature variations. This allowed a threefold increase in the maximum relative sensitivity from 0.3% K⁻¹ at 300K for GdScO₃:1%Nd³⁺,1%Er³⁺ to 0.96% K⁻¹ for GdScO₃:15%Cr³⁺, 1%Nd³⁺, 1%Er^{3+.}

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Near infrared hyperspectral imaging for biomedical applications including lipid visualization in liver and submucosal tumor detection <u>Kyohei Okubo^{1*}</u>, Masakazu Umezawa¹, Kohei Soga¹

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Hyperspectral imaging (HSI) is a powerful imaging technique for biomedical applications including disease detection, diagnosis, and image-guided surgery. The use of near infrared (NIR; 800-2500 nm) light enables to investigate deep parts of tissue due to its lower absorption and scattering. Especially, reflectance spectra in NIR range facilitate to identify chemical composition of targets because of overtone and combination vibrations of chemical bonds [1]. Our group is focusing on employing NIR-HSI to the following applications: (A) visualization of lipid distribution in the livers [2] and (B) distinction of surgically resected gastrointestinal stromal tumor (GIST) [3,4]. In presentation, we will show recent advances using NIR-HSI technologies combined with machine learning approaches.

(A) Lipid distribution in liver helps to diagnose nonalcoholic fatty liver disease (NAFLD) which can advance to liver cirrhosis and even hepatocellular carcinoma. Thus, a noninvasive, label-free and quantitative imaging technology is needed. We show NIR-HSI for quantitative visualization of lipid content in mouse liver using machine learning model called support vector regression (SVR). Analytical results indicate that SVR with standard normal variate pretreatment achieved $R^2 = 0.968$ with a mean absolute error of 8.5%. Color mapping of lipid content in the liver suggest uneven lipid distribution in liver, which may improve the diagnosis of NAFLD.

(B) The diagnosis of GIST using conventional endoscopy in visible range is difficult because a mucosal layer hinders the detection of submucosal tumors including GIST. NIR-HSI is a potent candidate to enhance the capability of endoscopy for distinguishing deep submucosal tumor. The images of surgically

resected GIST lesions are captured by the NIR-HSI system developed, and machine learning model revealed normal and GIST regions as color-coded areas. Furthermore, a laparoscopic imaging device based on multispectral imaging, which measures a small number (3-20) of spectral bands, is developed for preliminary demonstration in practical setup. Tumor delineation of tumor-bearing mice is achieved using the laparoscopic device.

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Figure. Lipid content distribution in mouse livers obtained by NIR-HSI technology.



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Shining a light on biomedical and energy applications

CuInS₂ quantum dots as pressure nanosensors

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Micro- and nano-Newton forces are involved in biological processes such as tumor progression or vasoconstriction that regulates the body temperature.^{1,2} Knowledge of the magnitude of these forces at the cellular level could provide tools for the diagnosis and treatment of diseases with marked impact on human health. Nanoparticles with pressure-dependent luminescence could afford a minimally invasive readout of such forces at the (sub)cellular level.

Semiconductor quantum dots (QDs) have attracted attention in the pressure sensing field due to the dependence of their photoluminescence peak position as a function of applied pressure and their nanoscale size.³ One of the best candidates as pressure sensor probes are copper indium sulfide $(CuInS_2)$ QDs because of their pressure-sensitivity (photoluminescence-wise) in the GPa-level.⁴ Besides, the CuInS₂ composition lacks heavy metals, making them non-toxic and thus suitable for applications in biological systems. In this work, we studied the response to pressure of CuInS₂ QDs specifically exploring how the size and the stoichiometry affect the QDs stress sensitivity. When pressure up to approximately 5 GPa is applied, the QDs exhibit a blueshift in the peak position of the emission spectrum. A complete recovery of the original peak position is observed upon releasing the pressure: a lack of hysteresis that is a fundamental requisite for effective pressure



Figure 1. Emission spectra of CuInS₂ QDs while applying 4.86 GPa of pressure (red) and without such applied pressure (yellow/before and orange/after), λ_{ex} .= 488 nm. Inset shows dependence of luminescence's peak position with applied pressure.

sensing. These pressure sensors could be used into biological systems, such as the analysis of mechanical forces at cellular level. This could suppose a big step into the understanding of the processes that take place at pathological level.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Mid-infrared Detection with Lanthanide Nanotransducers Liangliang Liang, Xiaogang Liu*

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Spectral conversion of mid-infrared (MIR) radiation to visible (VIS) and near-infrared (NIR) wavelengths is a fundamental technology for spectroscopy and imaging. However, current MIR-to-VIS/NIR conversion technology is limited to nonlinear optics with bulky crystals or resonant nanocavities. Here, we report lanthanide-based MIR-to-NIR nanotransducers that enable broadband MIR sensing at room temperature by harnessing ratiometric luminescence changes. The ratiometric luminescence of lanthanide nanotransducers in the NIR region can be incoherently modulated by MIR radiation in the 4.5-10.8 μ m wavelength range. Ratiometric modulation of luminescence enables a detection limit of ~ 0.3 nW/ μ m² with an internal quantum efficiency on the order of 3×10⁻³. The ratiometric sensor based on lanthanide nanotransducers does not require cryogenic cooling, polarization control, phase matching, or nanoantenna design for light confinement. We also developed a camera with lanthanide nanotransducers that enable room-temperature MIR imaging. We anticipate that these lanthanide nanotransducers can be extended to MIR light manipulation at the microscale for chip-integrated device applications.



