

# **PANIC**

# **Summer School 2023**

## **Book of Abstracts**

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International Conference**

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Karolina Saczuk  
Magdalena Wolak  
Kamil Bruchal  
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[zamawianie.ksiazek@pwr.edu.pl](mailto:zamawianie.ksiazek@pwr.edu.pl)

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# Summer School Programme

Monday – 15.05.2022	
Hours	Activity
9:00–9:30	Registration
9:30–9:45	Opening ceremony
Session I	
9.45–11:15	Invited lecture (I) – Prof. Carlos Marques
11:15–12:30	Poster session with a coffee break
12:30–14:00	Invited lecture (II) – Prof. Carlos Marques
14:00–15:00	Lunch break
Session II	
15:00–16:30	Invited lecture (I) – Prof. Thomas Bürgi
Tuesday – 16.05.2022	
Hours	Activity
Session I	
8.45–10:15	Invited lecture (III) – Prof. Carlos Marques
10:15–10:45	Coffee break
10:45–12:15	Invited lecture (I) – Prof. Bruno Therrien
12:15–12:30	Technical break
12:30–14:00	Invited lecture (I) – Prof. Ji-Seon Kim
14:00–15:00	Lunch break
Session II	
15:00–16:30	Invited lecture (II) – Prof. Ji-Seon Kim
19:30	Banquet



Wednesday – 17.05.2022	
Hours	Activity
<b>Session I</b>	
8.45–10:15	Invited lecture (I) – Prof. Neil Robertson
10:15–10:45	Coffee break
10:45–12:15	Invited lecture (I) – Dr Jean-Charles Ribierre
12:15–12:30	Technical break
12:30–14:00	Invited lecture (III) – Prof. Ji-Seon Kim <b>Leading and mentoring session (1/2)</b>
14:00–15:00	Lunch break
<b>Session II</b>	
15:00–15:45	Prof. Bruno Therrien <b>Leading and mentoring session (2/2)</b>
15:45–15:50	Technical break
15:50–16:30	<b>Flash presentations</b>
Thursday – 18.05.2022	
Hours	Activity
<b>Session I</b>	
8.45–10:15	Invited lecture (II) – Dr Jean-Charles Ribierre
10:15–10:45	Coffee break
10:45–12:15	Invited lecture (II) – Prof. Bruno Therrien
12:15–12:30	Technical break
12:30–14:00	Invited lecture (III) – Jean-Charles Ribierre
14:00–15:00	Lunch break <b>+ Phobia Student Photonics Symposium (PS)<sup>2</sup></b>
<b>Session II</b>	
15:00–16:30	Invited lecture (III) – Prof. Bruno Therrien

<b>Friday – 19.05.2022</b>	
<b>Hours</b>	<b>Activity</b>
<b>Session I</b>	
<b>8.45–10:15</b>	Invited lecture (II) – Prof. Neil Robertson
<b>10:15–10:45</b>	Coffee break
<b>10:45–12:15</b>	Invited lecture (II) – Prof. Thomas Bürgi
<b>12:15–12:30</b>	Technical break
<b>12:30–14:00</b>	Invited lecture (III) – Prof. Thomas Bürgi
<b>14:00–15:00</b>	Lunch break
<b>Session II</b>	
<b>15:00–16:30</b>	Invited lecture (III) – Prof. Neil Robertson
<b>16:30–17:00</b>	Closing ceremony

# Detailed list of PhD students' presentations

Wednesday – 17.05.2022	
Hours	Activity
15:00–15:45	Invited lecture – Leading and mentoring session Prof. Bruno Therrien
Session I – prof. Ji-Seon Kim	
12:30–12:45	<b>M. Ślemp</b> <i>“Hyper Rayleigh Scattering from metallic nanoparticles: Novel insight into interactions with elliptical polarization”</i>
12:45–13:00	<b>M. Lipok</b> <i>“Chiral fluorescence microscopy for studying linear and nonlinear properties of gold nanoclusters”</i>
13:00–13:15	<b>R. Kosman</b> <i>“Coupled colloidal molecules CdSe/ZnS@CdSe/ZnS and CdSe@CdSe”</i>
13:15–13:30	<b>K. Pyrchla</b> <i>“The optically detectible strain states in phosphorene nanostructures – ab initio study”</i>
13:30–13:45	<b>A. Hajda</b> <i>“Influence of donor position on one- and two-photon optical properties in amyloid markers”</i>
13:45–14:00	<b>S. Kozub</b> <i>“Single-chain folding of oligourethanes”</i>
Session II – prof. Bruno Therrien	
15:00–15:15	<b>L. Duda</b> <i>“Behavior of organic luminescent dyes in thermotropic liquid crystalline matrix – studies of novel diketofurofuran and selected dyes”</i>
15:15–15:30	<b>W. Zając</b> <i>“Surface modified photonic crystals for colorimetric gas detection”</i>
15:30–15:45	<b>A. Kabański</b> <i>“Highly sensitive luminescent thermometers based on hybrid formate perovskites containing dimethylammonium cations”</i>

<b>Session III (shotguns)</b>	
<b>15:50–15:55</b>	<b>M. Szatko</b> <i>“Development of Molecular Dynamics methodology to access receptor function in abiotic sequence-defined polymers”</i>
<b>15:55–16:00</b>	<b>K. Bruchal</b> <i>“Anti-Stokes cooling of lanthanide-doped nanoparticles”</i>
<b>16:00–16:05</b>	<b>D. Benkowska-Biernacka</b> <i>“The effect of pH on liquid crystalline properties of myelin-like structures”</i>
<b>16:05–16:10</b>	<b>M. Pieprz</b> <i>“Increasing the sensitivity of pressure readings based on Nd<sup>3+</sup> ion emission through Cr<sup>3+</sup> co-doping”</i>
<b>16:10–16:15</b>	<b>P. Źemojtel</b> <i>“First-principles analysis of the point-defects influence on CdSe nanoplatelets spectroscopic properties”</i>
<b>16:15–16:20</b>	<b>A. Zdubek</b> <i>“The Use of 5-aminolevulinic Acid in the Photodynamic Eradication of Psuedomonas aerugiinosa”</i>
<b>16:20–16:25</b>	<b>M. Piksa</b> <i>“The photosensitization of giant unilamellar vesicles assembled from bacterial lipid extracts”</i>
<b>16:25–16:30</b>	<b>M. Hancharova</b> <i>“Electrospun fibers in lighting nanotechnology”</i>

# List of PhD students' posters

Poster no.	Presenter	Title
P01	Zuzanna Korczak	Temperature dependence of photon avalanche emission in NaYF <sub>4</sub> :Pr <sup>3+</sup> Yb <sup>3+</sup> nanocrystals ions
P02	Martyna Majak	Influence of neodymium concentration on the photon avalanche and two-color emission from Tm <sup>3+</sup> in LiYF <sub>4</sub> 3% Tm <sup>3+</sup> microcrystals.
P03	Magdalena Dudek	Photon Avalanching in Pr <sup>3+</sup> and Yb <sup>3+</sup> co-doped NaYF <sub>4</sub> nanocrystals
P04	Kamila Lupińska	Linear and nonlinear properties of novel furan-based organic compounds exhibiting AIE behavior
P05	Patryk Rybczyński	Donor-acceptor fluorescent dyes for bioimaging
P06	Judyta Zielak-Milewska	The influence of donor change on TADF properties in difluoroborate-based dyes
P07	Agnieszka Siomra	Nonlinear optical properties of sulfur quantum dots for applications in heavy metal ions detection
P08	Maja Szymczak	Bimodal, ratiometric luminescence manometer based on Cr <sup>3+</sup> doped MgO nanoparticles
P09	Nina Tarnowicz-Staniak	Plasmonic Nanoparticles for Organic Photovoltaics – Synthesis and Postprocessing
P10	Małgorzata Policht	In the search for a perfect nanosilver stabiliser – ionic liquids with alkoxyethyl substituent?
P11	Przemysław Pietrusiak	Choline-based ionic liquids entrapped in nanocellulose matrix
P12	Maksymilian Dereniowski	Revealing the Hidden Beauty of Conjugated Polymers and Multilamellar Vesicles through the Lens of Third-Harmonic Generation Microscopy



# **Invited Lecturers**





## Prof. Thomas Bürgi



**Prof. Thomas Bürgi** studied chemistry and obtained his PhD in 1995, at the University of Bern, Switzerland. After a postdoc at Massachusetts Institute of Technology, he did his habilitation at Eidgenössische Technische Hochschule Zürich. He became an Assistant Professor at the University of Neuchâtel, Switzerland (2005) and a Full Professor at the University of Heidelberg, Germany (2008). In 2010, Prof. Bürgi moved to the University of Geneva, Switzerland, where he is a Professor of Physical Chemistry. His research focuses on fundamental aspects and applications of chiral metal clusters, surface chemistry and the development of in situ spectroscopy.

Prof. Thomas Bürgi, affiliated at University of Geneva, is going to deliver a series of lectures regarding the characteristics and applications of monolayer-protected metal clusters.

# Atomically precise monolayer-protected metal clusters: Chirality, dynamic nature and applications

Thomas Bürgi

*Department of Physical Chemistry, University of Geneva, 30 quai Ernest-Ansermet, 1211 Geneva, Switzerland  
E-mail: thomas.buergi@unige.ch*

Chirality at the nanoscale has gained considerable interest in recent years. Chiral nanomaterials have properties that are of interest for applications in chiral technology but also in materials science. In this contribution we will focus on a special class of materials: Monolayer-protected metal clusters [1]. As will be shown, these atomically well-defined objects could be used as building blocks for nanotechnology, as catalysts or as sensors. We will discuss the preparation of chiral gold clusters [2], their chiroptical properties studied by circular dichroism and vibrational circular dichroism and the transfer of chirality from cluster to ligand [3].

These clusters, although stable, turn out to be very dynamic. The latter is evidenced by the exchange of metal atoms and ligands between clusters as well as between clusters and surfaces. In addition, chiral clusters can undergo racemization. The latter property is usually unwanted but we will show that the interplay between racemization of a cluster and exchange of a chiral ligand can lead to amplification of enantiomeric excess [4].

## References

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- [3] Dolamic, Igor; Varnholt, Birte and Bürgi, Thomas, Chirality transfer from gold nanocluster to adsorbate evidenced by vibrational circular dichroism, *Nature Commun.* 6, 7117 (2015).
- [4] Wang, Yanan; Nieto-Ortega, Belen and Bürgi, Thomas, Amplification of enantiomeric excess by dynamic inversion of enantiomers in deracemization of Au<sub>38</sub> clusters, *Nature Commun.* 11, 4562 (2020).

## **Prof. Ji-Seon Kim**



**Prof. Ji-Seon Kim** is a Professor of Solid State Physics and the Director of the EPSRC Centre for Doctoral Training in Plastic Electronic Materials at Imperial College London. She also holds an Invited Professorship at Tokyo Institute of Technology (Japan) and held an Invited WCU Professorship at KAIST (Korea). Her research focuses on the Materials Physics of Molecular and Hybrid Semiconductor Devices, including the integration of structural and energetic spectroscopic techniques with simulation to elucidate the key processes determining device performance.

Prof. Ji-Seon Kim, from Imperial College London, will provide students attending PANIC Summer School 2023 with her latest work in the field of organic optoelectronic devices.

# Key Molecular Design Rules for High Performance Organic Optoelectronic Devices

Ji-Seon Kim

*Department of Physics & Centre for Processable Electronics, Imperial College London, United Kingdom*  
E-mail: [ji-seon.kim@imperial.ac.uk](mailto:ji-seon.kim@imperial.ac.uk)

Soft electronic materials such as organic semiconductors have attracted a huge interest for display, sustainable energy and healthcare applications. These applications include organic light-emitting diodes (OLED), photovoltaics (OPV), photodetectors (OPD), and electrochemical transistors (OECT). Although promising, there is still a lack of clear understanding of the impact of molecular structures and orientations in thin films on photophysical and electrochemical processes, which are critical for high-performance organic optoelectronic devices.

I will introduce our recent work in three main research areas such as OPV, OPD and OECT. First, I will discuss the importance of molecular design on efficiency and stability of OPV materials with a particular focus on non-fullerene acceptors. I will show the molecular structure-dependent photostability [1–3] and the molecular orientation-dependent energetic shift in NFAs, demonstrating the impact of NFA quadrupole moment on material energetics and thereby on the OPV performance [4]. Compared to sublimed small molecules where the molecular orientation control is relatively easy [5], there has been no report, to the best of our knowledge, demonstrating the orientation control of solution-processed NFA molecules leading to an energetic shift large enough to impact exciton separation for free charge generation. Second, I will discuss the molecular origin of high-performance in OPD devices, showing the key differences between OPD and OPV devices in terms of their operational mechanisms and requirements for molecular design [6]. Third, I will discuss the key molecular design rules for high-performance OECTs, where charge transport occurs via mixed electronic and ionic conduction [7]. As such, it is now critical to understand the molecular origins in much deeper detail than before to direct synthesis of organic semiconductors in more promising directions.

## References

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- [2] “Exceptionally low charge trapping enables highly efficient organic bulk heterojunction solar cells”, Wu J., et al., *Energy & Environmental Science*, (2020), 13(8), 2422-2430, doi: 10.1039/d0ee01338b
- [3] “Twist and Degrade-Impact of Molecular Structure on the Photostability of Nonfullerene Acceptors and Their Photovoltaic Blends”, Luke J. et al., *Advanced Energy Materials*, (2019), 9(15), doi: 10.1002/aenm.201803755.
- [4] “Molecular orientation-dependent energetic shifts in solution processed non-fullerene acceptors and their impact on organic solar cell performance”, Fu Y. et al., *NATURE COMMUNICATIONS* (in press).
- [5] “Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells”, Dong Y. et al., *Nature Communications*, (2020), 11(1), doi: 10.1038/s41467-020-18439-z.
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- [7] “The Role of Long-Alkyl-Group Spacers in Glycolated Copolymers for High-Performance Organic Electrochemical Transistors”, Tan, E., et al., *ADVANCED MATERIALS*, (2022) 34(27), doi: 10.1002/adma.202202574.

## Prof. Carlos Marques



**Prof. Carlos Marques**, a CNRS senior scientist, founded the MCube group at the Charles Sadron Institute in Strasbourg, France, where he geared experimental and theoretical research towards the understanding of the physical properties of self-assembled lipid bilayers. Trained as a polymer theoretician, he first got interested in membranes because of their interactions with polymers, and published the first prediction for the membrane changes expected when polymers adsorb on lipid bilayers. His group grew to include experiments and numerical simulations, and Prof. Marques has now published many papers based on research with giant unilamellar vesicles, including the first study of lipid oxidation in GUVs and the discovery of the so-called PVA method for vesicle growth. With his colleague, Rumiana Dimova, he edited *The Giant Vesicle Book*, the present reference textbook for these cell-size lipid platforms.

Prof. Carlos Marques, affiliated at the Charles Sadron Institute, is going to deliver lectures about the science of lipid membranes and light.

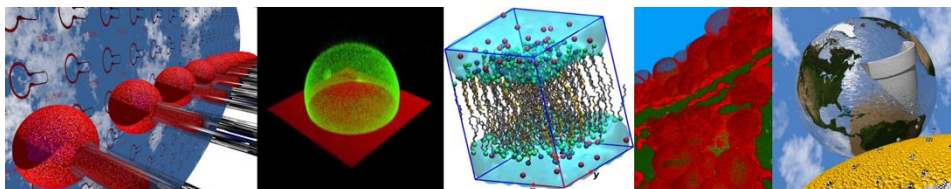
# Lipids and light: the fourth pillar of life under a microscope

Carlos M. Marques

University of Lyon, ENS-Lyon, CNRS UMR 5182, Chem. Lab., 69342 Lyon, France  
E-mail: [carlos.marques@ens-lyon.fr](mailto:carlos.marques@ens-lyon.fr)

From the standard point-of-view of biology, lipids are the dullest and the less interesting molecules amongst the four pillars of life: no well-defined molecular structure that would unveil directly the secrets of biological function like *DNA* and *proteins*, no high specificity like *carbohydrates*. Ole Mouritsen, in his book *Life as a matter of fat*, recalls as a teaser that lipids are considered as “[...] a structureless fatty material which is at best organized in a membrane structure that plays the role of a passive container of the cell and a solvent or container for the other important molecules of life.” Briefly, “lipids grease the functional machinery of the cells, controlled and run by proteins and DNA”.

But “there is a crack in everything, that is how light gets in”. We will meander thus in these lectures through the wide-open rifts of that standard view, exploring the unique properties of lipid self-assembly, phase behavior and functionality. Guided by what one can learn under an optical microscope about lipid structure and organization, we will micromanipulate lipid membranes subjected to photo-induced chemical reactions and phase transformations. Emerging from our meanderings, we will show why and how the modern science of lipids not only triggers many fundamental endeavors in biology, chemistry and physics, but also contributes to important technological progress in different areas and enlightens debates that permeate through present human societies.



From left to right: excess area of membrane oxidation [1], adhesion of giant vesicles, fatty alcohol bilayers, gel-supported vesicle formation [2, 3], oligomer pollution [4].

## References

- [1] Photo-induced Destruction of Giant Vesicles in Methylene Blue Solutions. Caetano, W. et al. *Langmuir*, 2007, 23, 1307.
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## Dr Jean-Charles Ribierre



**Dr Jean-Charles Ribierre** is the Reader in the School of Physics and Astronomy at the University of St Andrews in the UK. He received both his PhD degree in 2002 and his habilitation to supervise research in 2011 from the University of Strasbourg, France. His research activities mainly focus on the physics of organic semiconductors and their applications in organic electronics and photonics. His most recent important achievements involve the realization of high-efficiency near infrared thermally-activated delayed fluorescent (TADF) organic light-emitting diodes (OLEDs) and the first evidences of an influence of hyperbolic metamaterials on the charge transfer processes in organic thin films. He also played a key role in the development and the exploitation of a novel organic laser diode technology with the creation of a startup company, of which he was the CEO between 2019 and 2022.

