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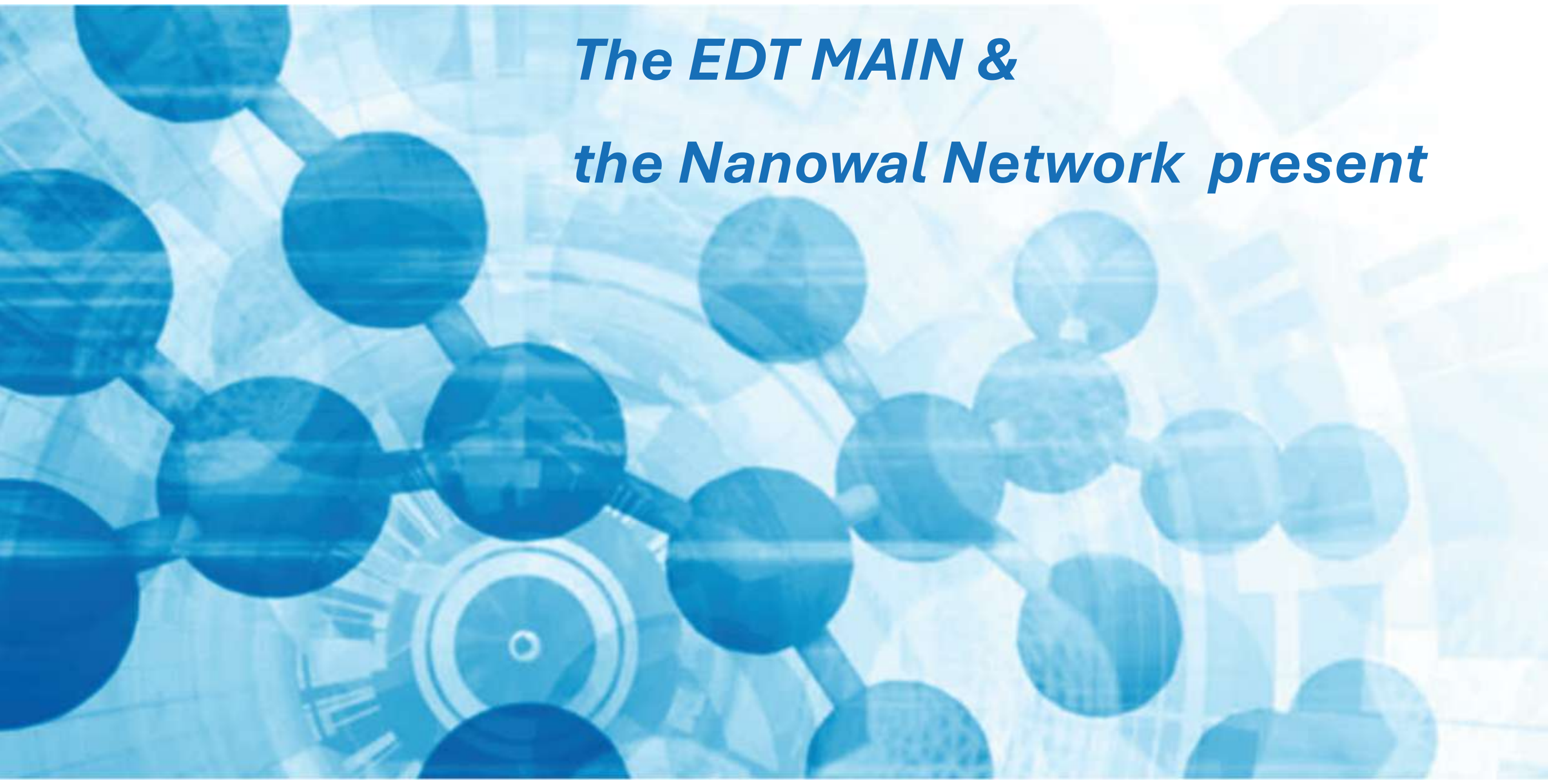