Figure 1. Working principles of detecting MIR light using lanthanide nanotransducers.

Anthracene for Molecular Solar Thermal Systems (MOST)

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The steadily increasing energy demand and the environmental impact of using fossil fuels have directed the world's focus on clean energy systems. Among all the renewable energy sources solar power systems are the most attractive option due to the abundance of energy the sun provides, consistency, and availability throughout the world. Classified among these systems is Molecular Solar Thermal system (MOST). It is a way to store solar energy in form of latent chemical bonds *via* a reversible photoinduced isomerization of organic and organometallic molecular photoswitches.^{1, 2} One such photoswitch is Anthracene. Using anthracene for solar energy storage was proposed as early as 1909.³ When exposed to sunlight, it isomerizes to the corresponding high-energy anthracene dimer. A thermal or photo back conversion can be used to release the stored energy in form of heat.^{4, 5}



Here we present different anthracene derivatives engineered with donor or acceptor substitution and alkylation to improve physical and photophysical properties such as solubility, absorption window, etc.. for future MOST applications.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Infrared emitting nanoparticles for thermal control in the brain

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Specify Technical Area: <u>✓</u>Biomedical ____ Energy and other Applications ____ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Temperature distribution has become an important subject in the study of brain physiology and in the possibility of diagnosing cerebral diseases. As traditional contact-based thermometers are not suitable for *in vivo* measurements,¹ luminescence thermometry presents itself as an alternative for efficient thermal control in the brain under *in vivo* conditions. By profiting from the high penetration depth of near-infrared light in biological tissues,^{2, 3} and the fact that fluorescence lifetime as a thermometric parameter is less prone to perturbations from the environment,⁴ one can then build a thermal probe for events taking place in the brain. Herein, we developed an Ag₂S-PEG2000-MeO (mAg₂S) thermometer with bright emission in the second near-infrared (NIR-II, 1000-1350 nm) window for noninvasive thermal reading in the brain (Figure 1a). Our results indicate that the fluorescence lifetime of mAg₂S is thermally dependent and that its calibration does not present any sign of thermal hysteresis (Figure 1b). Also, repeatability has been observed after 5 cycles of heating and cooling processes from 20 to 48 °C. Such characteristics of mAg₂S give them the potential of being applied in the brain for the diagnosis of diseases with noticeable thermal signatures.



Figure 1. (a) Fluorescence lifetime-based thermometry in the brain. (b) Fluorescent lifetime of mAg₂S in solution at different temperatures during heating and cooling process.

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SHIFT 2022 - Spectral sHaping For biomedical and energy applications TENERIFE, CANARY ISLANDS

10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Solar energy applications for Doped Transparent Metal Oxides

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Transparent Conductive Oxides (TCOs) are one of the main materials classes in optoelectronics and energy-related industries. These compounds achieve high optical transparency and electrical conductivity, making them fundamental for a wide range of applications, from solar cells to electrochromic windows. Commonly, these properties are developed by adding proper dopants in metal oxides. Some of the most used materials are Indium Tin Oxide (ITO), Fluoride Tin Oxide (FTO) and Aluminum Zinc Oxide (AZO)¹. Recently, materials like ITO and AZO have shown the ability to photodope^{2,3}, thus photo-generating electrons in the conduction band under illumination, making them interesting for light-driven energy generation/storage. In fact, these materials have shown the ability to accumulate and retain charges for a long period of time².

These metal oxides can be synthetized by colloidal approaches: this allows strict control over particle size, optical properties, and chemical composition⁴. Such particles can be employed to prepare low cost, large surface, and scalable coatings.

In this contribution, we will focus on doped metal oxides in the form of nanocrystals. We investigated the conditions for the ligand assisted synthesis in view of the possible modulation of the opto-electronic properties. Moreover, we analyzed the photodoping effect on the materials response, from the optical and electrochemical point of view. We will also present some results on the preparation of thin films, with the aim of future integration into solid-state devices for solar energy storage.

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Volumetric bioluminescence imaging of cellular dynamics with deep learning based light-field reconstruction

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In fluorescence microscopy, an external source of excitation light is required for photon emission and thereby sample visualization. Even though fluorescence imaging has provided a paradigm shift for cell biology and other disciplines, the sample might suffer due to high excitation light intensities, and spurious signals originating from autofluorescence. Bioluminescence imaging, on the contrary, does not need an external source of light for photon emission and visualization, bypassing the effects of autofluorescence, phototoxicity and photobleaching. This renders bioluminescence microscopy as an ideal tool for long term imaging. A major limitation of bioluminescence, compared to fluorescence imaging, is the low quantum yield of the bioluminescent proteins, which requires long exposure times and large collecting wells. Here, we work towards universal tools to overcome the main limitations of bioluminescence imaging: low spatiotemporal resolution and low SNR. To enhance spatiotemporal resolution, we have designed an optimized setup that boosts the optical efficiency and combine the photon starved, low SNR output with deep learning based content aware reconstruction methods. We trained a UNet architecture neural network with augmented fluorescent experimental data to denoise low SNR bioluminescent images. Next, we trained a subpixel convolutional network with synthetic Light Field data to perform 3D reconstruction from a single photographic exposure. We employed these CNN using the nematode C. elegans's mechanosensitive neural circuit during ageing and body-wall muscle to enhance the visualization of calcium activity in freely moving animals without the presence of autofluorescence. In addition, we demonstrate the denoising and 3D reconstruction on zebrafish epithelia and mouse embryonic stem cells.