Dr Jean Charles Ribierre, affiliated at the University of St Andrews, is going to deliver a series of lectures devoted to the physics of organic light-emitting materials and their applications in organic optoelectronics including OLEDs and organic semiconductor lasers.

# Organic light-emitting materials and their applications in optoelectronics

Jean-Charles Ribierre

*School of Physics and Astronomy, University of St Andrews,  
North Haugh, KY16 9SS St Andrews, United Kingdom  
E-mail: jr43@st-andrews.ac.uk*

Since the demonstration of the first organic light-emitting diode (OLED) by Tang and Slyke in 1987 [1], OLEDs have been the subject of intensive studies in both academia and industry. They became one of the dominant technologies for light-emitting displays used in full-color televisions and smartphones, and hold great promise for other applications in the fields of lighting, optical communication and healthcare. Another attractive and exciting feature of organic light-emitting molecules is their ability to amplify light and show a laser activity. Since 1995 and the first demonstration of organic semiconductor lasers [2], this class of devices has progressed significantly along with the development of high-efficiency OLED materials. In particular, the combined improvements in organic low-threshold laser materials and resonator structures have recently led to a clear indication of a current injection lasing from an organic electroluminescent device architecture [3].

In the first part of this lecture, I will provide an overview of the OLED technology and will discuss about the material development and the physical processes involved during the device operation. In particular, we will see how materials showing an efficient thermally-activated delayed fluorescence (TADF) can be engineered for the realization of high-performance OLEDs [4, 5]. With this knowledge, we will briefly discuss about the current challenges for the OLED technology and their future applications. In the second part of the lecture, I will then focus the discussion on the development and the recent advances of organic semiconductor lasers. After an introduction about the chemistry and physics of these devices, I will discuss more in details about the remaining challenges to operate them under long pulse photo-excitation [6] and to achieve an efficient lasing emission under current injection [3, 7].

## References

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- [2] N. Tessler, J.G. Denton, R.H. Friend, *Nature* 382, 695 (1996).
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## **Prof. Neil Robertson**



**Prof. Neil Robertson** graduated from the University of Edinburgh and worked in FU Berlin, University of Wales and Imperial College London before returning to University of Edinburgh. He leads research on new molecular and nanomaterials for solar photovoltaics, photocatalysis, electrical energy storage materials and devices, with around 230 peer-reviewed papers in international journals. He is Fellow of the Royal Society of Chemistry (RSC) and Fellow of the Higher Education Academy. He has previously served as Elected Member of RSC Dalton Council and RSC Materials Chemistry Division Council, and is Associate Editor of RSC Journal of Materials Chemistry C. He is Dean International Partnerships for Science and Engineering at the University of Edinburgh.

Prof. Neil Robertson from University of Edinburgh will acquaint Summer School attendees with the newest trends in nanomaterials for photocatalytic and photovoltaic applications.

# Nanomaterials for Electrical Energy Storage and Photocatalysis

Neil Robertson

*School of Chemistry, University of Edinburgh, King's Buildings, Edinburgh, Scotland, UK*  
E-mail: *neil.robertson@ed.ac.uk*

The presentation will focus on the design, synthesis, characterisation and application of nanomaterials for energy and environmental uses. We have recently studied bismuth-based anode materials in electrical energy storage and demonstrate ambient-pressure and moderate-temperature synthetic routes to nanocrystals and films of bismuth chalcogenides and halides, including  $\text{Bi}_{13}\text{S}_{18}\text{I}_2$  [1, 2],  $\text{BiSI}$  [2],  $\text{BiSI}$ -reduced-graphene-oxide [3] (Fig. 1), and  $\text{ABiI}_4$  (A = organic cation) [4]. We investigate their potential as anodes in super capacitors, pseudocapacitors, and lithium-ion batteries, showing high capacitance/capacity and excellent cycle stability.

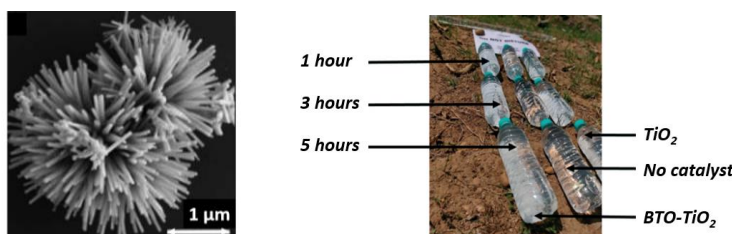


Figure 1: Hybrid  $\text{BiSI}$ -rGO material SEM (left); Photocatalytic drinking water treatment (right)

Contamination of water is increasingly problematic and we have studied photocatalysis for practical, real-world water treatment in rural areas [5]. We have applied simple solution-based approaches to create immobilized, nanocrystalline, photocatalyst films, with visible light harvesting and good charge separation [6]. Initial application to drinking water in rural India has been carried out and will be discussed [7].

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# Dye-Sensitised Solar Cells: Materials, Mechanisms and Applications

Neil Robertson

School of Chemistry, University of Edinburgh, King's Buildings, Edinburgh, Scotland, UK  
E-mail: neil.robertson@ed.ac.uk

Dye-sensitised solar cells (DSSCs) have recently attracted increasing interest for ambient light harvesting, with reported efficiencies now reaching 37% under indoor light [1]. A remaining challenge however, is the comparatively poor stability of devices containing a liquid electrolyte. One approach to overcome this involves drying of the Cu-complex based electrolyte to give a solid-state, so-called “zombie”, cell [2]. Although these can reach good efficiencies, the drying process is currently slow and poorly reproducible, thus impractical for real-world use. The presentation will give a background overview to DSSCs, including insights into the design of organic and inorganic materials for light absorption and charge transport, alongside understanding of the mechanism and characterisation of materials and devices. Following this, the talk will focus on our recent work into simple and stable zombie DSSCs. We have fabricated solid-state DSSCs by simply drying out the common liquid  $I^-/I_3^-$  electrolyte [3], and have demonstrated solar power-conversion efficiency for the solid-state cells over 5%, similar to that of the parent liquid cell before drying. In indoor light conditions (1000 Lux), power-conversion efficiencies were around 20%. We observed negligible degradation of efficiency after 12 months dark storage without encapsulation. Furthermore, we have developed a rapid process for cell fabrication, enabling larger area devices made on an open bench [4]. These findings establish a unique new approach to making very simple, stable, solid-state DSSCs of potential practical application.



Figure 1: Rapid drying process with quicker fabrication is quicker and improved stability

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# Design, Synthesis & Properties of Organic Materials for Photovoltaic Cells

Neil Robertson

School of Chemistry, University of Edinburgh, King's Buildings, Edinburgh, Scotland, UK  
E-mail: neil.robertson@ed.ac.uk

Organic materials have been widely applied in emerging photovoltaic technologies, including as dyes for dye-sensitised solar cells [1]; for light-harvesting and charge-transport in organic photovoltaics [2], for charge transport in perovskite solar cells [3] and as luminescent materials in luminescent concentrators and downshifting [4]. For all of these applications, attention must be paid to molecular design to achieve properties such as appropriate HOMO and LUMO energies; excited-state energy levels; hole and/or electron mobility; solubility and processing; cost; and stability to light and heat. The presentation will illustrate structure property relationships in organic and molecular materials, and show how these can be tuned to give the desired properties for various photovoltaic applications. This will be illustrated with examples from different solar technologies, also touching upon examples from other electronic and optoelectronic fields to show how understanding can be transferred between application areas.

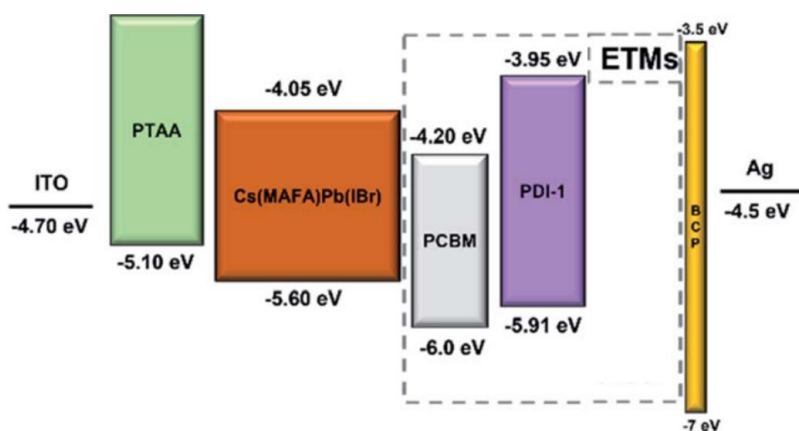


Figure 1. Energy level diagram of a solar cell based on perovskite absorber {Cs(MAFA)Pb(IBr)}, with PTAA as hole-transport material and a choice of materials, the commonly-used PCBM or the alternative PDI-1, for electron-transport [3]

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## **Prof. Bruno Therrien**



**Prof. Bruno Therrien** is a Professor within the Institute of Chemistry at the University of Neuchâtel, Switzerland, and since 2005 he runs the single-crystal X-ray structure facility, which is part of the Neuchâtel Platform of Analytical Chemistry. In the last twenty years, he has developed an independent career, and pioneered the biological side of arene ruthenium metalla-assemblies. His main research interests are the biological applications of water soluble metalla-assemblies and the use of hybrid ruthenium-porphyrin compounds in photodynamic therapy.

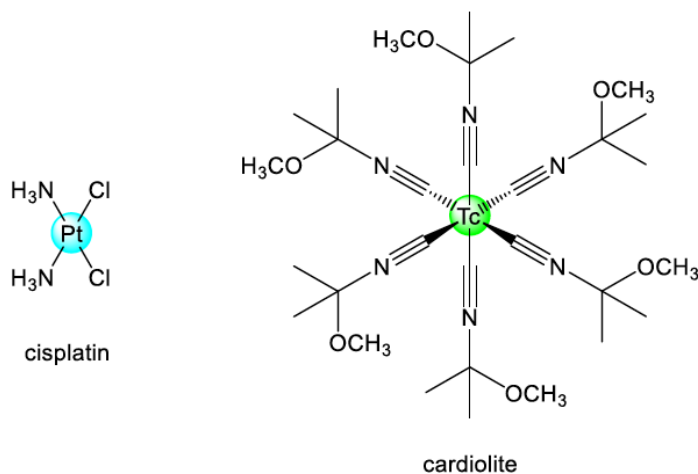
Prof. Bruno Therrien, affiliated at the University of Neuchâtel, is going to deliver a series of lectures regarding biological and biomedical applications of metal-based assemblies.

# Metal-Based Drugs – Past, Present and Future

Bruno Therrien

*Institute of Chemistry, University of Neuchatel, Switzerland  
E-mail: bruno.therrien@unine.ch*

The medicinal virtues of metals have been known for centuries [1]. Ancient civilizations have been often intrigued by metals, giving them sometimes magical properties, and the main objective of alchemists was to transform metals into gold. However, with the advent of modern medicine, metals have become an essential tool in the clinic, being involved in therapeutic and diagnostic procedures [2]. Nowadays, metals can be found in drugs and in imaging agents, especially when dealing with cancer. The nature of metals gives them properties and features that are not easily obtained with organic compounds, thus providing alternatives in targeted and rational approach to the development of innovative biological agents.



In this lecture, an overview of existing metal-based drugs and imaging agents will be presented, and new avenues where metals can play an important role will be discussed, thus giving to students a solid background to the exciting field of metal-based drugs.

## References

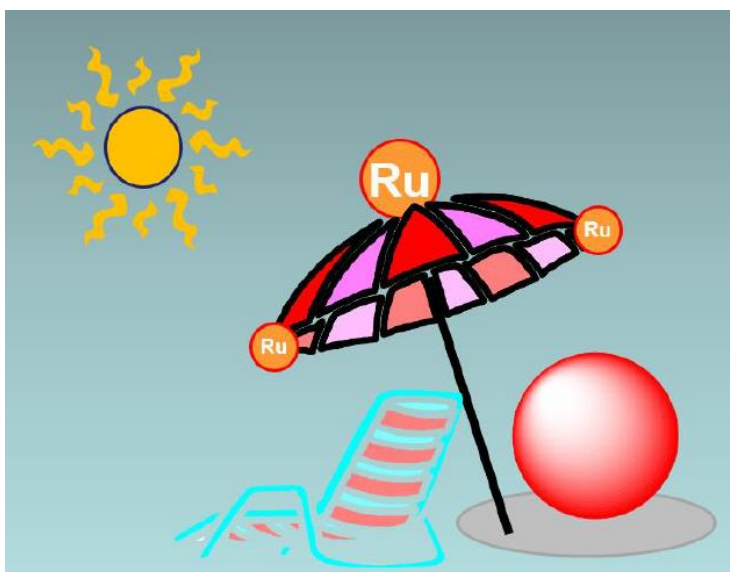
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# Ruthenium Complexes in Photo-Dynamic Therapy

Bruno Therrien

*Institute of Chemistry, University of Neuchatel, Switzerland  
E-mail: bruno.therrien@unine.ch*

Porphyrin derivatives are known to absorb light and they are often used as photosensitizing agents in light harvesting processes or photo-dynamic therapy (PDT) treatments. Despite being used in the clinic to cure cancer, these so called first and second generations of porphyrin-based photosensitizers are limited by hydrophobicity, aggregation, photobleaching and slow clearance [1]. Therefore, in recent years, new photosensitizers have emerged to overcome these limitations.



Of particular interest, those built around ruthenium complexes. The electronic and coordination properties of ruthenium provide several favorable characteristics to develop a new generation of photosensitizers. The rich photochemistry of ruthenium is well known and nicely exploited in light harvesting technology [2]. However, for biological applications such as PDT, the use of ruthenium-based photosensitizers remains in its infancy. During this presentation, recent results will be presented, showing the relevance of ruthenium complexes in PDT.

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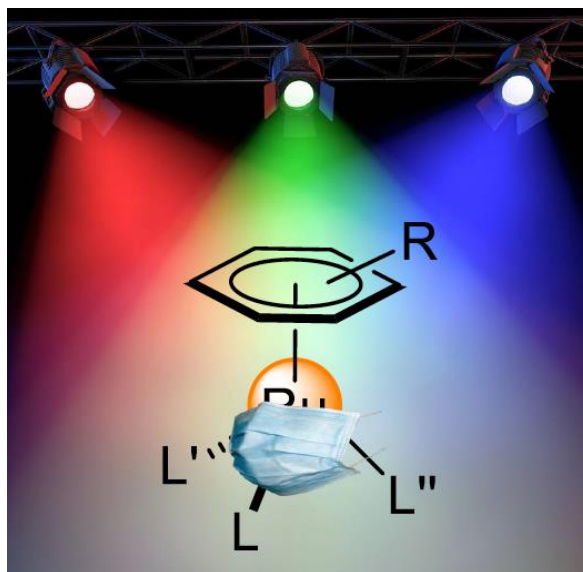
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# Biological Applications of Coordination-Driven Self-Assemblies

Bruno Therrien

*Institute of Chemistry, University of Neuchatel, Switzerland*  
E-mail: *bruno.therrien@unine.ch*

For nearly two decades, the use of arene ruthenium metalla-assemblies for biological and biomedical applications have flourished [1]. The synthetic strategies to generate arene ruthenium assemblies are well established and these compounds are offering tremendous possibilities in terms of structural diversities and chemical properties [2]. We have, like others, contributed to the development and to the popularity of arene ruthenium assemblies, and from early on, our research was driven by applications, mainly biological (therapeutic, drug delivery, DNA interactions, photodynamic therapy, imaging). During this presentation, we want to give the basic reasons behind our choice, and unmask our most successful examples, with an emphasis on applications.



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# Plenary Session



# Hyper Rayleigh Scattering from metallic nanoparticles: Novel insight into interactions with elliptical polarization

Michalina Ślęmp<sup>1</sup>, Estelle Salmon<sup>1</sup>, Vito Coviello<sup>2</sup>, Katarzyna Matczyszyn<sup>3</sup>,  
David Amans<sup>1</sup>, Vincenzo Amendola<sup>2</sup>, Pierre-Francois Brevet<sup>1</sup>

<sup>1</sup> Institut Lumière Matière ILM, UMR CNRS 5306, Université Claude Bernard Lyon 1,  
10 Rue Ada Byron, 69622 Villeurbanne cedex, France

<sup>2</sup> University of Padova UNIPD, Department of Chemical Sciences, Via 8 Febbraio, 2 - 35122 Padova, Italy

<sup>3</sup> Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology,  
Wyb. Wyspińskiego 27, 50-370 Wrocław, Poland

Hyper-Rayleigh scattering (HRS) is a for measuring second harmonic light from liquid media. By careful analysis of HRS technique signal, not only second-order non-linear optical polarizability (hyperpolarizability  $\beta$ ) can be measured, but also the role of the size and shape of the nanoparticles as well as the macroscopic origin of the response. This method has already been applied to molecules and nanoparticles albeit with linear polarization [1].

In this work, we analyse the response of metallic nanoparticles: principally containing gold obtained using laser ablation [2, 3]. The results are compared with those synthesised with metallic nanoparticles obtained by salt reduction method. Furthermore, the novel experiment involving quarter waveplate allows for deep understating of interactions between matter and circularly-polarized light. This work include insight into the behaviour of magnetic NPs that could be further used for sensing, selective imaging or in-situ targeting tumors or blood knots in the human body.