The EDT MAIN &
the Nanowal Network present

the 2024 PhD Scientific Day

Louvain-la-Neuve, October 31, 2024

Program & Abstracts

UCLouvain

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Program of the day

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12:05	**C2** - **Omaya Habli** (UNamur): *Numerical simulation of an inverse opal photonic crystal using the RCWA method*	p. 6
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14:00	**C3** - **Oriane de Leuze** (UCLouvain): *Charge transport in few-layer 2D crystals at micro and nanoscale: the case of* Ti_3C_2Tx *MXenes*	p. 7
14;20	**K3** - Prof. **Jean-Pierre Raskin** (UCLouvain), ***Information Communication Technology for the best and the worst***	p. 4
15:05	**C4** - **Eugenie Fomekong Louta** (ULiège): *Exploitation of Canarium Schweinfurthii core shells as carbon source for the case hardening of steels*	p. 8
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16:30	**C6** - **Victor Lepeintre** (ULB): *Calixarene-Coated Gold Nanorods as Robust Photothermal Agents*	p. 10
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Keynote talk 1

How will chemistry shape the materials of the future?

A personal perspective

Prof. Philippe Dubois
University of Mons - Materia Nova asbl, Place du Parc 23
B-7000 MONS (Be)
philippe.dubois@umons.ac.be

The ecological transition is a major challenge that society is facing. It requires profound changes in the way we produce, consume and live. Chemistry has an important role to play in this transition, helping to develop innovative solutions to environmental challenges.

The concrete contributions of chemistry include i) the production of new sources of energy, including storage technologies; ii) the development of sanitation processes to treat waste and wastewater; iii) the key role of pharmaceutical and medicinal chemistry, and iv) the production of sustainable materials such as recycled, intelligent/self-repairing, (super)conductive, catalytic and bio-sourced materials, etc.

To achieve this, scientific interdisciplinarity is essential, and the aim of this contribution is to illustrate this 'cross-fertilisation' and the involvement of chemistry in the production of new biosourced (nano)materials, i.e. materials derived from renewable resources. Not only are these materials, polymers and (nano)composites, derived from biomass, but they also have the property of controllable and even programmable biodegradation. To achieve this, disciplines as different and complementary as synthetic and catalytic chemistry, process engineering, nanotechnology, surface physics, biology and enzymology will be approached and combined.

Prof. Philippe Dubois is Rector of University of Mons, and 1st President of the European University Alliance EUNICE. As full professor he set up the Center of Innovation and Research in Materials & Polymers CIRMAP. His expertise covers organic chemistry; macromolecular chemistry; catalysis in polymer materials; and (reactive) processing of (nano)composites and nanohybrid materials, including bioplastics. He is President and scientific Director of Materia Nova Research Center ASBL in Mons. He is President/co-founder of GATE2 S.A., a spin-off company of UMONS. He has published 800+ peer-reviewed scientific articles, 11 books (H-index = 120, overall citations= 65,500+) and is the inventor of 76 patents. Ph. Dubois is invited professor in several Universities in Europe, US and China. He is elected member of the Royal Academy of Belgium (Class of sciences) and the European Academy of sciences EurASc (Engineering Division). In 2024, he became Doctor Honoris Causa of University of Montpellier, France.

Keynote talk 2

Supported transition metal catalyst preparation: Uses in energy-related reactions

Prof. Sébastien Royer
Université du Littoral Côte d'Opale, France
sebastien.royer@univ-lille.fr

The talk proposed introduces the preparation of supported catalysts, a major class of heterogeneous catalysts commonly encountered in the industry. Supported catalysts are composed of a porous support (several hundreds of square meter per gram of material), on which active elements are stabilized at its surface in the form of fine particles. Reaction thereafter occurs at the surface of these particles. Then, the dispersion of the active phase (that is the particle size of the active phase), and its accessibility to the reactants, conditions the activity of the catalyst and then the conversion/selectivities achieved. During the presentation, we will introduce some classical preparation procedures (wet impregnation, incipient wetness impregnation) and define the key properties of supported catalysts such obtained. Thereafter, alternative procedures of preparation (deposition precipitation, melt infiltration) will be presented and the properties obtained discussed. Finally, catalytic results obtained with supported transition metal for ammonia synthesis, CO2 methanation, CO2 reforming, biomass HDO will be presented, and the role of dispersion during reaction highlighted.