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Shifting NIR photons into UV-VIS radiation with rare-earth doped materials for photocatalytic pollutant degradation and water-splitting

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Enhancing the efficiency of solar energy harvesting schemes, particularly photocatalytic processes, by means of spectral converting materials stands up as an emerging route not yet fully explored. [1] In this context, there is a growing interest in harvesting energy from the large near-infrared (NIR) range of solar radiation (approx. 60% in terms of the photon number or 40% of the energy from the sun's total incoming radiation) for various energy and environmental applications. [2] The immediate goal is to bridge the gaps of photocatalysts by shifting NIR photons into UV-VIS ones through up-conversion photonic mechanisms. [3] Here we present different photonic nanostructured and crystalline-bulk RE-doped materials showing high intense NIR-to-UV-VIS upconversion luminescence. Photocatalytic degradation of organic dye methylene blue as a pollutant model has been successfully attained under NIR radiation. We have also successfully achieved hydrogen and oxygen evolution via water-splitting using Al-doped SrTiO₃ (STO:Al) photocatalyst, loaded with rhodium-chromium oxide (RhCrO_x) as a hydrogen evolution cocatalyst in order to enable the overall water-splitting reaction. Both experiments have been carried out under low-power commercial 980 nm laser irradiation. Up-conversion driven photocatalysis is proved, as a solely photonic effect, converting incident NIR radiation before reaching the contaminated solution.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Novel luminescence manometer based on Cr³⁺ emission in Li₂Mg₃TiO₆

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Luminescent manometers, in contrast to luminescent thermometers, are quite rarely described in the literature. However, it should be borne in mind, that pressure, as temperature, is a key physical parameter that determines both the physicochemical and spectroscopic properties of compounds and processes involving them [1,2]

The applied pressure causes changes in the local environment of the ions in the matrix, including an effect on the shortening of metal-oxygen distance, which in turn affects the strength of the crystal field. Among luminescent ions, Cr³⁺ ions have a unique potential in the context of use as luminescent pressure sensor, due to the high sensitivity of their spectroscopic properties to the change in the crystal field [3].

In view of the above, in this work, a novel luminescent manometer based on the emission of $Li_2Mg_3TiO_6:Cr^{3+}$ nanoparticles is developed. This sensor is based on the luminescence intensity ratio (LIR) of the broad band associated with the ${}^{4}T_2 \rightarrow {}^{4}A_2$ transition of Cr^{3+} , integrated within two spectral ranges. The relative sensitivity S_R determined from the LIR values shows a linear dependence in the range from 0 to 7.6 GPa, and reaches a maximum value of 4.6%/GPa. The effect of temperature on the proposed manometer was also investigated, in the *T*-range of 123-563 K. The obtained results revealed that temperature has no effect on the pressure readouts. Furthermore, the luminescence measurements during decompression cycle showed that the spectroscopic changes observed as a result of the applied isostatic pressure are not caused by irreversible structural changes, which were also investigated using Raman spectroscopy (0-10 GPa).

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Multilayer PE film with recycled filler

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Please indicate preference: X Poster __ Oral Specify Technical Area: __Biomedical X Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Composite film used in this work, containing polyethylene matrix and addition of recycled material was obtained using innovative manufacturing technology. Film was obtained in one process and combines 3 separate layers – films, into one multilayer film – polymer composite with new properties basing on benefits of particular layers. To obtain such composite, with thickness close to 100 microns, innovative blow molding system has been used. Work includes use of recycle material in aim to achieve - thanks to advanced manufacturing process - properties as good as properties of pure material obtained by conventional blow molding process. Use of accurate gravimetric dosimeters on three different extruders allows to vary final multilayer film with wide range of properties [1-3]

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Electrospinning and optical characterization of RE-doped ZnO nanofibers

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Please indicate preference: X Poster __ Oral Specify Technical Area: __Biomedical X Energy and other Applications __ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Doping of the zinc oxide crystal lattice is considered to be the most effective and the most widely used method, the aim of which is most often to improve the physico-chemical properties of ZnO nanostructures [1]. Many application possibilities of zinc oxide based nanomaterials depend primarily on the size of crystallites, stresses in the crystal lattice caused by the presence of atoms and/or ions of foreign elements, the extent of electromagnetic radiation absorption resulting from the concentration and form of admixtures [2]. Lanthanides are one of the groups of elements to which much attention is paid as structural impurities of ZnO, mainly due to much better optical properties of the obtained hybrid nanomaterials [3].