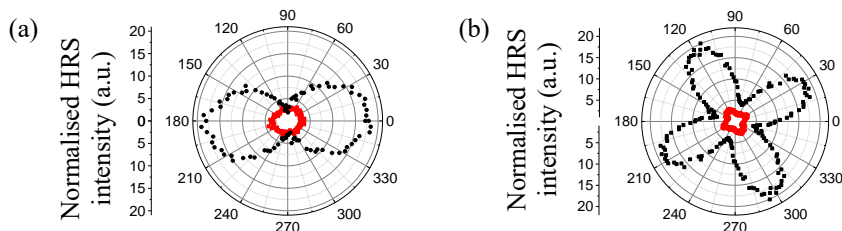


Fig. 1. Vertical (black) and (red) Horizontal polarization of the harmonic light as a function of the a) input polarization angle and b) input quarter waveplate rotation for AuNPs ( $\sim 5$  nm in diameter) obtained using laser ablation. Where quarter waveplate: 40 is linear polarization, 85 – circularly left- and 130 circularly right-polarized light

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# Chiral fluorescence microscopy for studying linear and nonlinear properties of gold nanoclusters

Maciej Lipok<sup>1</sup>, Anna Pniakowska<sup>1</sup>, Patryk Obstarczyk<sup>1</sup>, Joanna Olesiak-Bańska<sup>1</sup>

<sup>1</sup> Institute of Advanced Materials, Wrocław University of Science and Technology  
E-mail: maciej.lipok@pwr.edu.pl

Atomically precise gold nanoclusters (AuNC) are heavily studied nanomaterials because of their molecular-like structure, strong photoluminescence, and broad potential applications in catalysis, bioimaging, or sensing [1]. Moreover, assembling them using template-assisted methods provides benefits like controlled periodicity and controlled modulation of chiroptical properties [2]. However, very little is known about the influence of chirality on their linear and non-linear fluorescence.

To answer that, we built the fluorescence microscopy setup to collect circularly polarized luminescence from achiral gold nanoclusters Au<sub>25</sub>(PET)<sub>18</sub> helically assembled using liquid-crystalline template P-9-OPIMB, creating helical nanofilaments [3]. We discovered that the helical assembly of gold nanoclusters leads to the generation of strong circularly polarized luminescence depending on the chirality of domains revealed by 2D CPL maps and the maximum values of luminescence dissymmetry factors (Figure 1A) determined in our experiments were equal 0.32 and -0.37 for left-handed and right-handed circularly polarized light, respectively [4]. We also modified the excitation path of the multiphoton microscopy setup to assess the chiroptical properties exhibited by two enantiomers of arginine/6-aza-2-thiopyrimidine gold nanoclusters (Arg/ATT-AuNCs) and found out that exciting the samples with circularly polarized light leads to clear discrimination between two-photon excited luminescence exhibited by L- and D-Arg/ATT-AuNC nanoclusters (Fig. 1B) [5].

Overall, our results are an exciting example of the application of both one- and two-photon excited fluorescence microscopy methods for exploring chiroptical properties of atomically-precise nanoparticles and imaging their chiral assemblies.

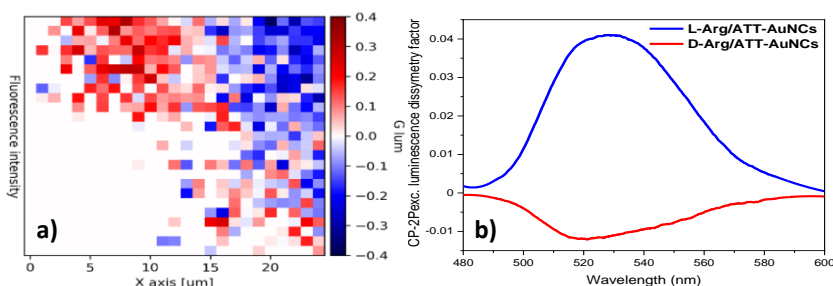


Figure 1. Luminescence dissymmetry factors calculated from (a) circularly polarized luminescence 2D map of helical assemblies of achiral Au<sub>25</sub>(PET)<sub>18</sub> gold nanoclusters and (b) circularly-polarized two-photon luminescence exhibited by L- and D-Arg/ATT-AuNC gold nanoclusters

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# Coupled colloidal molecules CdSe/ZnS@CdSe/ZnS and CdSe@CdSe

Rafał Krzysztof Kosman\*, Bartłomiej Cichy\*\*, Oleksii Bezkravnyj\*\*\*

<sup>1</sup> Institute of Low Temperatures and Structure Research, Polish Academy of Sciences,  
ul. Okólna 2, 50-422 Wrocław, Poland

E-mail: \* [r.kosman@intibs.pl](mailto:r.kosman@intibs.pl); \*\* [b.cichy@int.pan.wroc.pl](mailto:b.cichy@int.pan.wroc.pl); \*\*\* [o.bezkravnyj@int.pan.wroc.pl](mailto:o.bezkravnyj@int.pan.wroc.pl)

In analogy to atoms and molecules colloidal quantum dots (QDs) known as zero-dimensional objects can be used as building blocks of so called “artificial molecules”. In recent years, there has been increased interest in the synthesis of colloidal systems organized into superstructures. First syntheses of colloidal molecules were obtained on simple addition of difunctional dithiolate linkers to the colloidal QDs solution obtaining monomers, dimers, trimers and larger aggregates [1]. Higher selectivity and efficiency of the synthesis were obtained by using of silica template containing mercaptan surface ligands (MPTMS) to which QDs were attached. One of such syntheses was proposed by J. Cui et al. [2]. With modifications are presented in this work. In our procedure the TEOS silica surface modified by MPTMS is used as a template for combining colloidal QDs. It allowed for the synthesis of dimers composed of QDs without shell and obtained molecules with control distance regime with using linkers with different alkyl-chain lengths. Synthesized QDs dimers were characterized using single particle spectroscopy providing important physical premises on changes in the relaxation kinetics implicated by the QDs coupling represented here by exciton tunneling between them [3, 4]. More information on the impact of near field coupling on the relaxation kinetics is also gained by the Kinetic Monte Carlo (KMC) simulations. All reported results are here discussed using fluorescence lifetime-intensity distribution (FLID) maps showed in Fig. 1.

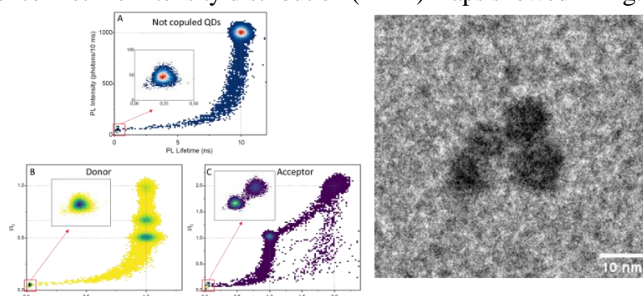


Fig. 1. FLID maps made from KMC calculation for (A) single QDs, and for dimers (B) QDs as perform role the donor and (C) acceptor in coupled system. (D) TEM image of CdSe/ZnS@CdSe/ZnS molecules

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# The optically detectible strain states in phosphorene nanostructures – ab initio study

Krzysztof Pyrchla

*Faculty of Electronics, Telecommunications and Informatics, Gdansk University of Technology,  
11/12 Gabriela Narutowicza Street, 80-233 Gdansk, Poland  
E-mail: krzpyrch@student.pg.edu.pl*

The non-electrical quantities despite being particularly hard to measure, are essential for many fields of science and technology. One of the possibilities to overcome sensor limitations is seen in the development of nanomaterials and nanosensors fabrication.

Two-dimensional crystals exhibit exciting properties under the influence of deformation. A unique and interesting material belonging to this group is phosphorene [1]. The Raman spectrum of phosphorene depends on the stress tensor of the structure. This effect has already been simulated for the pristine phosphorene monolayer [2]. Interestingly, the dependence on temperature is weaker than on stress. There is a possibility of distinguishing the deformation direction based on the change in the Raman spectrum.

This work is focused on studying the possibility of optical detection of strain states in phosphorene nanostructures. The conducted research consists of several stages. First, the material mechanical properties of small parts of phosphorene nanostructure were calculated using the ab-initio Density Functional Theory(DFT) approach. The Young modulus and Poisson ratio were calculated in a wide range of structure strains. Alongside, the changes in structural geometries at the atomic level were predicted using the energy/force minimization technique by the application of the limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm.

The second step is the calculation of the Raman scattering of the material. This calculation is based on the DFT and structure geometries predicted in the previous step. The “frozen-phonon” approach was utilized to simulate Raman spectra, so vibration modes were calculated as eigenvectors of the dynamic matrix. In order to determine which modes are actively involved in Raman scattering, it is still necessary to calculate, the matrix of dielectric susceptibility derivatives (in relation to the displacements of atoms). Based on these two matrices, it was possible to define the Raman tensor [3].

In last step, calculated material properties were used to simulate the behaviour of complex phosphorene nanostructure under external pressure using Finite Element Method. Based on the calculated dependency of the Raman spectrum on the strain, the change in the scattering spectrum of the nanostructure was predicted.

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# Influence of donor position on one- and two-photon optical properties in amyloid markers

Agata Hajda<sup>1</sup>, Patryk Rybczyński<sup>2</sup>, Manuela-Grelich-Mucha<sup>1</sup>,  
Borys Ośmiałowski<sup>2</sup>, Joanna Olesiak-Bańska<sup>1</sup>

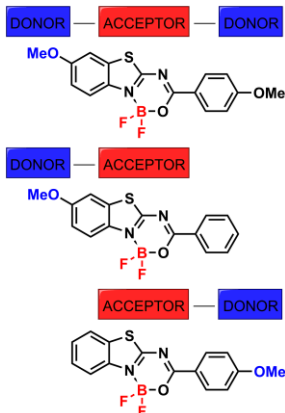
<sup>1</sup> Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland

<sup>2</sup> Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland

E-mail: joanna.olesiak-banska@pwr.edu.pl, agata.hajda@pwr.edu.pl

Emerging numbers of patients suffering from Alzheimer's, Parkinson's disease or Type 2 Diabetes cause the need to look for new therapies that are still beyond the reach of modern medicine. Mentioned pathologies have two things in common: they are incurable and their development is associated with protein aggregates called amyloids [1]. In order to be able to construct therapies that will give satisfactory results, it is first necessary to understand better the amyloids formation. New strategies for amyloids detection involve one-photon (1P) and two-photon (2P) microscopy, which are non-invasive and suitable to observe amyloids formation in vivo [2].

We investigate a potential of BF<sub>2</sub>-functionalized benzothiazoles with additional electro-donating functional methoxy group as amyloids fluorescent markers. We examine three dyes with a weak electron-donating group -OMe located on one or both terminals of benzothiazole-based fluorophores (Fig. 1) Dyes presented various Fluorescence Quantum Yield (FQY) on surrounding environment [3]. Compounds are based on BF<sub>2</sub>-functionalized benzothiazoles.



We investigated optical properties like UV-Vis absorption, fluorescence, FQY, and fluorescence lifetime, for neat dyes and those interacting with bovine insulin amyloids. We observed over 50-fold increase of FQY upon binding to amyloids. Comparison of fluorescence changes to different types of amyloids was also studied. The probes were sensitive to various microenvironment of amyloids formed from different proteins. We calculated radiative ( $k_r$ ) and non-radiative ( $k_{nr}$ ) decay constant changes upon binding and compared them for dyes in different solvents allowing to better understand one-photon optical properties. Moreover, we evaluated two-photon absorption cross-sections of dyes in the presence of amyloids. The obtained results confirm that the dyes have amyloid detection potential. Moreover, difluoroborate benzothiazoles are prominent for further development as markers for one and two-photon microscopy.

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# Single-chain folding of oligourethanes

Sara Kozub, Roza Szweda<sup>1\*</sup>

*Lukasiewicz Research Network – PORT Polish Center for Technology Development  
Stablowicka 147, 54-066 Wrocław, Poland,*

\* E-mail: [Roza.Szweda@port.lukasiewicz.gov.pl](mailto:Roza.Szweda@port.lukasiewicz.gov.pl)

Biomolecules are essential components of living organisms, and their structures and functions are intricately linked. The primary structure of biomolecules, which refers to the sequence of amino acids or nucleotides, plays a crucial role in determining the three-dimensional structure of the molecule. This, in turn, determines the functionality of the molecule. For example, the specific shape of an enzyme's active site enables it to catalyze a particular reaction. Therefore, understanding the factors that control the shape of macromolecules is crucial for developing new materials and therapies. In recent years, there has been progress in synthesis of sequence-defined, abiotic polymers to create materials with specific properties [1]. However, to achieve complex functionalities of materials using non-biological building blocks, it is necessary to understand the principles of single-chain folding of macromolecules.

In this study we investigated stereochemistry as a tool for controlling the shape of sequence-defined oligourethanes. We synthesized a series of stereocontrolled oligourethanes [2] and analyzed their conformation using combination of various NMR methods. The results showed that stereochemistry plays a crucial role in the folding behavior of oligomers and each diastereoisomer exhibited unique folding patterns that resulted in the stabilization of specific conformations. The findings have significant implications for the design of materials with specific functionalities. Further research in this area could lead to the creation of more complex materials that mimic the properties of natural biomolecules.

## Acknowledgement

This project was supported by the Polish National Science Centre (2018/31/D/ST5/01365)

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# Behavior of organic luminescent dyes in thermotropic liquid crystalline matrix – studies of novel diketofurofuran and selected dyes

Ł. Duda<sup>1,2</sup>, M. Czajkowski<sup>1</sup>, S. Czarnocki<sup>1</sup>, M. Guzik<sup>1,2</sup>, M. Skoreński<sup>1</sup>, B. Potaniec<sup>1</sup>, and J. Cybiska<sup>1,2</sup>

<sup>1</sup>Łukasiewicz Research Network – PORT Polish Center for Technology Development, ul. Stabłowicka 147, 54-066 Wrocław, Poland

<sup>2</sup>University of Wrocław, Faculty of Chemistry, ul. F. Joliot-Curie 14, 50-383 Wrocław, Poland  
E-mail: lukasz.duda@port.lukasiewicz.gov.pl

Maintenance of high photoluminescence quantum yield (QY) in various matrices (e.g., liquid crystalline) is undoubtedly a desirable property of luminescent organic dyes, when thinking of their application in optical sensors (e.g., thermofluorochromic) and light amplification systems. However, the number of dye classes studied in the liquid crystalline matrices is limited to the most known pyromethanes, merocyanines, coumarins and rhodamines. Recently, it was shown that dyes from less-known chemical group, such as diketofurofuranes may exhibit also very high QY in solution and liquid crystal matrices [1].

Here we present the crystal structure and luminescent properties of a novel diketofurofuran dye (DFF) of structure presented in Fig. 1. Detailed studies of its solubility in liquid crystals as well as QY determination in crystal and liquid crystal matrices were performed. Spectroscopic properties of the synthesized dye were compared with the analogous dye from the diketopyrrolopyrrole (DPP) family. For both dyes high values of the QY (up to 95%) in liquid and liquid crystalline matrices were found. On the other hand, lower values of QY and appearance of additional absorption band were observed for these dyes in solid matrices. High contrast of the QY in different phases was a motivation for preparation of a thermofluorochromic indicator. In the selected thermotropic liquid crystalline matrix a visible change of the luminescent properties upon heating from crystalline (Cr) to nematic (N) or isotropic (Iso) phase was found for the DFF dye. Its performance was compared with the analogous DPP dye and other commercially available dyes. The DFF dye turned to be one of the best among the studied dyes.

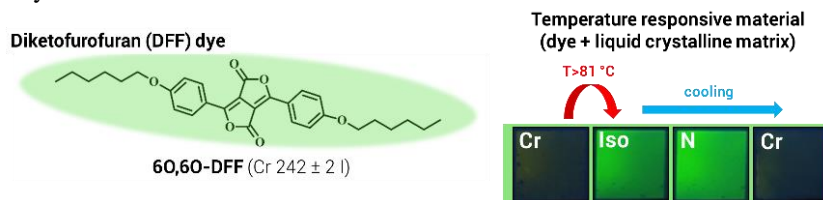


Fig. 1. Structure of the studied DFF dye together with photographs of the obtained liquid crystalline temperature responsive (thermofluorochromic) material

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The research was supported by the National Science Centre of Poland (NCN) under grant OPUS 16 no. 2018/31/B/ST8/02832. Ł. D. would like to thank the Ministry of Science and Higher Education in Poland for Grant No. DWD/4/64/2020 in the frame of Implementation Doctorate Programme.

# Surface modified photonic crystals for colorimetric gas detection

Weronika Zajac<sup>1,2</sup>, Maciej Czajkowski<sup>1</sup>, Joanna Cybińska<sup>1,2</sup>

<sup>1</sup>Lukasiewicz Research Network – PORT Polish Center for Technology Development, Wrocław, Poland

<sup>2</sup>Faculty of Chemistry, University of Wrocław, Wrocław, Poland

E-mail: weronika.zajac@port.lukasiewicz.gov.pl

Due to the continuous growth of industry, many dangerous gas vapors can be released in places such as large factories, research laboratories or warehouses. Sensitive, rapid and cost-effective systems are needed to detect and report hazardous vapors that could affect human health and safety and the environment [1, 2].

In this study, we demonstrate the synthesis of opals from silica nanospheres with a surface modified by covalently bound pH-responsive azo dyes. Size of the nanospheres forming the synthesized opals was determined by SEM. An azo dye (methyl red) has been permanently combined with 3-aminopropyltriethoxysilane (APTES) in a chemical reaction [3]. The resulting opals show a rapid color change in the presence of acid vapors. These changes do not disappear immediately when the vapor is removed. However, when exposed to ammonia vapor there is no color change visible to the naked eye. Opal's color change is reversible, so it can be used more than once. Simple and rapid detection of acid vapors can be very useful, for example, in factories producing nitrogen fertilizers.