Based on the above-described possibilities of producing ZnO nanofibers doped with lanthanide elements in the electrospinning process, the authors of this paper presented a method of producing thin fibrous polymer-ceramic mats, which were then subjected to a high-temperature thermal treatment process in order to obtain ceramic nanofibers. An attempt was made to dope the ZnO crystal structure with foreign atoms in the form of ytterbium (Yb), europium (Eu) and both of these elements, and the effect on the morphology and structure of electrospun nanomaterials was determined (SEM, TEM, FTIR, Raman, UV/Vis). In order to determine the optimal calcination temperature, a thermogravimetric analysis of the fibrous films was performed (TGA, DTG, DTA). The structural tests were performed based on the analysis of X-ray diffraction patterns (XRD), absorbance spectra obtained with the use of infrared spectroscopy and transmission electron microscopy. The average size of the 1D crystallites of ZnO nanostructures doped with lanthanides and the stresses in the zinc oxide crystal lattice caused by the presence of atoms and/or foreign ions were determined based on the Halder-Wagner (H-W) method.

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Exfoliation and transferring of 2D materials for potential energy conversion and storage applications

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Poster Technical Area: Energy Applications

In the last ten years, two-dimensional materials from layered van der Waals crystals have attracted a wide range of research interests. These 2D materials have electrical and structural features due to the low dimensionality and high correlations of 2D systems. Among them, transition metal dichalcogenides (TMDCs) have sizable bandgaps that change from indirect to direct in single layers, allowing applications such as transistors, photodetectors, and incredibly exciting potential for flexible electronics and optoelectronics.

Several strategies have been developed to prepare 2D TMDCs and among them, conventional mechanical exfoliation using scotch tape provides high-quality monolayers with lateral dimensions of tens of microns. The Au-assisted mechanical exfoliation is a high-yield facile method to disassemble TMDC crystals into single layers with dimensions limited only by bulk crystal sizes.

Together with band-gap engineering that can be carried out by changing the number of layers, heterostructure systems constructed by these materials can open up new design opportunities for electronics and optoelectronics. To integrate 2D materials for creating artificial structures, it is necessary to preserve the cleanliness and morphology of 2D monolayers. In this work, we transferred the monolayers mechanically which gave us the opportunity to build the heterostructure device on the substrate of our interest without worrying about the quality change of the individual layers.



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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Depletion Layer Engineering in Core-Shell Metal Oxide Nanocrystals

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The optical and electronic properties of metal oxide nanocrystals (MO NCs) strongly depend on the surface depletion regions, derived from the presence of surface states. MO NCs exhibit a localized surface plasmon resonance (LSPR), offering tunable characteristics enabled by doping, or via electrochemical or photochemical charging. Dynamic control over the LSPR makes MO NCs promising for several optoelectronic and storage applications. [1] By manipulating the NC depletion width, it is possible to control the features of the NCs. The mechanism behind this phenomenon is very complex, and not yet fully understood. [2] In particular, it is possible to engineer the depletion region by varying several parameters, including the material under consideration, the size of the NCs, the presence of multiple core-shell systems, etc. To do this, it is possible to calculate the energy band and carrier density profiles for NCs with different features. In this work, a new framework has been introduced in order to predict the behavior and physics under the MO NCs photodoping process, revealing that the charging mechanism is based on the electronic rearrangement of the energy bands. Numerical simulations were experimentally supported by studying the case of a core-shell structure of ITO/In₂O₃ NCs, by tuning the thickness of the shell, as well as post-synthetically, both by photodoping and reversible chemical reactions. The engineering of the depletion layer and the consequent manipulation of the electronic structure allows to significantly increase the sensitivity of LSPR and to target specific properties in MO NCs. The fine-tuning of the NCs band structure has enabled an improvement in the charge storage capacity, which represents a step towards fully light-driven energy storage devices. [2]

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10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Multi-Layer Optical Model for Metal Oxide Nanocrystals

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Engineering the carrier density profile is fundamental to tailor the optoelectronic properties and to design new devices based on metal oxide (MO) semiconductor nanocrystals (NCs). [1,2] In particular, the tuning of the depletion layer present at the surface of MO NCs has been demonstrated to improve the charge storage capabilities of the NCs upon photodoping. [3] Modelling the optical absorption response of a colloidal solution of NCs allows to access information on the internal structure and carrier density profile of the NCs without direct measurements.

In this work, we propose a detailed application of multi-layer optical model to describe NCs system based on Sn-doped Indium Oxide (ITO). We identified the minimum number of parameters able to simulate the experimentally observed spectra. We validated the multi-layer model by considering spectra evolution with core-shell structural tuning. Then, we considered spectra transformation by post-synthetic modification via photodoping, explaining the double peak appearance and evolution related to charge storage. We highlighted in both cases the importance of depletion layer, which plays a key role in determining a reasonable physical explanation of the spectrum evolution [4]. We foresee that the multilayer model can represent a useful tool for designing core-shell NCs systems with specific optoelectronic properties based on energy band and depletion layer engineering.

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Lanthanide-doped core-shell nanostructures with enhanced VIS-to-UVC upconverted emission for biomedical applications

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The anti-Stokes process of upconversion occurs when a few low-energy photons are sequentially absorbed by lanthanide ions and, as a result, one photon of higher energy is emitted. The first mention of such a phenomenon was provided by F. Auzel in 1966 for Yb³⁺, Er³⁺-doped phosphate glasses [1]. Since then, it has become more and more attractive to be investigated in materials bearing other lanthanide ions, as their abundant energy level structure allows for any desired wavelength generation [2]. The research accelerated when the first upconverting nanostructures were successfully synthesized in the late 1990s, which opened up the possibility to utilize them for *in vivo* biomedical applications, e.g. biosensing systems or cancer treatment. [3]

UV radiation (100-380 nm), having the tremendous impact on biologically active compounds (e.g. dsDNA), tissues, and living organisms is achievable to be generated *via* upconversion process in Tm^{3+} , Gd^{3+} or Pr^{3+} -ions doped nanomaterials. It is feasible upon visible excitation or upon energy transfer from sensitizer ions (e.g. Yb³⁺ or Nd³⁺) excited with NIR photons to the UV emitting lanthanide one [4]. Nevertheless,

the both processes are insufficiently effective, especially the NIR-to-UVC upconversion due the necessity of multiple photon sequential absorption [5]. Therefore, this study is focused on various core-shell NaYF₄ nanoparticles doped with lanthanide ions at optimized concentrations which exhibit considerably enhanced UV upconverted emission upon VIS excitation. Their performance is critically reviewed in the dsDNA photodegradation proof-of-concept experiment. The degraded dsDNA content is estimated with the dsDNA intercalating dye emission intensity changes, based on fluorescence analysis of DNA unwinding assay. Obtained within the research scope, the results provide a significant feedback concerning efficient UV emitting nanoparticles and their biomedical applications.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Investigation of the composite structures for organic solar cells (OSCs) based on bulk heterojunction (BHJ)

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Article present investigation of the structure and properties of the layered solar cells architecture containing composite (hybrid) bulk heterojunction (BHJ). The heterojunction - active layer of the solar cell, determines the photovoltaic effect through absorption of photons, separation and transport of electric charge. The authors of the Article focused on the study of p-n volumetric (bulk) heterojunctions consist of the combination of nanostructural inorganic semiconductor and semiconducting polymer matrix of (Poly [2.6- (4,4-bis- (2-ethylhexyl) -4H-cyclopenta [2,1 -b; 3,4-b '] dithiophene) -alt-4,7 (2,1,3-benzothiadiazole). The materials of the heterojunction were selected on the basis of their optical and electrical properties (absorption of solar radiation, width of the energy gap). The share of the materials were optimized in order to maximize the effect of the formation and transfer of the charges (electrons and holes). The improvement of charge transfer in the layer was achieved by the addition of a highly conductive metal nanostructures. Another innovative solution proposed by the authors is single-stage production process of the heterojunction layer requiring only prior preparation of the solution of starting materials. The final structure of OPVs was composed of a layered system including: glass substrate/ conductive indium tin oxide layer (ITO) - anode/ electron transporting layer (ETL)/ composite-BHJ / hole transporting layer (HTL)/silver (Ag) cathode.

The work include investigation of the changes in properties of active layers caused by nanoparticles additives and process parameters. The research was carried out structure and surface morphology of produced layers (with use energy-dispersive X-ray spectroscopy (EDS), scanning electron microscopy (SEM), atomic force microscopy (AFM)) as well as its optical and electrical properties (with use UV-Vis spectrometry and elipsometry). Subsequently obtained test OPVs were subjected the tests of electrical properties based on current-voltage characteristics (with maintaining standard conditions AM 1.5 with light power of 100 mW/cm²)

Presented research results fits the research on increasing the efficiency of OPV, which has an extremely significant impact on the extension of their application possibilities.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Investigation of Rylene-Based Dyes for Application in Dye-Sensitized Solar Cells

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Singlet fission (SF) has been a topic of investigations to elevate the Shockley-Queisser limit of photoconversion efficiency (PCE) from 33% to 44%.^[1] This is possible through the process of multi-exciton generation, where two charges are generated for every absorbed photon.^[2] On one hand, pentacenes and tetracenes are the more known SF sensitizers and studies in n-type solar cells have been conducted.^[3,4] On the other hand, rylenes are interesting compounds due to their application in p-type dye-sensitized solar cells.^[5] Most importantly, in terms of constructing highly efficient and cheap tandem cells, p-type devices have lagged behind in terms of generated current and PCE.^[6]

Due to the way p-type DSSC work, with the charge carrier being injected into the valence band (VB) of the semiconductor, this would suggest that SF should be a favorable process in such devices. To this end, a rylene derivative was synthesized and investigated. Devices consist of a p-type semiconductor like, for example, CuO or NiO, a standard I_2/I_3^- redox mediator, and a counter electrode, sandwiched between two conductive glass substrates. CuO exhibits higher average layer thicknesses and higher J-V values compared to NiO. On the downside, the high absorption of the CuO layers renders transient absorption pump-probe measurements rather difficult. Therefore, we focused on the more transparent NiO as a semiconductor.^[7] The goal was to optimize the device composition, to obtain the highest J-V values possible for rylenes, as well as, to study interfacial processes utilizing electrochemical impedance spectroscopy. Finally, the optimized devices were used to monitor the processes following photoexcitation in a time-resolved manner and to corroborate SF as well as charge injection from the corresponding triplet excited state.