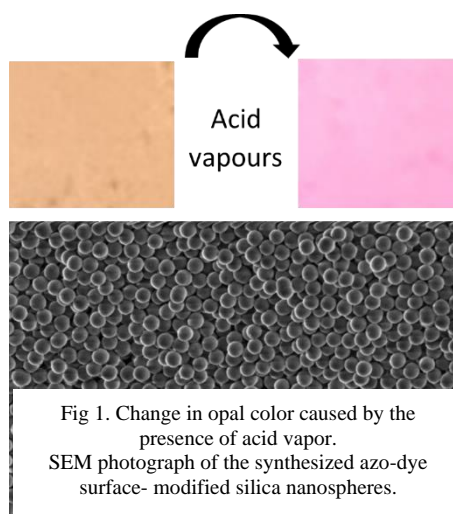


Fig 1. Change in opal color caused by the presence of acid vapor.  
SEM photograph of the synthesized azo-dye surface-modified silica nanospheres.

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These studies were supported by the National Centre for Research and Development (Poland) within the framework of the 12th edition of the LIDER programme – project contract no. LIDER/39/0203/L-12/20/NCBR/2021. W.Z. would like to thank the Ministry of Science and Higher Education in Poland for the Grant No. DWD/6/0316/2022, „Fabrication of photonic crystals with sensor properties” in the frame of Implementation Doctorate Programme.

# Highly sensitive luminescent thermometers based on hybrid formate perovskites containing dimethylammonium cations

Adam Kabanski, Thi Hong Quan Vu, Maciej Ptak, Dagmara Stefańska

*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, 50-422, Poland*  
E-mail: [a.kabanski@intibs.pl](mailto:a.kabanski@intibs.pl)

Materials with perovskite-like architecture have attracted a lot of attention due to their extraordinary structural, magnetic, and optical properties [1, 2]. Among various materials, organic-inorganic structures exhibit particularly interesting characteristics, where temperature-dependent luminescence is one of the most significant [1].

The influence of the temperature on spectroscopic characteristics of hybrid perovskites is well visible in the example of  $[\text{DMA}]\text{M}_{1-x}\text{Cr}_x(\text{HCOO})_3$  ( $\text{M} = \text{Zn}, \text{Mn}, \text{Mg}$ );  $x \in (0, 0.01, 0.03, 0.05)$  series. Performed measurements show that an increase in temperature leads to the reduction of the dominant narrow spin-forbidden  ${}^2\text{E}_g \rightarrow {}^4\text{A}_{2g}$  transition, which is the basis of the emission near 700 nm. What is more, the progressive temperature rise induces the emergence of the broad emission near 750 nm, originating from the spin-allowed  ${}^4\text{T}_{2g} \rightarrow {}^4\text{A}_{2g}$  transition. The obtained results enable to describe thermometric parameters, such as fluorescence intensity ratio (FIR), absolute sensitivity ( $S_a$ ) as well as relative sensitivity ( $S_r$ ). Calculated values of  $S_r$  (up to  $2.49\% \cdot \text{K}^{-1}$ ) indicate the usefulness of the investigated materials as highly sensitive luminescent thermometers.

The presentation will be focused on the preparation of investigated materials as well as structural and optical characterization. Particular attention will be paid to the influence of temperature on the spectroscopic properties and thermometric parameters. Moreover, the potential of the implementation of investigated materials as non-contact thermometers will be detailed and discussed.

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# **Flash Presentation Session**



# Development of Molecular Dynamics methodology to access receptor function in abiotic sequence-defined polymers

Maksymilian Szatko<sup>1</sup>, Weronika Forysiak<sup>1</sup>, Sara Kozub<sup>1</sup>,  
Tadeusz Andruniów<sup>2</sup>, Róża Szweda<sup>1</sup>

<sup>1</sup> *Łukasiewicz Research Network – PORT Polish Center for Technology Development,  
Stabłowicka 147, 54-066 Wrocław, Poland*

<sup>2</sup> *Department of Chemistry, Wrocław University of Science and Technology,  
Wybrzeże Wyspińskiego 27, 50-370 Wrocław, Poland  
E-mail: Roza.Szweda@port.lukasiewicz.gov.pl*

Sequence-defined polymers (SDPs) are macromolecules that possess a uniform structure with a precisely defined monomeric sequence [1]. This characteristic is also shared with biopolymers; like them, SDPs can exhibit advanced functions such as folding and binding to target ligands [2]. The implementation of advanced functionalities in SDPs requires the precise selection and specific arrangement of monomers. A vast array of abiotic monomers presents a high potential for fine-tuning the properties of the polymer to suit various applications. However, the exhaustive exploration of the entire sequence space is not experimentally feasible due to the sheer number of possible combinations.

In this study, we present a theoretical methodology with an experimental verification for assessing the binding of bisphenol A (BPA) to oligocarbamates. The developed methodology enables evaluating the binding energy of the SDP-BPA complex using a Molecular Dynamics in silico approach. Experimental verification was performed based on fluorescence quenching fitted to the Stern-Volmer model. The results demonstrate that the binding affinity of the SDPs to BPA was influenced by the stereochemical center arrangement, with some SDPs exhibiting a lower binding constant than others. Our findings suggest that low-cost theoretical methods coupled with fluorescence measurements are viable for the assessment of functionalities in SDPs.

## Acknowledgment

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# Anti-Stokes cooling of lanthanide-doped nanoparticles

Kamil Bruchal, Paweł Karpiński, Dominika Wawrzyńczyk

*Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology*  
E-mail: [kamil.bruchal@pwr.edu.pl](mailto:kamil.bruchal@pwr.edu.pl)

Laser cooling is the process of lowering the thermal energy of a physical system by illuminating it with a laser beam. In 1929, Peter Pringsheim proposed the use of anti-Stokes luminescence to cool solids [1].

Here, we present the experimental study on anti-Stokes cooling of lanthanide-doped nanoparticles  $\text{NaYF}_4:\text{Yb}^{3+}$ . We demonstrate this phenomenon using thermometry technique based on liquid crystal phase transition [2]. Our investigation reveals a reduction in temperature of the nanoparticles upon laser irradiation, indicating anti-Stokes cooling. The dependence of the cooling effect on laser power, wavelength, size and concentration of lanthanide ions is explored. The results suggest that anti-Stokes cooling of ytterbium-doped nanoparticles can be a promising strategy for achieving efficient cooling in a variety of applications. This work provides valuable insights for the development of new cooling technologies.

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# The effect of pH on liquid crystalline properties of myelin-like structures

Dominika Benkowska-Biernacka, Katarzyna Matczyszyn

Wrocław University of Science and Technology, Institute of Advanced Materials,  
Wyb. Wyspiańskiego 27, 50-370 Wrocław  
E-mail: dominika.benkowska@pwr.edu.pl

An important aspect of biological soft matter research is the development of new approaches to understanding membrane-associated processes [1, 2]. A well-known example of biologically relevant mesophases is the myelin sheath, which plays a crucial role in action potential propagation [3]. Here, we investigated myelin-like structures composed of phosphatidylcholines [4, 5]. The important advantage of the sample made of a single type of biomacromolecule was obtaining a simplified model of the biological membrane.

The combination of polarized light microscopy and fluorescence microscopy provided detailed information about the effect of pH on the thermal stability of myelin figures (MFs). Furthermore, different structural morphologies of multilamellar assemblies were also examined using two-photon excited fluorescence microscopy. Our results revealed that the pH of the aqueous phase shows a significant correlation with the liquid crystalline properties of MFs.

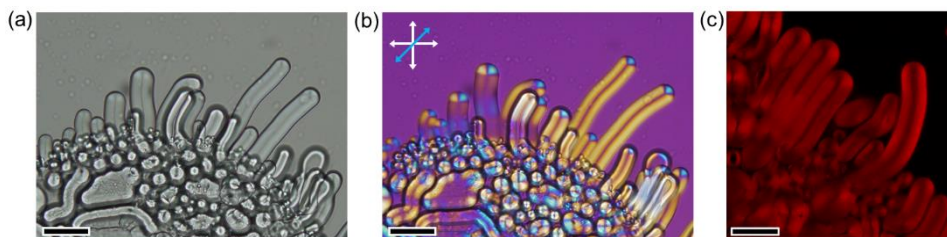


Fig. 1. (a) Bright field and (b) polarized light microscopy images of myelin figures (MFs). White and blue arrows represent the polarizers and slow axis of the full-wavelength retardation plate, respectively, (c) Confocal fluorescence microscopy image of MFs ( $\lambda_{\text{ex}} = 488 \text{ nm}$ ). Scale bars are (a-b)  $50 \mu\text{m}$  and (c)  $20 \mu\text{m}$

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# Increasing the sensitivity of pressure readings based on Nd<sup>3+</sup> ion emission through Cr<sup>3+</sup> co-doping

Mateusz Pieprz, Łukasz Marciniak

<sup>1</sup> *Institute of Low Temperature and Structure Research, Polish Academy of Sciences,  
Okólna 2, 50-422 Wrocław, Poland  
E-mail: m.pieprz@intibs.pl*

Luminescence manometry is a pressure sensing method that holds great promise due to its real-time response and low invasiveness of the measurement. The technique is based on examining the spectral response of a system under applied pressure. Most often, observations of the emission band maximum shift are used, where two groups of phosphors can be distinguished: narrowband and broadband. Narrowband emission shift analysis is most often used because of its high precision. However, these bands shift only slightly with applied pressure which reduces the sensitivity of the readout. Alternatively, the spectral shift of broadband emission can be used, which is more sensitive, but less precise, due to the difficulty in accurately determining the band maximum.

This work presents a mixed approach, combining the broadband emission shift of chromium associated with the  ${}^4T_2 \rightarrow {}^4A_2$  electronic transition with the narrow-band emission of neodymium ( ${}^4F_{3/2} \rightarrow {}^4I_{11/2}$  transition), as observed in the spectrum of  $\text{La}_3\text{Ga}_5\text{GeO}_{14}$ . The resulting Nd<sup>3+</sup>-based optical manometer shows an absolute sensitivity of 2.92 cm<sup>-1</sup>/GPa for the  ${}^4F_{3/2} \rightarrow {}^4I_{11/2}$  electron transition. [1]

## Acknowledgement

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# The Use of 5-aminolevulinic Acid in the Photodynamic Eradication of *Pseudomonas aeruginosa*

Anna Zdubek<sup>1</sup>, Irena Maliszewska<sup>1</sup>

Politechnika Wroclawska, Wydział Chemiczny,  
ul. Wybrzeże Wyspiańskiego 29, 50-370 Wrocław, Polska  
E-mail: [anna.zdubek@pwr.edu.pl](mailto:anna.zdubek@pwr.edu.pl)

The problem of antibiotic resistance is a major concern around the world. The increasing number of antibiotic-resistant pathogens is the reason for the development of other methods to combat bacteria. Antimicrobial photodynamic therapy (aPDT) is an alternative to antibiotics for the treatment of bacterial infections [1].

The purpose of the study was to evaluate the effect of 5-aminolevulinic acid on the photosensitisation efficacy of bacteria.

The study was carried out with the bacterial strain *Pseudomonas aeruginosa*. In antimicrobial photodynamic therapy, 5-aminolevulinic acid (5-ALA) was used as a precursor of the specific photosensitiser, protoporphyrin IX (PpIX). 5-ALA is converted in the heme biosynthesis pathway to protoporphyrins including protoporphyrin IX [2]. To enhance the effect of aPDT, glucose was used as an adjuvant in various concentrations. The light sources that have been used for light activation of photosensitiser are lasers. In this study, lasers emitting red (635 nm) and blue light (405 nm) were applied. The effect of 5-aminolevulinic acid with an adjuvant on the viability of *Pseudomonas aeruginosa* cells was estimated by determining the amount of ATP by measuring the luminescence intensity at 560 nm. The quantity of ATP is proportional to the number of metabolically active cells in a given suspension [3]. Additionally, cultures were performed to quantify colonies that formed after treatment.

The use of blue laser light in antimicrobial photodynamic therapy is more effective than the use of red light. Exposure of 10 minutes to blue light resulted in a lethal effect. On the contrary, this cannot be achieved with red light, even after prolonged exposure. Glucose significantly increases the efficiency of aPDT. The incubation of bacteria in 2% and 1% glucose solutions reduces the irradiation time required to obtain a lethal effect to 1 min for the blue laser and to 15 min for the red laser.

The results obtained indicate that the use of 5-ALA, particularly in combination with glucose, has a positive impact on the effectiveness of antimicrobial photodynamic therapy.

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# The photosensitization of giant unilamellar vesicles assembled from bacterial lipid extracts

Marta Piksa<sup>1</sup>, Krzysztof Pawlik<sup>1</sup>, Katarzyna Matczyszyn<sup>2</sup>, Baptiste Fourmaux<sup>3</sup>, Patricia Daira<sup>3</sup>, Sigolène Lecuyer<sup>4</sup>, Carlos M. Marques<sup>4</sup>

<sup>1</sup> *Hirszfeld Institute of Immunology and Experimental Therapy PAS*

<sup>2</sup> *Wroclaw University of Science and Technology*

<sup>3</sup> *Institut National des Sciences Appliquées de Lyon*

<sup>4</sup> *École Normale Supérieure de Lyon*

E-mail: [marta.piksa@hirszfeld.pl](mailto:marta.piksa@hirszfeld.pl)

Giant unilamellar vesicles (GUVs) are cell-sized lipid bilayer capsules widely used as biomimetic models of cellular membranes [1]. In this project, we self-assembled GUVs from bacterial lipid extracts to study the mechanism of bacteria photoinactivation, also called Antimicrobial Photodynamic Therapy (APDT).

APDT is based on the oxidation of biological structures caused by reactive oxygen species produced during the photoactivation of a chemical compound called photosensitizer (PS). Although the chemical pathways of APDT are well described, the exact biological mechanism is still unknown. Since the bacterial cell membrane is the first barrier in the path of oxidation processes, and its fundamental component is lipid fraction, we consider that their role is crucial, if not the key in the destruction of the cell by APDT [2, 3].

To investigate the role of bacterial lipids in photoinactivation and the response of their lipid bilayers to photosensitization, GUVs were prepared with lipids extracted from *Escherichia coli*, and their photosensitization and observation was performed under contrast microscopy. Methylene blue was chosen as the photosensitizer, and activated directly during observation under the microscope. Additionally, confocal microscopy observation was performed with NBD (1,2-dioleoyl-sn-glycero-3-phosphoethanolamine-N-(7-nitro-2-1,3-benzoxadiazol-4-yl)) to visualize the GUVs 3D structure. To induce lipid composition changes in bacterial cells the culture medium was modified by the addition of mannitol.

The formation of GUVs was achieved independently on medium modification. Changes in lipid composition were measured by liquid chromatography-mass spectrometry and gas chromatography-mass spectrometry. The photosensitization effect was found to be dependent on GUVs lipid composition. The vesicles assembled from the lipid extract of modified culture medium were not sensitive to photosensitization, while the control group showed an important photosensitizing effect. The results presented here thus provide background for further research and forms the basis for describing the biological mechanism of APDT.

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# Electrospun fibers in lighting nanotechnology

Marharyta Hancharova, Kinga Halicka-Stępień, Dorota Zajac,  
Joanna Cabaj, Lech Sznitko<sup>1</sup>

Wrocław University of Science and Technology  
E-mail: marharyta.hancharova@pwr.edu.pl

The electrospinning (ES) technique is relatively simple, low-cost, and useful for micro/nano-scale fiber fabrication. Other methods, e.g. precipitation [1], solid-state field-assisted diffusion [2], and pulsed laser deposition method [3], compared with ES, are not such easy and versatile. Electrospun polymer fibers can be applied in molecular recognition [4], sensors [5], luminescent semiconductors [6], enzyme immobilization [7], tissue engineering [8], filtration [9], etc. ES method allows improving of the physicochemical properties of fibers by surface modification of manufactured materials and easy functionalization of fibers. The last one is possible due to using inorganic compounds (metal ions [10], lanthanides [11]), organic (luminescent dyes [12],  $\pi$ -coupled polymers), or by admixture of polymers. Very promising systems for ES purposes are heterocyclic compounds [13], especially those containing benzothiadiazole which already have been applied in optoelectronics and medical diagnostics. In lighting technology, membranes made of luminescent materials produced by ES can be integrated into optical sensors, field effect transistors, or lasers significantly improving the performance of this equipment. In my shotgun, I want to introduce the ES technique as a way to produce polymer fibers doped with organic semiconductors for application in lighting technology and my own results so far.

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# Poster Session





# Temperature dependence of photon avalanche emission in NaYF<sub>4</sub>: Pr<sup>3+</sup> Yb<sup>3+</sup> nanocrystals ions

Z. Korczak<sup>1\*</sup>, M. Szalkowski<sup>1,2</sup>, M. Dudek<sup>1</sup>, M. Majak<sup>1</sup>, M. Misiak<sup>1</sup>, A. Bednarkiewicz<sup>1\*</sup>

<sup>1</sup> Institute of Low Temperature and Structure Research PAS, ul. Okólna 2, Wrocław, 50-422 Wrocław, Poland

<sup>2</sup> Nicolaus Copernicus University, ul. Grudziądzka 5, 87-100 Toruń, Poland

E-mail: [z.korczak@intibs.pl](mailto:z.korczak@intibs.pl); [a.bednarkiewicz@intibs.pl](mailto:a.bednarkiewicz@intibs.pl)

Lanthanides trivalent ions exhibit remarkable properties such as non-toxicity, photostability, emission well-fitted into biotissues optical window and long emission lifetimes. Therefore, they have found applications in many fields, including bioimaging and super-resolution imaging. Moreover, a very special up-conversion (UC) process of photon avalanche (PA) can occur in these ions. A characteristic feature of PA is a steep, very nonlinear relationship between the excitation laser power density ( $I_{ex}$ ) and the luminescence intensity ( $I_L$ ),  $I_L = (I_{ex})^S$ , with  $S > 10$ , which occurs above a certain critical excitation power density (PA threshold), resulting in S-shaped power dependence diagram. In order to observe PA emission, the material must be pumped with photons matching excited state absorption but far from resonance with any ground state absorption transition. Although this phenomenon has been studied in fibers and bulk crystals, it has only recently been demonstrated in nanocrystals [1–3]. Importantly, also utilization of avalanching nanomaterials for temperature sensing was predicted recently [4].