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Dispersion of Persistent Luminescent Particles using Different Strategies to Enhance their Antimicrobial Properties

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The synthesis process of nano- and microparticles usually involves high working temperatures that directly affect to their fastdegree of agglomeration and rapid precipitation. This aspect becomes a constraint for the different *in vitro* and *in vivo* tests and consequently for their final biomedical application. With the alteration of the surface of these nanomaterials, their dispersion properties in an aqueous solution can augment significantly. The availability of particles in solution is key for the successful development of the European project Light4Lungs (L4L), which aims to develop a novel photodynamic therapy by using inhalable luminescent particles to kill the lungs bacteria. For this purpose, three different strategies have been used to disperse the persistent luminescent particles. On one hand, the silica-shell assisted (1) has been applied during the synthetic route to avoid the formation of aggregates during the annealing step (**Fig. 1a**). On the other hand, two different molecules –glutamic acid (GA) and a polyethylene glycol derivative (MeO-PEG-COOH)– have been attached on the nanoparticles' surface in order to stabilize the particles in solution (2,3). The different particles have been characterized by dynamic light scattering (size average and Z-potential), electron microscopy, X-ray powder diffraction and several spectroscopic techniques. The results have shown significant differences in terms of stability when the as-cast materials and the modified surface materials are compared, as can be seen in **Fig. 1b**.



Figure 1. (a) TEM image of ZrO_2 :Ti⁴⁺ particles inside a silica matrix and **(b)** stability studies of ZrO_2 :Ti⁴⁺ particles (left tube) and ZrO_2 :Ti⁴⁺@GA (right tube) in an aqueous solution.

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Shining a light on biomedical and energy applications

Synthesis, structural characterization and optical studies on the perovskitetype mixed oxide SrFe_{1-x}Co_xO₃ (x=0.25, 0.50, 0.75) doped with rare-earth elements.

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Perovskite-type oxides show interesting properties that make them very versatile materials for multiple applications. $SrFe_{1-x}Co_xO_3$ (x=0.25, 0.50, 0.75) oxides doped with La, Pr, Sm, Eu, and Er have been synthesized by different methods and a detailed structural study by means of X-ray diffraction has been carried out [1-2]. The dopant occupies the Sr atoms sites in the structure. In addition, others properties as UV-Vis diffuse reflectance has been studied. The bandgap for these semiconductors was determined by means of a Tauc plot [3]. Preliminary results indicate that the materials are electrical conductors with a suitable bandgap for use as catalysts and components in solar cells. The bulk of the material is porous and this fact is key for other applications such as the removal of contaminants and dyes.



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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Temperature-dependent up-conversion luminescence in core/shell nanoparticles doped with Ho³⁺ and Er³⁺ ions upon 1151 nm excitation

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Materials revealing the up-conversion (UC) phenomenon, which is a conversion of low energetic photons to higher energetic ones^[1], have attracted considerable attention in luminescence thermometry due to the possibility of precise and remote optical thermal sensing^[2]. The most widely studied type of luminescent thermometry is the ratiometric approach, which is based on changes in the UC luminescence intensity of thermally coupled energy levels of Ln³⁺ ions^[3].

In our work, core/shell nanoparticles (NPs) with the core based on sodium-yttrium fluoride with an admixture of only Ho^{3+} or Ho^{3+} and Er^{3+} ions and shells based on the undoped sodium-yttrium fluoride were synthesised using the co-precipitation method. The obtained samples were characterised by hexagonal, crystalline structures and contained nanoparticles of sizes around 22.5 nm. The spectroscopic properties of obtained NPs were investigated by measurements of the UC emission under 1151 nm excitation in the temperature range from 295 to 378 K. The mechanism responsible for the observed UC behaviour based on the energy transfer (ET) processes from Ho^{3+} to Er^{3+} ions were proposed. For the first time, thermometric sensing properties based on luminescence intensities ratio (LIR) between energy levels of Ho^{3+} and Er^{3+} ions responsible for the near-infrared emission were evaluated.



Temperature-dependent UC emission spectra of the NaYF₄:7.5%Ho³⁺,7.5%Er³⁺/NaYF₄ NPs under 1151 nm excitation.

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Shining a light on biomedical and energy applications

Zirconia nanofibers – from synthesis to optical properties characterization

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The physicochemical properties of ZrO₂ strongly depend on its crystal structure, which is influenced by the production technique used. Zirconia has three polymorphic varieties at ambient pressure: monoclinic (m-ZrO₂ <1150 °C), tetragonal (t-ZrO₂ 1150-2300 °C), cubic (c-ZrO₂ >2300 °C) and orthorhombic (o-ZrO₂) formed at high pressure. Recent advances in nanotechnology have paved the way for the successful production of one-dimensional zirconium oxide nanostructures using the hydrothermal method, sol-gel, ablation, chemical vapor deposition (CVD), direct electrochemical anodization and electrospinning. The studies conducted so far have shown that electrospinning allows for simple, scalable and repeatable production of one-dimensional nanostructures from metal oxides [1-4].

The authors of this paper presented a method of producing thin fibrous PVP/ZrOCl₂ mats using electrospinning device DOXA Microfluidics Electrospinning Startup Machine, which were then subjected to a high-temperature thermal treatment process at 500 and 600°C in order to obtain ceramic zirconia nanofibers. The morphology and structure of fibrous nanomaterials were analyzed using electron microscopy (SEM, TEM), X-ray diffraction spectroscopy (XRD), infrared spectroscopy (FTIR) and Raman spectroscopy. The influence of calcination temperature on the average crystalline size and strain were examined based on Halder – Wagner method (H-W). Moreover, based on the absorbance vs. wavelength graphs, the optical band gaps of the obtained nanostructures were calculated.

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TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Hybrid TiO₂ NPs-SnO₂ NWs photoanode for developing the performance of DSSC

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The aim of the work was to use the facile electrospinning method with subsequent calcination in 500 and 600 °C to produce one-dimensional SnO₂ nanostructures and use them as a supplement to TiO₂ photoanode in order to increase the efficiency of dye-sensitized solar cell. An analysis of the morphology and structure of nanowires using scanning and transmission electron microscopy (SEM, TEM) was carried out. The chemical composition and crystallographic structure were determined using Fourier transform infrared spectroscopy (FTIR), Raman and X-Ray diffraction (XRD), respectively. In addition, the specific surface area and porosity of the obtained nanostructures were measured by the BET and BJH methods. In order to investigate the influence of the SnO₂ nanowires calcination temperature on their optical properties, a UV-Vis spectrophotometer was used and the optical energy gap was determined.

The obtained SnO_2 nanowires in various amounts were added to TiO_2 nanoparticles and applied to the FTO substrate by screen printing. The topography of the produced layer was analyzed by SEM (Fig.1). Then, the dye, electrolyte and electrode were placed on the SnO_2/TiO_2 layers and the performance of the finished DSSCs was investigated. It was shown that the use of nanowires calcined at 600 °C improves the efficiency of the cell by 13%. It was also observed that higher concentration of SnO_2 nanowires in TiO_2 paste decreased DSSCs performance.



Fig. 1. Manufactured DSSC with SEM image of SnO₂/TiO₂ composite layer



Photoisomerization of Push-pull Functionalized Norbornadiene/Quadricyclane Couples for Solar Energy Storage

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The norbornadiene (NBD) / quadricyclane (QC) couple is a very well-known solar energy storage system. By means of functionalizing the NBD double bonds with electron-donating and/or -accepting groups, the absorption is shifted with ease from the UV to the visible range of the solar spectrum.¹⁻³ As a function of push-pull strength, different electronic states are populated during irradiation. Using transient absorption spectroscopy, we follow the generation of these states and their fate within the context of photo-isomerization. This enables constructing, for the first time, the full reaction coordinate of photo-isomerizing NBD to afford QC.⁴ This includes the fact that the photo-isomerization is tunable by, for example, irradiating either into the localized NBD absorption or the delocalized charge-transfer absorption. A strong push-pull character goes hand-in-hand with facilitating a light-triggered back-isomerization from QC to NBD.^{4,5} A particularly prominent example is NBD featuring an electron-accepting perylenediimide (PDI). Here, the QC to NBD back-isomerization proceeds via a charge-separated state rather than a charge-transfer state in QCs with poorer electron accepting ability.

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The influence of vanadate host material on the relative sensitivity and brightness in the single band ratiometric thermometry

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Poster

Technical Area: Energy and other Applications

In recent years, it has been found that crucial to understanding the course of many thermodynamic processes, both in liquids and solids, is the spatial determination of temperature. However, among conventional methods, most offer the possibility of determining temperature only point-wise or surfacewise, and that too may require the direct introduction of a temperature probe into the investigated system in the invasive way. Therefore, techniques termed luminescence thermometry, which overcome these limitations, are thriving. Nowadays it found the applicability for both in vivo thermal imaging [1], as well as monitoring the temperature of microelectronic components [2]. One of the methods developed in luminescent thermometry is the single band ratiometric approach, which uses the ratio of emission intensities coming from a single band at two excitation wavelengths [3]. An example of the use of this strategy was performed in AVO₄ (A = Lu, Y, Gd, La) nanocrystals doped with Eu³⁺ [4]. It was found that ${}^{1}E({}^{1}T_{1}) \rightarrow {}^{1}B_{2}({}^{1}T_{2})$ absorption band in these host materials is thermally enhanced with respect to the ${}^{1}A_{2}({}^{1}T_{1}) \rightarrow {}^{1}B_{2}({}^{1}T_{2})$ of the V⁵⁺ ion. As a result, due to (VO₄)³⁻ to Eu³⁺ charge transfer, the ratio of observed Eu³⁺ emission intensities recorded upon two different excitation wavelengths is temperature dependent. Therefore, two wavelengths, i.e. 266 nm and 342 nm, were selected to obtain thermal evolution of intensities for ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ emission band of Eu³⁺ ions with opposite monotonicity. Example emission band intensities are shown for YVO₄:Eu³⁺, where the opposite monotonicity was observed in the range from ~220 to 520 K (Figure 1). This guarantees a satisfactory relative sensitivity of luminescent

thermometer, which exceeded 1.0% K⁻¹ in the range from 180 to 350 K in the case of YVO4:Eu³⁺ with a maximum sensitivity of 3.0% K⁻¹ at 230 K. The results obtained for different host material with general formula of AVO₄:Eu³⁺, where A = Lu, Y, Gd, La, were compared to find correlations between spectroscopic and structural properties.