In this work we present studies of the PA phenomenon in NaYF<sub>4</sub> nanocrystals doped with praseodymium and ytterbium ions. The nanocrystals were excited at 1059 nm and multicolor emission with the main lines centered 610 nm and 482 nm was observed. In our experiments we were focused on the relationship between the power density of the excitation laser and the intensity of the luminescence. We demonstrated characteristic S-shaped relationship in this dependence, confirming photon avalanche origin of this emission. In addition, these relationships were examined for various temperatures ranging from  $-175^{\circ}\text{C}$  to  $175^{\circ}\text{C}$ . Interestingly, we found strong temperature dependence of the essential parameters describing the PA, such as the intensity, slope and threshold power. Corresponding relative temperature sensitivities were calculated, reaching the values up to  $7.5\% \text{ }^{\circ}\text{C}^{-1}$ . Presented research reveals potential of the avalanching nanostructures for applications in the luminescence thermometry, including also the temperature sensing based on the new type of the thermometric parameter – the PA threshold power.

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# Influence of neodymium concentration on the photon avalanche and two-color emission from $\text{Tm}^{3+}$ in $\text{LiYF}_4$ 3% $\text{Tm}^{3+}$ microcrystals

M. Majak<sup>1</sup>, M. Misiak<sup>1</sup>, A. Bednarkiewicz<sup>1\*</sup>

<sup>1</sup> Institute of Low Temperature and Structure Research Polish Academy of Science, ul. Okólna 2, Wrocław, 50-422 Wrocław, Poland

\* Corresponding author, e-mail: a.bednarkiewicz@intibs.pl

Lanthanides are a group of materials known and valued for their up-conversion properties and used for vast applications from active centers in lasers to bioimaging. Among many up-conversion mechanism there is one, that requires special remark.

Photon avalanche (PA) is a highly nonlinear case of an anti-stokes up-conversion process, which can be observed in lanthanide doped crystals [1]. In the process, emitted photons have higher energy than absorbed photons. Moreover, due to the phenomena named cross-relaxation between adjacent ions of lanthanides, luminescence intensity ( $I_L$ ) has steep and nonlinear excitation power dependence ( $I_P$ ) following  $I_L = (I_P)^S$  within photon avalanche regime. While S factor in other up-conversion processes achieve 2–5, in PA up-conversion can go far beyond these values and even reach 46 [1–3].

PA process, due to its very complex dynamics, can be obtained only by carefully designed architecture and composition of lanthanide ions [3]. This process can be either enhanced or hindered by admixture of different lanthanide ions [4]. Here, we are presenting influence of different  $\text{Nd}^{3+}$  concentrations in  $\text{LiYF}_4$  3%  $\text{Tm}^{3+}$  on PA mechanism and two-color emission intensity of  $\text{Tm}^{3+}$  ions. We measured luminescence intensity versus excitation power showing that addition of  $\text{Nd}^{3+}$  ions undermine 800nm and 450nm PA emission of  $\text{Tm}^{3+}$ . Additionally, obtained up-conversion luminescence spectra corresponds with aforementioned effect, showing decrease in  $\text{Tm}^{3+}$  emission intensity with increasing  $\text{Nd}^{3+}$  concentration. We assume that effect is a consequence of the energy migration from  $\text{Tm}^{3+}$ :  $^3\text{H}_4$  ( $^3\text{F}_4$ ) to  $\text{Nd}^{3+}$ :  $^4\text{F}_{3/2}$  ( $^4\text{I}_{11/2}$ ). These measurements shed light on the complex and composition dependent PA process.

## Acknowledgements

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# Photon Avalanching in Pr<sup>3+</sup> and Yb<sup>3+</sup> co-doped NaYF<sub>4</sub> nanocrystals

M.Dudek<sup>1</sup>, Z.Korczak<sup>1</sup>, O.Bezkrovnyi<sup>1</sup>, M.Szalkowski<sup>1,2</sup>, M.Misiak<sup>1</sup>, A.Bednarkiewicz<sup>1</sup>

<sup>1</sup> Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław,  
ul. Okolna 2, 50-422, Poland

<sup>2</sup> Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun,  
ul. Grudziadzka 5, 87-100, Poland

E-mail: M.Dudek@intibs.pl; A.Bednarkiewicz@intibs.pl

Among different up-conversion processes Photon Avalanche (PA) is unique, because luminescence intensity of investigated materials increases rapidly in response to tiny increase of excitation source power density. The dependence is illustrated by s-shaped curve characterized by slope and PA threshold indicating minimal value of pump power density necessary for PA existence. Until now, the PA phenomenon was observed in bulk as well as micro and nano-sized crystals. While PA in bulk materials was widely investigated in many matrices doped different lanthanide ions [1], PA in smaller scale was obtained relatively recently in fluorides doped with Tm<sup>3+</sup> [2, 3] as well as co-doped with Pr<sup>3+</sup> and Yb<sup>3+</sup> ions [4]. Here we present PA in Pr<sup>3+</sup> and Yb<sup>3+</sup> co-doped NaYF<sub>4</sub> nanocrystals, synthesized by thermal decomposition of lanthanide salts method in two architectures: as core and core-shell samples. Measurements of the dependence of luminescence intensity as a function of excitation wavelength power density were performed on a custom-built optical microscope system. Nanocrystals were excited with 852 nm laser diode and PA emission was observed at 482 nm and 607 nm, which corresponds <sup>3</sup>P<sub>0</sub>→<sup>3</sup>H<sub>4</sub> and <sup>3</sup>P<sub>0</sub>→<sup>3</sup>H<sub>6</sub> transitions in Pr<sup>3+</sup> ions, respectively. Slope and threshold values were determined. Comparing core and core-shell samples, higher slopes values and lower thresholds were obtained for core-shell nanocrystals. As an optimal sample, i.e. with the biggest average slope reaching around 9 and the smallest threshold value, approximately 280 kW/cm<sup>2</sup>, NaYF<sub>4</sub>: 15%Yb<sup>3+</sup> 0.5%Pr<sup>3+</sup>@ NaYF<sub>4</sub> was found. Beyond experimental results, theoretical calculations for Yb<sup>3+</sup> and Pr<sup>3+</sup> ions system were performed using Matlab. The computations were aimed at showing, how different parameters, such as absorption cross sections, energy transfers between ions as well as lifetimes of excited levels influence PA features. The presented results provide a solid foundation for further development and applications of new optimized PA materials, which can be potentially used in bioimaging and biodetection.

## Acknowledgements

Research was supported by project 2021/43/B/ST5/01244 funded by the National Science Centre, Poland.

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# Linear and nonlinear properties of novel furan-based organic compounds exhibiting AIE behavior

Kamila Łupińska<sup>1</sup>, Agnieszka Siomra<sup>1</sup>, Chantal Andraud<sup>2</sup>, Lech Sznitko<sup>1</sup>, Marcin Nyk<sup>1</sup>

<sup>1</sup> *Institute of Advanced Materials, Wrocław University of Science and Technology,  
Wyb. Wyspińskiego 27, 50-370, Wrocław (Poland)*

<sup>2</sup> *Univ. Lyon, ENS de Lyon, CNRS UMR 5182, Laboratoire de Chimie, F69342, Lyon, France  
E-mail: kamila.lupinska@pwr.edu.pl*

The push-pull molecules are gaining scientific interest due to their easy polarization by external electric fields carried by incident light. Thus, they show a relatively low threshold for nonlinear optical (NLO) phenomena compared to other dyes. From the application point of view, NLO could be utilized, for instance, in diagnostic and medicine (2-photon imaging), in material processing (2-photon excited photodynamic polymerization), or in optics (as optical limiters) [1– 3], etc.

The mentioned molecules exhibit an effect called Intramolecular Charge Transfer (ICT). To properly describe the absorption and emission of ICT molecules, it is necessary to use a four-level-energy diagram. This layout of energies is very beneficial to obtain laser action of low pumping thresholds. However, the main mechanism limiting high laser materials development is aggregation-caused quenching. Discovering materials showing Aggregation-Induced Emission (AIE) phenomena could lift the mentioned restriction. Recently, it was proven that AIE materials might enhance laser emission intensity [5].

Herein, we would like to describe the optical properties of a newly synthesized family of furan-based organic compounds. All of the studied compounds were synthesized using Knoevenagel condensation with satisfactory reaction yields (~85% for 2,4,6-OBn-TCF). For mentioned molecules, we were able to obtain 2-photon absorption (TPA), Optical Kerr Effect (OKE), and light amplification. For instance, one of the studied compounds – 2,4,6-OBn-TCF – showed a considerable TPA cross-section around 2000 GM. Moreover, all of the presented molecules exhibit the AIE phenomenon.

To summarize, we want to present a spectroscopic characterization of a novel family of molecules based on furan derivatives, including linear and nonlinear studies. As their synthesis is relatively easy to obtain and low-costed compared to other types of laser materials, they seem to be very promising nonlinear dyes for two-photon lasing and photonic applications.

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# The influence of donor change on TADF properties in difluoroborate-based dyes

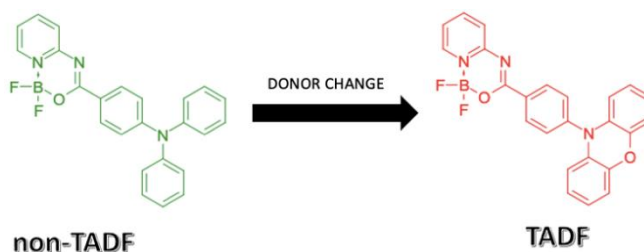
Judyta Zielak-Milewska<sup>1</sup>, Borys Ośmiałowski<sup>1</sup>, Sudhakar Pagidi<sup>2</sup>,  
Abhishek Gupta<sup>2</sup>, Eli Zysman-Colman<sup>2</sup>

<sup>1</sup> Faculty of Chemistry, Nicolaus Copernicus University, 87-100, Toruń, Poland

<sup>2</sup> University of St Andrews, St. Andrews, Scotland, United Kingdom

E-mail: jzielak@doktorant.umk.pl

Organic compounds that show Thermally Activated Delayed Fluorescence (TADF) are being given increasing attention in research nowadays as next-generation emitters in organic light emitting diodes (OLEDs). Compared to existing liquid crystal displays (LCDs), OLEDs provide better image quality and contrast, faster response times/refresh rates, are thinner, and can be seen from wider viewing angles [1]. Organoboron compounds have been extensively studied and widely used as optoelectronic materials due to their diverse optical and electronic properties. In tetracoordinated difluoroboron materials boron can adjust the electronic properties of the acceptor and increase the molecular rigidity to achieve high photoluminescence quantum yield [2].



The present work describes and the synthesis of compounds belonging to difluoroborate (BF<sub>2</sub>) group and donors used in TADF exhibiting dyes. Considering the emission of studied dyes the change of the donor (phenoxazine vs diphenylamine) causes shift of emission bands and switch on and off the TADF, meaning the phenoxazine-substituted dyes exhibited TADF while diphenylamine-substituted did not. This was confirmed experimentally and by performing theoretical calculations.

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# Nonlinear optical properties of sulfur quantum dots for applications in heavy metal ions detection

Agnieszka Siomra, Dominika Wawrzyńczyk, Marcin Nyk

<sup>a</sup>*Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław*

E-mail: [agnieszka.siomra@pwr.edu.pl](mailto:agnieszka.siomra@pwr.edu.pl); [dominika.wawrzynczyk@pwr.edu.pl](mailto:dominika.wawrzynczyk@pwr.edu.pl); [marcin.nyk@pwr.edu.pl](mailto:marcin.nyk@pwr.edu.pl)

The potential applications of cadmium-based quantum dots [1] are significantly limited due to the presence of heavy metals in the chemical composition. Therefore, metal-free sulfur quantum dots (SQDs) represent an interesting alternative, as they exhibit not only desired optical properties, but also antimicrobial activity, high biocompatibility, low toxicity and excellent water dispersibility [2]. However, there are only a few reports in the literature on the nonlinear optical properties of SQDs. The presented results demonstrate the ability of this nanomaterial to exhibit nonlinear optical responses, shedding light on its potential applicability as two-photon active optical sensors for metal ions detection - including heavy metal ions. Third-order nonlinearities of SQDs were investigated with the two-photon luminescence excitation method using a tunable femtosecond laser pulses. This allowed for quantitative determination of two-photon absorption cross-sections in an expanded spectral range, which has not been described in the literature before. The quenching of two-photon excited emission of SQDs in the presence of  $\text{Fe}^{3+}$  was explored – the results are presented in Fig. 1. The observations confirm that SQDs are attractive materials for applications as highly sensitive sensors for metal ions detection and could be a promising alternative to the nonlinear absorbers currently used, for example, as markers for nonlinear microscopy [3]. This study can also facilitate the design of new nanomaterials based on sulfur QDs for use in photonics and biophotonics in the future.

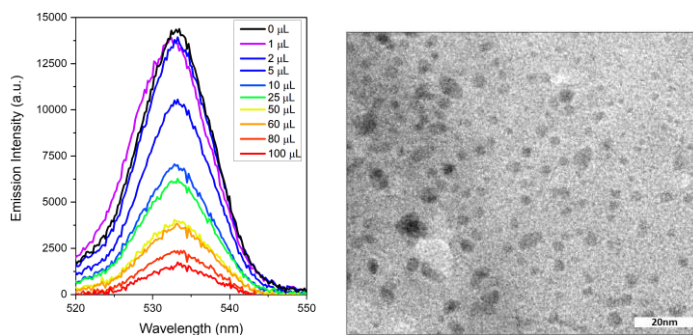


Figure 1. Two-photon excited emission spectra at  $\lambda_{\text{EXC}} = 780 \text{ nm}$  demonstrating the quenching of fluorescence upon addition of  $\text{Fe}^{3+}$  (left) and representative TEM image of SQDs (right)

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# Bimodal, ratiometric luminescence manometer based on Cr<sup>3+</sup> doped MgO nanoparticles

Maja Szymczak\*, Lukasz Marciniak\*

*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*  
E-mail: [m.szymczak@intibs.pl](mailto:m.szymczak@intibs.pl); [l.marciniak@intibs.pl](mailto:l.marciniak@intibs.pl)

In various industries, it is necessary to strictly control parameters such as temperature or pressure during technological processes. Due to the increasing automation of processes, non-contact parameter readout that provides non-invasive and fast, real-time measurement, is becoming essential. Research on pressure sensing, in contrast to temperature, is not so widely conducted. An important class of non-invasive pressure sensors mentioned above are those based on the luminescence of lanthanide and transition metals ions. Among them, in the context of application in luminescence manometry, transition metal ions stand out, due to the possibility of easy luminescence tuning by changing the strength of the crystal field, which depends on the pressure applied to the material [1].

Hence, we present a ratiometric luminescence manometer based on MgO:Cr<sup>3+</sup> nanoparticles emission. By choosing a Cr<sup>3+</sup> dopant concentration that provides an intermediate crystal field, it was possible to propose two ratiometric pressure readout modes – one using the luminescence intensity ratio (LIR) of emission bands associated with the <sup>2</sup>E→<sup>4</sup>A<sub>2</sub> and <sup>4</sup>T<sub>2</sub>→<sup>4</sup>A<sub>2</sub> transitions, and another based on a novel approach exploiting the LIR of two spectral ranges of <sup>4</sup>T<sub>2</sub>→<sup>4</sup>A<sub>2</sub> emission band. Both modes provide an extremely high sensitivity of 40 and 9.8%/GPa, respectively. A comparison was also made between the two modes in terms of temperature-dependent emission. Despite the lower sensitivity to pressure changes, the proposed mode based only on the <sup>4</sup>T<sub>2</sub> emission band provided a temperature-invariant pressure readout, in contrast to the approach based on the emission from the <sup>2</sup>E level, due to the thermal coupling of the <sup>2</sup>E and <sup>4</sup>T<sub>2</sub> states that is widely exploited in luminescence thermometry [2].

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# Plasmonic Nanoparticles for Organic Photovoltaics – Synthesis and Postprocessing

Nina Tarnowicz-Staniak, Katarzyna Matczyszyn

Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology,  
Wyb. Wyspiańskiego 27, 50-370 Wrocław  
E-mail: nina.tarnowicz-staniak@pwr.edu.pl

Improvement in the power conversion efficiency (PCE) of organic solar cells [1, 2] and their benefits, such as flexibility, make organic photovoltaics (OPVs) a promising technology for wearable electronics [3]. However, the overall efficiency is often compromised by the ultrathin architecture of the devices. Various strategies have been proposed to overcome this obstacle, and one of them is the absorption enhancement induced by the incorporation of plasmonic nanoparticles [4].