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Highly Stable Lead-Free Perovskite Single Crystals with NIR Emission beyond 1100 nm

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Please indicate preference: Poster Specify Technical Area: NIR imaging

Materials that emit in the near-infrared (NIR) region are at the forefront of both research and industry, mainly due to their wide applications in national security, non-destructive bioimaging, long-wave communications, and photothermal conversion for medical care. As a key member of the luminescent materials family, metal halide perovskites have been intensively demonstrated to emit light in ultraviolet and visible regions. However, NIR-emitting perovskites suffer from severe limitations, such as low photoluminescence quantum yield and poor chemical/optical stability, thereby preventing them from practical applications. Herein, we report the synthesis and growth of Cs₂MoCl₆ and Cs₂WCl₆ perovskite single crystals with ultrahigh chemical and optical resistance to heat, moisture, polar solvents, and high-energy radiation. Upon ultraviolet or blue excitation, these lead-free single crystals emit light beyond 1100 nm, the longest wavelength ever reported for perovskite hosts. Mechanistic studies indicate that self-trapped excitons are responsible for the NIR emission. We also fabricate optoelectronic devices using these



single crystals and demonstrate their broad applications in noninvasive palm vein imaging, night vision, and non-destructive food analysis. These results may stimulate research in the development of highefficiency near-infrared perovskite phosphors for fast, accurate biometric identification food and inspection.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

Lanthanide-nucleotide Coordination Nanoparticles for STING Activation Zichao Luo, Xiaogang Liu*

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Please indicate preference: Poster Specify Technical Area: Biomedical Satellite Meeting "Doing Biology with Light"

Activation of the stimulator of interferon genes (STING) is essential for blocking viral infections and eliciting antitumor immune responses. Local injection of synthetic STING agonists, such as 2'3'-cGAMP, is a promising approach to enhance antiviral functions and cancer immunotherapy. However, the application of such agonists has been hindered by complicated synthetic procedures, high doses, and unsatisfactory systemic immune responses. Herein, we report the design and synthesis of a series of 2'3'-cGAMP surrogates in nanoparticle formulations formed by reactions of adenosine monophosphate, guanosine monophosphate, and coordinating lanthanides. These nanoparticles can stimulate the type-I interferon (IFN) response in both mouse macrophages and human monocytes. We further demonstrate that the use of europium-based nanoparticles as STING-targeted adjuvants significantly promotes maturation of mouse bone marrow-derived dendritic cells and MHC class I antigen presentation. Dynamic molecular docking analysis revealed that these nanoparticles bind with high affinity to mouse STING and human STING. Compared with soluble ovalbumin, subcutaneously immunized europium-based nanovaccines exhibit significantly increased production of primary and secondary anti-ovalbumin antibodies (~180-fold) in serum, as well as IL-5 (~28-fold), IFN- γ (~27-fold) and IFN- α/β (~4-fold) in splenocytes *ex vivo*. Compared with the 2'3'-cGAMP/ovalbumin formulation, subcutaneous administration of nanovaccines significantly inhibits B16F10-ovalbumin tumor growth and prolongs survival of tumor-bearing mice in both therapeutic and protective models. Given the rich supramolecular chemistry with lanthanides, this work will enable a readily accessible platform for potent humoral and cellular immunity while opening new avenues for costeffective, highly efficient therapeutic delivery of STING agonists.



Figure 1. Scheme of Ln-GAMP-NPs for STING activation.



TENERIFE, CANARY ISLANDS 10-14TH OCTOBER, 2022

Shining a light on biomedical and energy applications

SYNTHESIS AND CHARACTERIZATION OF MIXED OXIDES WITH RARE EARTH

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In the last years, perovskites containing rare earth elements have been extensively studied for their incredible properties as solar cells components and in the field of hydrogen production. In this project, the main objective is the synthesis and structural characterization of perovskite-type oxides A'_xBa_{1-x}Mo_{0.8}Ni_{0.2}O₃ (A'= Yb, Er // x= 0.1; 0.2; 0.4) and the study of their magnetic and electrical properties as superconductivity, test whether these compounds are useful for catalysis and PCS. Furthermore, a comparison between synthesis methods by different optical techniques such as SEM and AFM have been carried out.









AFM



Shining a light on biomedical and energy applications

Synthesis, structural characterization and optical studies on the perovskitetype mixed oxide $SrFe_{1-x}Co_xO_3$ (x=0.25, 0.50, 0.75) doped with lanthanides.

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Please indicate preference: X Poster _ Oral Specify Technical Area: _ Biomedical X Energy and other Applications _ SHIFT-DBL (Satellite Meeting "Doing Biology with Light")

Perovskite-type oxides show interesting properties that make them very versatile materials for multiple applications. $SrFe_{1-x}Co_xO_3$ (x=0.25, 0.50, 0.75) oxides doped with La, Pr, Sm, Eu, and Er have been synthesized by different methods and a detailed structural study by means of X-ray diffraction has been carried out [1-2]. The dopant occupies the Sr atoms sites in the structure. In addition, others properties as UV-Vis diffuse reflectance has been studied. The bandgap for these semiconductors was determined by means of a Tauc plot [3]. Preliminary results indicate that the materials are electrical conductors with a suitable bandgap for use as catalysts and components in solar cells. The bulk of the material is porous and this fact is key for other applications such as the removal of contaminants and dyes.



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