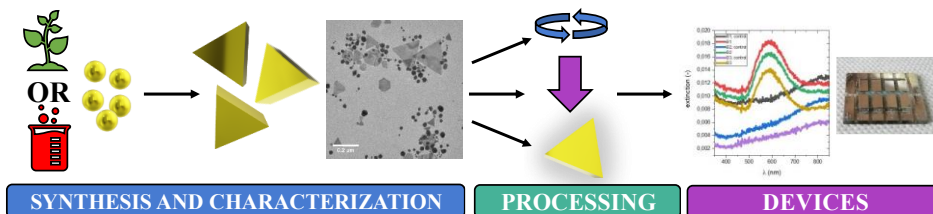


Fig. 1. Schematic workflow of the project.

The main focus of this work is the incorporation of triangular gold nanoplates (AuNTs) in the architecture of organic solar cells. Two approaches to the synthesis are tested – biological [5] and chemical [6]. Further studies concern the most efficient postprocessing approach (including centrifugation [5], depletion flocculation [6], and polymer coating [7]) in order to facilitate the incorporation process [7] and optimize the concentration of nanostructures. Subsequently, the extinction pre-tests of the PEDOT:PSS layers doped with as-prepared AuNTs were performed, and the final devices were prepared and tested.

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# In the search for a perfect nanosilver stabiliser – ionic liquids with alkoxyethyl substituent?

Małgorzata Policht, Anna Bastrzyk, Joanna Feder-Kubis

Wrocław University of Science and Technology, Faculty of Chemistry  
E-mail: malgorzata.policht@pwr.edu.pl

Stable nanodispersions have been a challenge in chemical technology since the advent of nanoscience. Metal nanoparticles (NPs) in water solutions tend to agglomerate easily and form micrometre-sized aggregates that exhibit altered properties compared to their nano form and have a higher toxicity profile. Therefore, several compounds, including polymers, surfactants and ionic liquids (ILs) have been tested as additives for metal NPs suspensions [1, 2]. ILs, which are organic compounds composed entirely of ions, can be employed not only as NPs stabilisers and templates but also as reaction media, functionalising agents, or even reducing agents and metal precursors. The other issue is the supporting function of ILs for bioactive NPs; in this context, imidazolium salts with alkoxyethyl substituent are highly recommended as they possess various bioactive functions [3].

Here, we present the synthesis of two aprotic ILs, namely 1-butoxymethyl-3-ethylimidazolium chloride (IL-C<sub>4</sub>) and 1-decyloxymethyl-3-ethylimidazolium chloride (IL-C<sub>10</sub>), and their application as stabilising additives to silver NPs derived from green tea. We discuss the influence of the length of the side carbon chain on the optical and physicochemical properties of NPs, as well as the ecological factors of the process.

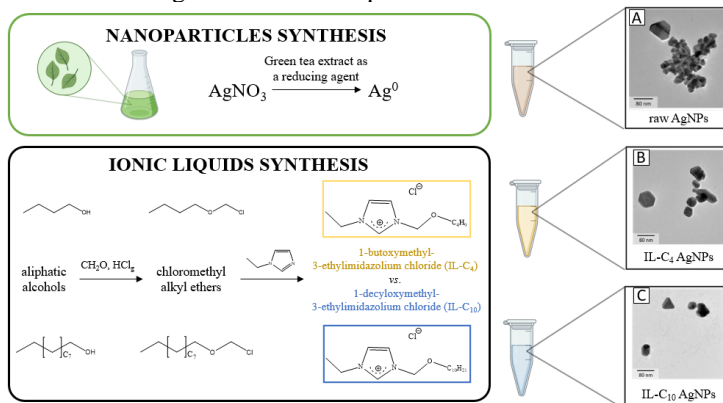


Figure 1. A scheme of the synthesis of ionic liquids with alkoxyethyl substituent and silver nanoparticles along with TEM photomicrographs of: raw-AgNPs, IL-C<sub>4</sub> AgNPs and IL-C<sub>10</sub> AgNPs

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# Choline-based ionic liquids entrapped in nanocellulose matrix

Przemysław Pietrusiak, Aleksandra Gersz, Joanna Feder-Kubis

Wroclaw University of Science and Technology, C. K. Norwida Street 4/6, 50-373 Wroclaw, Poland  
E-mail: przemyslaw.pietrusiak@pwr.edu.pl

Scientific research has been increasingly focused on finding novel, green, and sustainable materials. Environmental constraints have driven researchers to seek valuable products with low environmental impact. To achieve this goal, the combination of cellulose nanofibers' hydrogel with appropriately designed compounds with important functions appears to be a justified approach for many possible applications. In this study, we explored the use of choline-based ionic liquids (ILs) in combination with cellulose nanofibers as a carrier. From a structural point of view, presented ionic compounds are a group of quaternary ammonium salts composed of choline cation and various types of anions. Numerous choline-based ILs are fully biodegradable, biocompatible, water-soluble, and non-toxic compounds with a wide range of applications. Furthermore, economic considerations related to choline-based ILs are beneficial, as they utilize cheap and readily accessible substrates and can be produced under favourable conditions.[1]. Additionally, cellulose nanomaterials are an ideal choice as an IL carrier due to their renewable source, biodegradability, and chemical inertness [2]. In this work, we synthesised various choline derivatives, including choline salicylate, choline saccharinate, and choline bis(trifluoromethylsulfonyl)imide. We 3D printed the obtained ILs and other commercially available choline salts (choline chloride, choline hydroxide, and choline bicarbonate) in a hydrogel matrix based on cellulose nanofiber (CNF). The main stages of this research are presented in Figure 1.

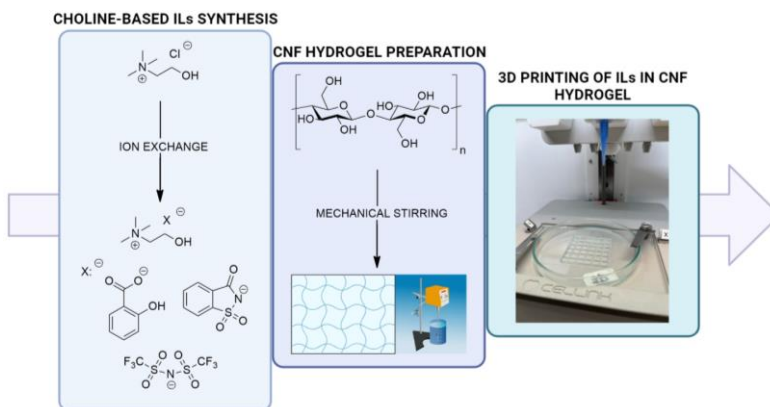


Figure 1. Three stages leading to 3D printed ILs in CNF hydrogel.

This research was financed by the National Science Centre, Poland (grant no. UMO-2020/37/B/NZ9/04201).

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# Revealing the Hidden Beauty of Conjugated Polymers and Multilamellar Vesicles through the Lens of Third-Harmonic Generation Microscopy

Maksymilian Dereniowski<sup>1</sup>, Karen Aerts<sup>1</sup>, Thierry Verbiest<sup>1</sup>,  
Katarzyna Matczyszyn<sup>2</sup>, Koen Clays<sup>1</sup>, Yovan de Coene<sup>1</sup>

<sup>1</sup>Department of Chemistry, University of Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium  
<sup>2</sup>Institute of Advanced Materials, Wrocław University of Science and Technology, Wrocław, Poland  
maksymilian.dereniowski@kuleuven.be

Nonlinear optical techniques base on the nonlinear optical behavior of materials under intense electromagnetic fields and require pulsed (high peak, short duration) infrared wavelength lasers. As a result multiple photons of light can interact with material at the same time and thus generate higher-energy photons. **Double (second harmonic, SH)** or even **triple frequency (third harmonic, TH)** scattered light phenomena may be seen in such circumstances. In THG, **three** identical photons interact with a substance or material to scatter a photon that has three times the frequency (i.e., one third the wavelength) of the original photons. At the molecular level, third-harmonic generation is governed by the **second hyperpolarizability ( $\gamma$ )**, which is equivalent to the molecules third-order nonlinear optical response to an applied electric field. Unlike second-harmonic generation (SHG) (which is a symmetry-dependent process and occurs only in non-centrosymmetric structures), **THG** is associated with any material due to fact that every material possess **non-zero third order susceptibility** and is susceptible to THG. In theory TH signal appears in two cases: 1) **relatively big  $\gamma$  of the molecule**, present in conjugated poly(3-hexylthiophene-2-5-diyl) (P3HT), due to its high density of polarizable  $\pi$  electrons and 2) **at the interface of components with different refractive indexes** [1]. These interfaces are actually present in every biological system; membrane-cytosol e.g. myeline. THG is significantly enhanced when many membranes are present inside the focus volume, what is observed in case of the multilamellar vesicles (MLVs). As it was presented at the Fig. 1 we will be able to generate label-free images which have origin in: left – overlapping of THG and multiphoton fluorescence, showing the bulk origin of the TH; right – importance of the interface. Our research is focused at an assessment of the relative importance of both mechanisms for materials with large gamma.

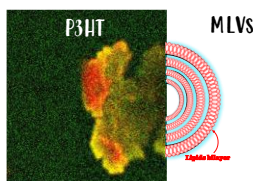


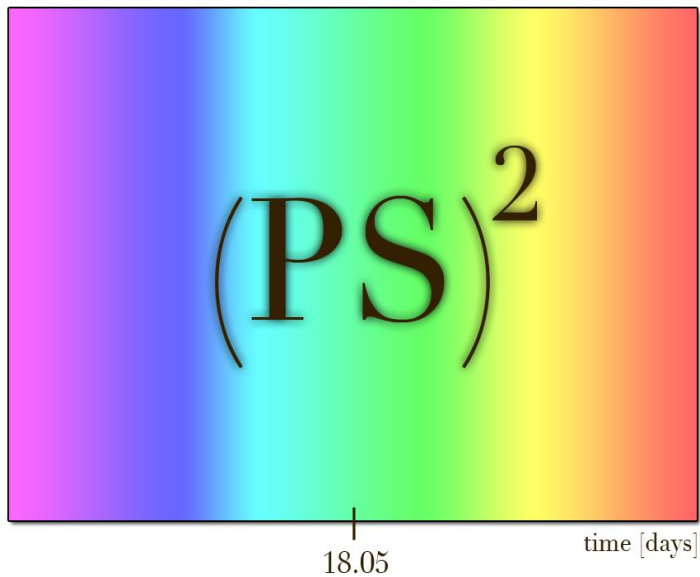
Figure 1: Left: P3HT polymer; using label-free THG microscopy at 1140 nm; imaged with Insight® DS+ fs laser™. Right: A scheme of multilamellar vesicle irradiated with 1140nm excitation wavelength.

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# PhoBiA Student Photonics Symposium 2023



- |        |                             |
|--------|-----------------------------|
| What?  | Poster session for students |
| When?  | 18.05                       |
| Where? | D-20 building, WUST         |

# PhoBiA Student Photonics Symposium

## List of students posters

Poster no.	Presenter	Title
P01	Piotr Kuich	Synthesis and morphology characterization of lanthanide doped NaYF <sub>4</sub> core-shell nanomaterials
P02	Dominika Czekanowska	Biocompatible fluorapatites co-doped with terbium(III) and rubidium(I) ions as highly functional materials for biomedical applications
P03	Marek Adaszyński	A novel composite based on Eu <sup>2+</sup> doped phosphors for high quality white light generation
P04	Julia Osmólska	Non-linear absorption measurements of Au <sub>25</sub> nanoclusters linked with a bidentate dithiol via z-scan technique
P05	Jan Pytel	Time resolved reflectivity and absorption measurements of Ti <sub>3</sub> O <sub>5</sub> thin film
P06	Aleksandra N. Piasecka	A Novel Technique of Probing the Local Spectral Temperature in Semiconductor VCSELs
P07	Antonina Bieganowska	Investigating the Dynamics and Interactions of a Photonic Condensate in an Optical Trap
P08	Natinael Koyra	Effect of process parameters on amorphous DLC thin film coating using PECVD technique on silk fabric for medical applications
P09	Aleksandra Dupla	Synthesis of linear benzothiadiazole derivatives for use in optoelectronics
P10	Ioanna-Yustyna Shpak	Production of valeric acid based on polyene antibiotic lucensomycin polyketide synthase
P11	Marek Czyszczon	Synthesis of fluorene-based organic building blocks for the design of new fluorophoric dyes

<b>P12</b>	<b>Weronika Antworka</b>	Liposomes from DLPC
<b>P13</b>	<b>Julia Wątor</b>	CpkL as a potential participant of malonyl-CoA synthesis in <i>Streptomyces coelicolor</i> A3(2)
<b>P14</b>	<b>Piotr Kruszyński</b>	Production of nanoparticles by fungi
<b>P15</b>	<b>John Vincent Tumaneng</b>	From Nature For Nature: Supporting the Development of Stimulus-Responsive Ionogels for Agrochemistry
<b>P16</b>	<b>Tymotuesz Mrozek</b>	Finite field method with harmonic potential
<b>P17</b>	<b>Diego M. Juela</b>	Cellulose nanocrystals in copolymeric composites with self-healing and piezoelectric properties





# Synthesis and morphology characterization of lanthanide doped NaYF<sub>4</sub> core-shell nanomaterials

Piotr Kuich<sup>1</sup>, Patryk Fałat<sup>1</sup>, Min Ying Tsang<sup>2</sup>, Marcin Nyk<sup>1</sup>, Dominika Wawrzyńczyk<sup>1</sup>

<sup>1</sup> Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology, 50-370 Wrocław, Poland

<sup>2</sup> Institute of Functional Materials, Department of Chemistry, University of Vienna, 1090 Vienna, Austria  
E-mail: 246085@student.pwr.edu.pl

Proper design of the lanthanide doped core@shell nanomaterials can be used to tune or enhance their optical properties, and at the same time integrating several applications [1]. Those nanocrystals (NCs) can be in general divided into two categories, either as multishell (with more than one shell) or single-shell structures [2]. Epitaxial shells can be obtained with the same synthetic procedure used to obtain the core-nanoparticles, except that growth takes place on the surface of the previously synthesized core nanoparticles, not in the liquid phase. There are two main routes by which epitaxial growth of shells can be achieved – either by injecting shell precursors into the reaction in progress (hot-injection method) or by adding pre-obtained core nanoparticles into the reacting mixture before starting the reaction heating (heat-up strategy) [3].

In this work, three core@shell@shell@shell materials based on the NaYF<sub>4</sub> matrix have been obtained by solvothermal synthesis, with different lanthanide ions doped in the core, i.e., 1% Nd<sup>3+</sup>, 1% Tm<sup>3+</sup>, 10% Yb<sup>3+</sup>, respectively. For all materials, the second shell contained 1% Pr<sup>3+</sup>, whereas first and last shell stayed undoped. Shell growth was obtained by heat-up strategy. The matrix which has been used to obtain mentioned nanomaterials was NaYF<sub>4</sub> and remained unchanged for all layers.

The morphology of the core@shell NCs have been characterized by the transmission electron microscopy and based on the obtained images – mean size and size distribution has been measured and compared.

Despite the fact that all syntheses were based on the same protocol, nanoparticles differing in average size and size distribution were obtained. The measured histograms directly confirmed the formation of successive shells after each synthesis, due to an increase in size.

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# Biocompatible fluorapatites co-doped with terbium(III) and rubidium(I) ions as highly functional materials for biomedical applications

Dominika Czekanowska<sup>1,2</sup>, Nicole Nowak<sup>3</sup>, Rafał Wiglusz<sup>1</sup>

<sup>1</sup>*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, s50-422 Wrocław, Poland*

<sup>2</sup>*Refectio Students' Scientific Society, Department of Biostructure and Animal Physiology, Wrocław University of Environmental and Life Sciences, ul. Kozuchowska 1/3, 51-631 Wrocław, Poland*

<sup>3</sup>*Department of Biostructure and Animal Physiology, Wrocław University of Environmental and Life Sciences, ul. Norwida, 31, 50-375 Wrocław, Poland*  
E-mail: [d.czekanowska@intibs.pl](mailto:d.czekanowska@intibs.pl)

Recent successes in nanotechnology are reported about diversity of nanomaterials that can be successfully used in the various fields of biology and nanomedicine. Multifunctional nanomaterials are become especially desirable in tissue engineering field as factors leading to increased regeneration of fractured tissues, and as luminescent nanoprobes in bioimaging or bio-detection. One of the materials opening above possibilities are the basic elements of dentin and bone, the fluorapatites ( $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2$  - FAp), characterized by exceptional biocompatibility, bioactivity, and mechanical properties. Due to the similarities in ionic radii values between  $\text{Ca}^{2+}$ ,  $\text{Tb}^{3+}$  and  $\text{Rb}^+$  ions, the replacement of  $\text{Ca}^{2+}$  ions in the crystal lattice of fluorapatite with dopants can be successfully incorporated. In the case of terbium dopants, this substitution results in the addition of luminescent properties to the matrix [1], [2], and in the case of rubidium, in the stimulation of the cell's biological regenerative properties and an increase in bone cells proliferation [3].

In our research, the basic structural, physicochemical, and biological properties of hydrothermally synthesized fluorapatites co-doped with terbium(III) and rubidium(I) ions were thoroughly investigated. The studies focused on the luminescent and biological properties of our materials, by measuring excitation spectra, emission spectra and fluorescence lifetimes, and the in vitro studies on selected cell lines (L929 mouse fibroblasts, 3T3 mouse fibroblasts, 7F2 mouse osteoblasts, THP-1 human monocytes). In conclusion, obtained fluorapatite-based nanocomposites can be successfully used in biomedicine, both as a bio-labelling material and as a potential material for use in treatments involving regenerative medicine and tissue engineering.

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# A novel composite based on $\text{Eu}^{2+}$ doped phosphors for high quality white light generation

Marek Adaszyński<sup>1</sup>, Damian Szymański<sup>1</sup>, Dagmara Stefańska<sup>1</sup>

<sup>1</sup>*Institute of Low Temperature and Structure Research Polish Academy of Science, Wroclaw, 50-422, Poland  
m.adaszynski@intibs.pl*

Nowadays new highly efficient and energy saving lighting devices are desired. One of the most promising technologies currently available in the market are Light Emitting Diodes (LED). However, although their high power efficiency, the diodes itself usually produce light with poor quality of emission. This can be evaluated by Color-Rendering Index (CRI), which is the parameter indicating the ability to reproduce the colors of objects as seen under ideal white light sources, for example, the Sun. To increase the CRI value, besides the semiconductor chip, a phosphor mixture embedded in a polymer is added. Their role is to absorb some or the whole emitted light from the chip and emit a broad band which overall will cover the whole visible spectral range [1, 2]. An example of such a system is a blue LED chip, covered with a composite containing YAG:  $\text{Ce}^{3+}$ , which luminescence complements the chip emission. For UV LED chips a mixture of different phosphors is used, which entirely absorbs the emission of the chip and emits a more balanced white emission than in the first example. As a result higher CRI index can be reached [2].

In this work, a new composite material for UV LED chips will be presented. It consists of two phosphors an aluminosilicate doped with  $\text{Eu}^{2+}$  and a borate  $\text{LiSr}_4(\text{BO}_3)_3: \text{Eu}^{2+}$ , for which the synthesis process was optimized, and spectroscopic properties such as luminescence excitation, emission, lifetimes, and quantum yield were extensively investigated. As a matrix for the composite, the Sylgard 184 resin was used and the layers with different ratios of the phosphors were prepared. Finally, the colorimetric parameters were calculated. The highest CRI value equal to 92 was achieved for the composite with a 90% concentration of  $\text{LiSr}_4(\text{BO}_3)_3$  and the Correlated Color Temperature was equal to 3227 K.

In conclusion, these parameters make the final material suitable for use in LED lighting at home, especially in bedrooms, where a warm white light with a low amount of blue emission component is preferred. This could minimize a disruptive influence on the circadian rhythm, and melatonin production and leads to a better quality of sleep [3].

This work was funded by The National Centre for Research and Development in Poland (LIDER/19/0103/L-12/NCBR/2021).

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# Non-linear absorption measurements of Au<sub>25</sub> nanoclusters linked with a bidentate dithiol via z-scan technique

Julia Osmólska<sup>1</sup>, Patryk Obstarczyk<sup>1</sup>, Michał Świerczewski<sup>2</sup>,  
Thomas Bürgi<sup>2</sup>, Joanna Olesiak-Bańska<sup>1</sup>

<sup>1</sup>*Institute of Advanced Materials, Wrocław University of Science and Technology, Wrocław, Poland*

<sup>2</sup>*Department of Physical Chemistry, University of Geneva, Geneva, Switzerland*  
E-mail: 250152@student.pwr.edu.pl

In this poster, we present broad range (600 – 1500 nm) two-photon absorption (TPA) spectra measurements using the z-scan technique on atomically-precise gold nanocluster (AuNC) monomers, dimers, and trimers linked with a 1,1'-binaphthyl-2,2'-dithiol ligand. Previous studies of organic and organometallic molecules have demonstrated that the two-dimensional and three-dimensional arrangements of monomers as well as oligomeric and dendritic structures can enhance their two-photon absorption cross-sections [1]. Therefore, we studied the impact of gold nanocluster oligomerization on their nonlinear properties. AuNCs are molecule-sized nanomaterials composed of well-defined number of gold atoms, ranging in size up to 2 nm in diameter. They exhibit unique optical and electronic properties, including significant nonlinear optical properties, due to core size and quantum confinement effects [2, 3]. In this study, we investigated the nonlinear optical properties of Au<sub>25</sub>PET<sub>18</sub> (PET = phenylethanethiol, SC<sub>2</sub>H<sub>4</sub>Ph) monomers, dimers and trimers linked with ((1R, 1'R)-6,6'-(1,4-phenylene)di-1,1'-binaphthyl-2,2'-dithiol) (diBINAS), reported previously by M. Swierczewski et al. (2023) [4]. Using a femtosecond laser and an open- and closed-aperture z-scan setup, we measure their TPA cross-sections. Our results indicate that the TPA cross-sections of the Au<sub>25</sub> oligomers strongly depend on their size, which may be attributed to the increased rigidity within the ligand shell of each cluster caused by the bidentate bonding. Moreover, we observed that the TPA cross-sections of the Au<sub>25</sub> dimer and trimer were significantly larger than those of individual Au<sub>25</sub>PET<sub>18</sub> clusters, suggesting a cooperativity effect in such structures, with nonlinearly enhanced TPA cross-sections as a function of the number of linked nanoclusters. These findings provide valuable insights into the TPA properties of gold nanoclusters, optical properties of nanoparticle oligomers and hold promise for the potential applications in nonlinear optical devices and bioimaging.

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# Time resolved reflectivity and absorption measurements of $\text{Ti}_3\text{O}_5$ thin film

Jan Pytel<sup>1</sup>, Maciej Lorenc<sup>2</sup>, Vinh Ta Phuoc<sup>3</sup>

<sup>1</sup> Faculty of Chemistry, Wrocław University of Science and Technology

<sup>2</sup> Univ Rennes, CNRS, IPR (Institut de Physique de Rennes)–UMR 6251, Rennes, France

<sup>3</sup> GREMAN–UMR 7347 CNRS, Université de Tours, Tours, France

E-mail: 258825@student.pwr.edu.pl

Trititanium pentoxide undergoes a reversible, photoinduced phase transition at room temperature between  $\lambda$ - $\text{Ti}_3\text{O}_5$ , a near-metallic conductor and  $\beta$ - $\text{Ti}_3\text{O}_5$ , a semiconductor [1]. The favourable properties of this transition may be useful for applications in fields of optical memory devices and heat storage [2]. The dynamics of the transition were previously explored by a number of time-resolved methods [3, 4]. Strain wave propagation has been suggested as the underlying cause of this photoinduced switching [4].

In our work, we performed time-resolved pump-probe measurement in absorption and reflectivity setups at room temperature on a  $100 \pm 20$  nm thick film of  $\lambda$ - $\text{Ti}_3\text{O}_5$ . White light, generated in a sapphire via nonlinear optical effects, was used as probe. A strain wave, traveling from the thin film into a quartz substrate, was observed as a time-resolved Brillouin scattering signal. The changes in reflectivity at given delays in 10 ps timescale, associated with the propagation of the strain wave in the film, appear to depend linearly on the pump fluence. The results may be used as foundation for future measurements at higher pump fluences or different probe wavelengths.

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# A Novel Technique of Probing the Local Spectral Temperature in Semiconductor VCSELs

Aleksandra N. Piasecka<sup>1</sup>, Marcin Gębski<sup>2</sup>, Michał Wasiak<sup>2</sup>,

Tomasz Czyszanowski<sup>2</sup>, and Maciej Pieczarka<sup>1</sup>

<sup>1</sup>*Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology,  
Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

<sup>2</sup>*Institute of Physics, Łódź University of Technology, ul. Wólczajska 219, 90-924 Łódź, Poland  
235452@student.pwr.edu.pl*

The occurrence of Bose-Einstein condensation of bosons has been theoretically introduced in early 1920's by A. Einstein [1]. Yet only recent experimental study confirmed that a thermalized gas of the most fundamental bosons, i.e., photons, trapped in optical microcavity can display signatures of Bose-Einstein condensation [2]. However, the aspect of ununiform temperature distribution still needs to be investigated to determine if semiconductor lasers can act as Bose-Einstein condensate of photons.

The most commonly used measurement method to characterize temperature of laser microcavity by monitoring the thermally induced shift in the lasing wavelength provides only information on the average temperature distribution across the entire microcavity surface and more sophisticated techniques for probing local temperature have been developed [3]. However, the inhomogeneity of local temperature distribution and nonuniform current density affects the whole emission spectrum of electrically pumped semiconductor vertical-cavity surface-emitting lasers (VCSELs). This inhomogeneity effect also changes the effective local width of cavity, which is directly connected to the effective inhomogeneous confining potential for the photons, and therefore changes the density of states function and influences extracted values of the Bose-Einstein distribution. The assumption that the density of states has purely 2D-like character and has a fixed value over the whole VCSEL resonator may be an insufficient approximation. Here, we present a new technique for measuring local spectral temperature distribution in wide aperture oxide-confined VCSELs by locally fitting the Boltzmann distribution to the high-energy tail of the spontaneous emission spectrum. Additionally, through measurement of the local fundamental mode energy by filtering the spontaneous emission in the wavevector space close to the normal incidence  $k_{\parallel} \approx 0$ , we probed the local resonance of the cavity, which allows us to deduce the local effective potential change of the microresonator. The resulting data can be compared to theoretical simulations of the influence of local temperature and current density on the local potential shape.

Studies on the thermalized boson gas of trapped photons in electrically pumped VCSEL microresonators may provide devices that act as Bose-Einstein condensate of photons, allowing for a new research in Bose-Einstein photon condensation physics.

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# Investigating the Dynamics and Interactions of a Photonic Condensate in an Optical Trap

Antonina Bieganowska, Marcin Syperek, Maciej Pieczarka

Department of Experimental Physics, Faculty of Fundamental Problems of Technology,  
Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370  
E-mail: 255489@student.pwr.edu.pl

Both exciton polaritons and photons can achieve Bose-Einstein condensation (BEC) due to their bosonic nature, resulting in macroscopic coherence. The study of polariton and photon condensates has explored the nature of equilibrium and non-equilibrium BEC. In the high density regime, the exciton-photon coupling weakens, leading to a transition to weak coupling and the emergence of a photonic condensate or a photon laser, which is a non-equilibrium state. Interactions between exciton polaritons arise from the excitonic component, while interactions between photons may originate from nonlinearities in the active material, such as the nonlinear refractive index, which has not been studied in semiconductor microresonators in this context. These interactions are expected to manifest as a collective Bogoliubov spectrum of excited states measured in the dispersion of the emitted photons.

In this study, we experimentally investigate the dynamics of a high-density photonic condensate in an optically induced trap and the effects of photon-photon interactions using GaAs-based microcavity. We excite the sample with a pulsed laser shaped into a ring, which creates an optical trap for photons. By measuring the momentum dispersion using time-resolved spectral tomography on a streak camera, we track the time dynamics of the photon dispersion and observe its modification at the highest particle densities in the system, which may indicate the presence of effective photon-photon interactions. The photonic condensate is driven-dissipative, and our experimental results show a dissipative Bogoliubov spectrum, Figure 1 [1]. Our findings provide insights into the dynamics and nature of photonic condensates.

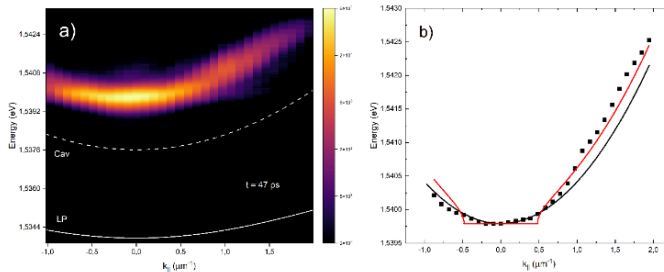


Fig. 1. (a) Measured dispersion of a photonic condensate at highest pumping power at time after pulse corresponding to the highest photon density. Theoretical photon and polariton curves are marked with Cav and LP. (b) Extracted energies from (a) (squares), with blueshifted theoretical cavity mode (black line) and fit with the dissipative Bogoliubov dispersion (red line)

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We would like to thank prof. Christian Schneider (University Oldenburg), prof. Sebastian Klemmt and prof. Sven Höfling (University Würzburg) for providing microcavity samples used in this study.

# Effect of process parameters on amorphous DLC thin film coating using PECVD technique on silk fabric for medical applications

Natinael Koyra<sup>1</sup>, Katarzyna Matczyszyn<sup>1</sup>, Rina G.Mbankeu<sup>2</sup>, Omar Benzine<sup>2</sup>.

<sup>1</sup>Wroclaw University of Science and Technology,

<sup>2</sup>AGC Interpane R & D centre

[natinaelkokeb88@gmail.com](mailto:natinaelkokeb88@gmail.com), [katarzyna.matczyszyn@pwr.edu.pl](mailto:katarzyna.matczyszyn@pwr.edu.pl), [rinambankeu@yahoo.com](mailto:rinambankeu@yahoo.com), [Omar.Benzine@interpane.com](mailto:Omar.Benzine@interpane.com)

In the present study, amorphous DLC thin films using gaseous methane as a carbon precursor were developed on the surface of silk fabric for medical applications. We used the PECVD technique to deposit an amorphous DLC thin film layer using Ar, Ar/He, N<sub>2</sub>, and Ar/N<sub>2</sub> process gases to ignite plasma, whereas, with pure helium, it was not possible to ignite plasma.

Figure 1A illustrates, a film coated by Ar and Ar/He plasma gas shown low the surface energy (WCA range of ~90 to 115 deg) and the thickness range of the film was 35 nm to 70 nm, while N<sub>2</sub> and Ar/N<sub>2</sub> plasma increased the surface energy (WCA range of ~50 to 70 deg) of the film and shown lower thickness. The thickness of the film was mainly influenced by the time or speed of coating, whereas process gas (Fig. 1B) and precursor gas (Fig. 1D) also has effect on thickness. The FTIR spectra (Fig. 1F) shown the C-C (1800 cm<sup>-1</sup>, 2150 cm<sup>-1</sup>) and C-H (850 cm<sup>-1</sup> up to 1600 cm<sup>-1</sup>, 2900 cm<sup>-1</sup>) bonding exist in the film. From the UV-VIS spectra (Fig. 1E), we observe that, increasing the chamber gas pressure (~2.5 kPa to 3.5 kPa), increased the light absorbance (~45.5% to 48%) with maximum absorbance at 595 nm. The SEM image (Fig. 1C) affirms the film has smooth with few spots. Since antibacterial activities are strongly related to the surface properties [1] of the film, the current DLC films can be promising for medical applications.

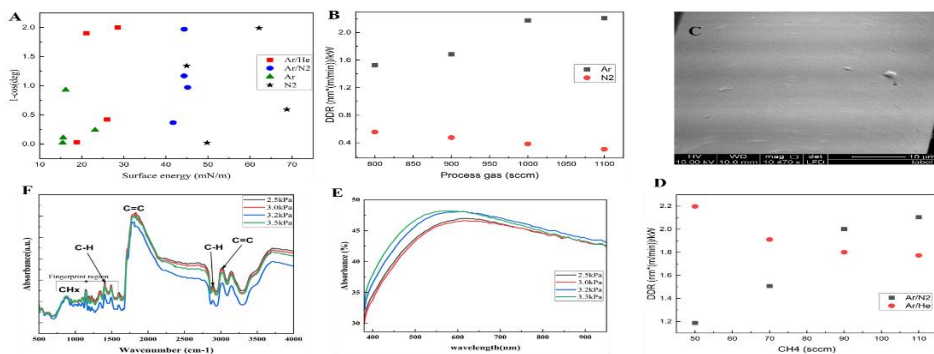


Figure 1: A, WCA as a function of surface energy of DLC films using variety of plasma gases; B&D, thickness as a function of process and precursor gas flow, respectively; C, SEM of the film on textile substrate; E, UV-Vis absorbance of the film deposited with variety pressure; F, FTIR spectra of the film on textile substrate

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# Synthesis of linear benzothiadiazole derivatives for use in optoelectronics

Aleksandra Dupla, Dorota Zajac

Wroclaw University of Science and Technology, Faculty of Chemistry, Institute of Advanced Materials  
E-mail: 269774@student.pwr.edu.pl

This present work focuses on the synthesis of linear benzothiadiazole derivatives for use in optoelectronics. The specific compound (E)-4-(3,4-ethylenedioxythiophen-5-yl)-7-(7-(2-(thiophen-2-yl)viny)))-3,4-ethylenedioxythiophen-5-yl)benzo[c][1,2,5]thiadiazole will be obtained as a result of a four-step synthesis (Fig. 1). The derivative's acceptor properties suggest potential applications in medical diagnostics, optoelectronics (e.g., photovoltaic cells, light-emitting diodes, and sensors), and medical imaging [1].

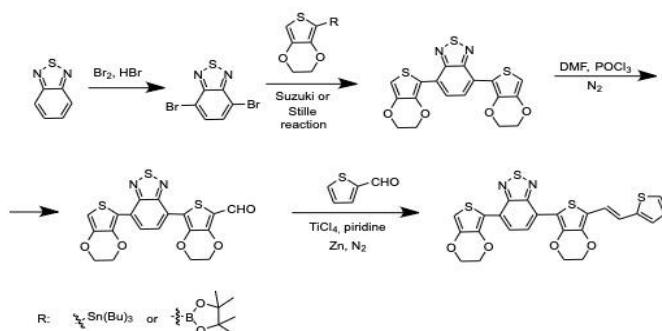


Fig. 1 Synthesis routes of (E)-4-(3,4-ethylenedioxythiophen-5-yl)-7-(7-(2-(thiophen-2-yl)viny)))-3,4-ethylenedioxythiophen-5-yl)benzo[c][1,2,5]thiadiazole

The synthesis process involves the substitution of bromine atoms into the benzothiadiazole unit in the first stage, using the bromine solution ( $\text{Br}_2$ ) together with hydrobromic acid (HBr), followed by C-C coupling reaction using palladium catalyst to expand the molecule with 3,4-ethylenedioxythiophene rings. The Vilsmeier-Haack reaction was then used to synthesize the aldehyde using N, N-dimethylformamide and phosphorus(V) oxychloride, and the final product was obtained using the McMurry reaction to allow the reaction between two carbonyl compounds. The research is ongoing to optimize the reaction and choose between the Stille and Suzuki reactions for the best performance.

The next stages of the project will involve testing the semiconducting and optical properties (absorbance and fluorescence) of the monomer and subjecting the compound to electro polymerization, creating a polymer film, to the potential use as a matrix in biosensors.

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# Production of valeric acid based on polyene antibiotic lucensomycin polyketide synthase

Ioanna-Yustyna Shpak\*<sup>1,2</sup>, Mateusz Wenecki<sup>2</sup>, Sofia Melnyk<sup>1</sup>,  
Magdalena Kotowska<sup>2</sup>, Krzysztof J. Pawlik<sup>2</sup>, Bohdan Ostash<sup>1</sup>.

<sup>1</sup> Ivan Franko National University of Lviv, Faculty of Biology, Department of Genetics and Biotechnology,  
Lviv, Ukraine

<sup>2</sup> Hirsztfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Wrocław, Poland.

\* E-mail: yustyna.shpak@hirsztfeld.pl

*Streptomyces*, Gram-positive bacteria, are producers of secondary metabolites, for instance antibiotics. One of the type of the metabolites are polyketides whose biosynthesis is based on repeated condensation of short acyl residues (acetyl-CoA, malonyl-CoA and propionyl-CoA etc.). The polyketides have a wide structural diversity and types of biological activity. However, they are all produced by a class of enzymes called polyketide synthases. This project is focused on synthesis of short carboxylic acids by a fragment of lucensomycin synthase from *Streptomyces cyanogenus* S136.

Genes for lucenomycin (Lcm) biosynthesis are encoded within the genome of *Streptomyces cyanogenus*. Lcm modular polyketide synthase consists of three subunits. The project investigates the first protein in the assembly line, LcmA. According to the prediction of the LcmA domain structure, this protein should catalyse synthesis of valeric acid (pentanoic acid), which has a characteristic scent. So far, the product release mode of polyketide chain from LcmA is unknown. It can happen spontaneously or via hydrolysis catalysed by thioesterase protein or domain.

In order to investigate LcmA production capability several expression vectors were constructed: for LcmA protein expression alone; LcmA protein fused with thioesterase domain; LcmA protein and thioesterase type II protein ScoT expressed from two different plasmids. Created plasmids were introduced into the production strain *Streptomyces albus* (*albidoflavus*) J1074.

# Synthesis of fluorene-based organic building blocks for the design of new fluorophoric dyes

Marek Czyszczoń<sup>1</sup>, Nicholas Richy<sup>2</sup>, Frederic Paul<sup>2</sup>, Olivier Mongin<sup>2</sup>

<sup>1</sup> *Wroclaw University of Science and Technology, Faculty of Chemistry*

<sup>2</sup> *Université de Rennes 1, Institut des Sciences Chimiques de Rennes (UMR 6226)*

E-mail: 258818@student.pwr.edu.pl

New organic materials can be synthesised in a bottom-up approach using building blocks – functionalized organic molecules. This approach is a useful method which may facilitate the synthesis of various compounds including dyes, metal-organic frameworks and supra-molecular complexes.

Three multi-step syntheses of fluorene-based building blocks were performed. Most of the reactions gave high yields (over 80%). Each of the final compounds had different functional groups: TIPS-C<sub>2</sub>- and H-C<sub>2</sub>-; I- and -NPh<sub>2</sub> or two I- groups. The synthesised compounds presented fluorescence under UV irradiation. Then, two of the obtained building blocks underwent Sonogashira cross-coupling reaction which resulted in a highly blue-fluorescent compound.

The presented reactions provide a promising way to easily synthesise building blocks useful in the design of new dyes with fluorophoric properties. However, it is needed to optimize the conditions of some lower-yield reactions to maximize the efficiency of the multi-step syntheses.

# Liposomes from DLPC

Weronika Antworka

*Institute of Advanced Materials, Faculty of Chemistry, Wrocław University of Science and Technology  
E-mail: 252642@student.pwr.edu.pl*

Due to the bilamellar structure of the liposome with hydrophilic and hydrophobic endings, they can be used to transport various types of active substances into the skin. Hydrophilic molecules will be placed inside the membrane, while hydrophobic molecules can be placed outside it. The fact that liposomes are very compatible with the structure of cell membranes and are not toxic to the body makes them suitable structures to be used as drug carriers. In addition, the structure of the liposome protects unstable ingredients from degradation, for example under the influence of UV rays or enzymes.

The lipid DLPC, i.e., 1,2-dilauroyl-sn-glycero-3-phosphocholine dissolved in chloroform at a concentration of 1 mg/ml, was used to create the liposomes. The very process of liposome formation was based on pouring 100 microliters of 5% PVA polyvinyl alcohol solution, which had been prepared and stored in a safe place, on a cleaned glass slide (sonication 3x10 min in succession: acetone, isopropyl alcohol, distilled water). The slide then had to be heated so that the water in the solution evaporated leaving only a thin, even layer of PVA. Such a slide had to be cooled to room temperature and 7–10 microliters of the lipid solution in chloroform were applied (usually it was 9 to increase the amount obtained). The sample prepared in this way was placed in the desiccator for 2 hours or even for a whole day if a “wet” layer of chloroform was still visible. After this time, the step was to place a previously prepared sucrose solution with a concentration of 90 mM/dm<sup>3</sup> in the amount of 150 microlitres on the surface of the plate and wait an hour for the liposomes to form. After that time, they were transferred to the Eppendorf and flooded to the entire volume with a 90-mol glucose solution so that they could sink to the bottom, from where it would be easier to collect them for testing using a polarizing microscope, and there would be more liposomes.

After checking the samples with a polarizing microscope, it was possible to obtain an image with bright circular structures with a dark cross in the middle. This proves a positive result of the experiment and obtaining a lamellar liquid crystal structure. The presence of such a structure is a clear indication of the appearance of the phospholipid bilayer in the liquid crystal sample of which the liposomes are composed. Different amounts of these layers were obtained. Different forms of liposomes were observed. They were most likely to show single liposomes composed of one bilayer (LUV) and a cluster of liposomes built of one or more bilayers (MVV) could be also seen.

# CpkL as a potential participant of malonyl-CoA synthesis in *Streptomyces coelicolor* A3(2)

Julia Wątor<sup>1</sup>, Mateusz Wenecki<sup>1</sup>, Magdalena Kotowska<sup>1</sup>, Krzysztof Pawlik<sup>1</sup>

<sup>1</sup>Hirschfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Wrocław, Poland  
julkawator29@gmail.com

*Streptomyces* are Gram-positive, soil-dwelling filamentous bacteria that are able to produce a variety of secondary metabolites. Many of the produced compounds have antibiotic, antitumor or immunosuppressant activities important for human and veterinary medicine. One type of the metabolites are polyketides (PKs), that consist of a carbon skeleton, a polymer of acyl residues. PKs biosynthesis is carried out by a huge proteins – polyketide synthases (PKS), which use malonyl-CoA as a building blocks [1].

Precursors of polyketides synthesis come from the primary metabolism of the cell. Malonyl-CoA biosynthesis occurs through carboxylation of acetyl-CoA, which is catalyzed by acetyl-CoA carboxylase (ACCase). ACCase is a biotin-dependent enzyme, which is well described in the model strain *Streptomyces coelicolor* A3(2). There are two types of ACCases in *S. coelicolor* A3(2) that consist of subunits: I.  $\alpha$  and  $\beta$  subunits II.  $\alpha$ ,  $\beta$  and  $\epsilon$  subunits. Two of the subunits,  $\alpha$  (AccA) and  $\beta$  (AccB), have catalytic activities: biotin carboxylase (BC) and carboxyltransferase (CT), respectively. The third one,  $\epsilon$  subunit (AccE, SCO5536), acts as an adaptor protein, which strengthens ACCase catalytic activity. It is possible that all of the subunits have at least one homologous protein in *S. coelicolor* A3(2) [2, 3].

*S. coelicolor* A3(2) can produce a yellow polyketide – coelimycin (CPK). Genes necessary for its biosynthesis form a cluster, so far, not all of them are fully characterised.

Proposed study aims to elucidate the role of CpkL, putative  $\epsilon$ -like protein (33% identity to AccE), which hypothetically can be involved in synthesis of malonyl-CoA from acetyl-CoA by acting as a part of ACCase. The research covers generation of deletion and overexpression mutants, as well as utilizing bacterial two-hybrid system for protein-protein interaction screening.

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# Production of nanoparticles by fungi

Alicja Grzegorzek<sup>1</sup>, Piotr Kruszyński<sup>1</sup>, Beata Greb-Markiewicz<sup>2</sup>

<sup>1</sup> Students' Science Club "Bio-Top", Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże S. Wyspiańskiego 27, 50-370 Wrocław, Poland

<sup>2</sup> Laboratory of Biochemistry and Molecular Biology, Department of Biochemistry, Molecular Biology and Biotechnology, Faculty of Chemistry, Wrocław University of Science and Technology, Faculty of Chemistry, Wybrzeże S. Wyspiańskiego 27, 50-370 Wrocław, Poland  
E-mail: beata.greb-markiewicz@pwr.edu.pl

Nanoparticles (NPs) are the type of particle substances with at least one dimension less than 100 nm. At such scales, nanomaterials can add specific characteristics to their macro counterparts including electronic, optical, magnetic, mechanical, thermal or biological properties [1]. Some of interesting applications of nanoparticles are: Ti NPs in sunscreen, ZnO NPs in lithium-ion batteries and improving the mechanical properties and durability of concrete [1]. Typically, different chemical compounds (such as NaBH<sub>4</sub>) and methods, including UV radiation, aerosol technologies, laser ablation, ultrasonic fields, and photochemical reduction are used to create nanoparticles [2]. Depending on the type of nanomaterial and the production process, toxic compounds like metal oxides, as well as pollutants in the form of volatile organic substances can be produced and enter the natural environment affecting ecosystems and human health. To reduce costs and to preserve environment, new strategies based on the plant, bacterial and fungal systems as catalysts were developed, reducing application of various inorganic salts. Plant based approaches generally involve extracts from leaves or fruits, while bacterial and fungal systems involves various intracellular/extracellular compounds [2]. Fungal lysates, in comparison to bacterial, can produce selected nanoparticles using more differentiated enzymes leading to different sizes [3]. The use of fungi can be advantageous because of the simple cultivation conditions, and well-known pathways. Especially interesting application seems to be the use of the produced biomass of entomopathogenic fungi and their properties for extracellular biosynthesis of silver nanoparticles against insects to create bioinsecticides [4]. Future progress in the green synthesis of nanoparticles will not only result in broader spectrum of cheap and more biocompatible nanomaterials, but it will also reduce the use of toxic chemicals, leading to the reduced contamination of the environment.

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# From Nature For Nature: Supporting the Development of Stimulus-Responsive Ionogels for Agrochemistry

John Vincent Tumaneng<sup>1</sup>, Anna Jakubiak-Marcinkowska<sup>1</sup>, Joanna Feder-Kubis<sup>1</sup>

<sup>1</sup>Faculty of Chemistry

Wroclaw University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wroclaw

E-mail: 269604@student.pwr.edu.pl; tumanengjv@gmail.com

The growing resistance of microorganisms to known antiseptics has led to a strong industrial demand for new active substances, among which those with ionic character appear to be one of the most promising options. Additional immobilisation of such chemicals in a polymeric matrix is beneficial for their stability and effective transport of substances to the target location. In this seminal work on bioactive polymers, terpene-based ionic liquids and functionalized biopolymers were prepared and combined to create ionogels – ionic liquid gel materials that offer symbiosis between the dispersed ionic liquid phase and the solid continuous phase [1]. The preliminary investigation of select ionic liquids' sorption-desorption profiles show successful control over the release of the ionic liquid. In a system that more closely mimics the acidic nature of fertile soil, a faster release is observed. Such behavior is ideal for agrochemistry since release due to degradation can be neglected and reusability of the polymer is not undermined. Once the optimization of conventional polymer preparation is completed, the use of more recent additive manufacturing techniques like 3D printing can be explored to form green biotechnological ionogels that build functionality at every scale (Fig. 1).

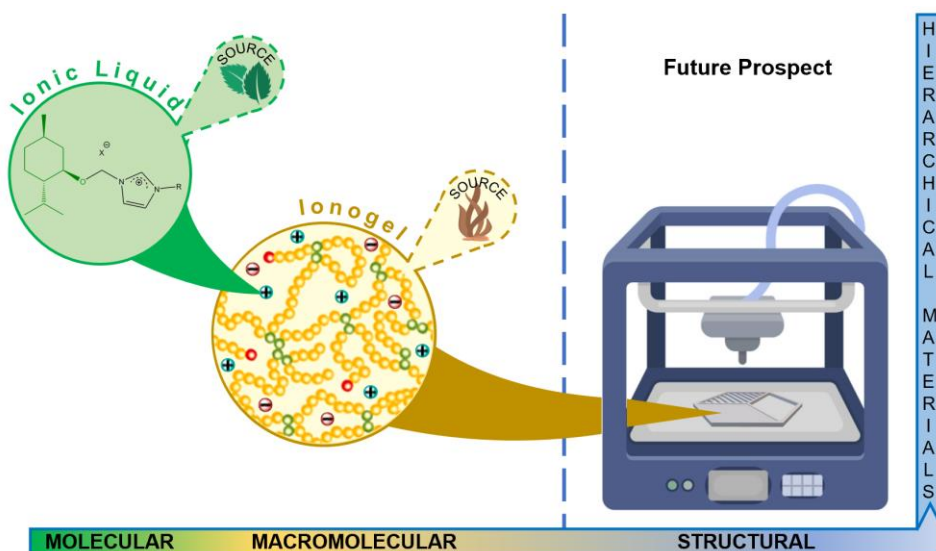


Figure 1. Illustration of the atom-to-bulk physicochemical functionality of green ionogels

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# Finite field method with harmonic potential

Tymotuesz Mrozek

Wroclaw University of Science and Technology

E-mail: [tymekmrozek97@gmail.com](mailto:tymekmrozek97@gmail.com)

The purpose of this work is to introduce a modification of the finite field method [1]. In the original method the energy of the molecule is calculated with a method of quantum chemistry for varying intensity of the electric field. Hamiltonian in these calculations is unlimited from below and so are the spectra of its eigenvalues. Proposed modification consists in replacing the homogenous electric field with the harmonic potential  $V(x) = 0.5k(x - X_0)^2 = b(x - X_0)^2$ . Two approaches were tested. One with double perturbed energy series and the second one that is using the dependence of appropriate coefficients upon  $X_0$ , that describe response of the system to the harmonic potential. Every computation was performed in aug-pc-2, aug-pc-3 and Hy-pol basis sets with MP2 and HF-SCF method. The properties of water, lithium hydride and the helium atom were calculated. Obtained values of dipole moment  $\mu$ , dipole polarizability  $\alpha$  and dipole hyperpolarizability  $\beta$  are close to the cited literature [2–4], which proves that the modification is indeed correct. However, there are several problems that appear in calculations mainly with numerical precision of the hyperpolarizability.

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# Cellulose nanocrystals in copolymeric composites with self-healing and piezoelectric properties

Diego M. Juela<sup>1,2\*</sup>, Talia Tene<sup>3</sup>, Jorge Fajardo<sup>2</sup>

<sup>1</sup> Chemical Nano-Engineering master's program, Wroclaw University of Science and Technology, Wroclaw 50-370, Poland

<sup>2</sup> Research Group in New Materials and Transformation Processes (GIMaT), Polytechnique Salesian University, Cuenca 010203, Ecuador

<sup>3</sup> PharMaterials Research Group, Private Technical University of Loja, Loja 110102, Ecuador

\* E-mail: [diego.juela\\_tb@outlook.com](mailto:diego.juela_tb@outlook.com)

The production of wearable microelectronics devices has made great advances in recent years for its use in prosthetics, health condition sensors, electronic skins, and human motion detectors, consequently increasing the demand for batteries. Piezoelectric nanogenerators (PENGs), which generate electricity when squeezed or twisted, are a more effective and sustainable power source for these portable devices, replacing the conventional batteries. This study reports a new PENG produced combining poly(vinyl alcohol-g-lactic acid) (PVA-g-LA) and cellulose nanocrystals (CNCs). We hypothesized that the integration of CNCs into the polymeric matrix could boost the piezoelectric response and mechanical properties. First, CNCs were isolated from bamboo fibers by acid hydrolysis and characterized by FTIR, XRD, TEM and AFM. In parallel, PVA-g-LA copolymers at several lactic acid (LA) concentrations (1.0 - 2.5 PVA/LA molar ratios) were prepared. <sup>1</sup>H-NM analysis detected the presence of methyl and methine protons in the copolymeric chains, confirming the grafting of LA onto PVA. Piezoelectric response was then measured in these four copolymers, where the voltage output increased with the LA concentration, reaching the highest value of 24.8 V with a 2.0 PVA/LA molar ratio (copolymer PVA-g-LA-2.0). Afterwards, the composites in the form of films were produced by drop casting mixing the PVA-g-LA-2.0 and CNCs at different ratios (2–14 wt.%). The introduction of 14 wt% CNCs improved the piezoelectric response by 75%, the main justification is their polar hydroxyl groups that form asymmetric dipoles and endows the composite with electron donating capacity. An addition of 10 wt.% CNCs improved the tensile strength of the PVA-g-LA-2.0 film by 65%. Finally, the presence of PVA provided the composite with self-healing activity; the film was self-healed within 1 h when wetted with deionized water, and the strain at break slightly decreased by only 11 %. This stretchable, self-healable and piezoelectric film shows promising properties for electronic skins and motion sensors.

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