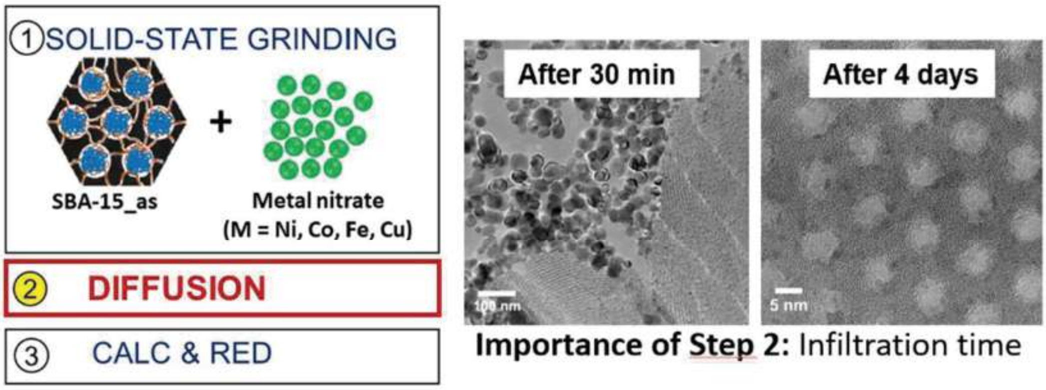

Illustration of melt infiltration preparation procedure

Ciotonea et al. Catal. Sci. Technol. 7 (2017) 5448; Chen et al. Catalysis Today 334 (2019) 48

Sebastien Royer is professor at the Université du Littoral Côte d'Opale, France, since 2024, after being professor at Université de Lille in the UCCS Laboratory (2015-2024). He leads a research group working on the synthesis of heterogeneous catalysts, and develops researches in the fields of porous materials (mesostructured solids, zeolites, MOFs, carbons), oxides and mixed oxides, supported nanoparticles syntheses, with applications in green chemistry, energy and environment. The group also study small catalyst scale-up and shaping in view of industrial application. For more information on the recent activities:

https://uccs.univ-lille.fr/index.php/en/heterogeneous-catalysis/matcat

Keynote talk 3

Information Communication Technology for the best and the worst

Prof. Jean-Pierre Raskin
ICTEAM Institute, Université catholique de Louvain, 1348 Louvain-la-Neuve
Jean-pierre.raskin@uclouvain.be

Electronics is increasingly introduced in our society and ICT contributes extensively to this trend. Although this could enable positive effects both on our society and our environment through optimization and monitoring, the massive deployment of ICT comes together with an undeniable environmental burden which is often overlooked.

In the talk, we will begin by questioning the vision of progress shared by our societies. We will lift the veil on the invisibles of the digital world. It shows that the exponential trends such as Moore’s law or Cooper’s law will very unlikely lead to an absolute decrease of greenhouse gas emission and a reduction of our appetite for a wide variety of minerals if sobriety is not considered together with efficiency improvements.

Faced with the societal challenges of today and tomorrow, teaching and disciplinary research must reinvent themselves. Based on the assessed impacts of ICT, we will question the merits of certain technological choices made in the name of the transition. A holistic, transdisciplinary and pragmatic approach must be put in place in order to think, design and innovate within the constraints of our ecosystem limits. Concrete examples of current research will be shared, such as a critical look at the deployment of connected objects, the eco-design of sensors, a reflection on the pursuit of Moore's law and its environmental consequences, and the strategies to minimize e-waste.

Prof. Jean-Pierre Raskin received the M.S. and Ph.D. degrees in applied sciences from Université catholique de Louvain (UCLouvain), Louvain-la-Neuve, Belgium, in 1994 and 1997, respectively. In 1998, he joined the EECS Department of The University of Michigan, Ann Arbor, USA, for a post-doc of two years. In 2000, he joined the Microwave Laboratory of UCLouvain, Louvain-la-Neuve, Belgium, as Associate Professor, and he has been a Full Professor since 2007. His research interests are the modeling, wideband characterization and fabrication of advanced SOI MOSFETs as well as micro and nanofabrication of MEMS / NEMS sensors and actuators, including the extraction of intrinsic material properties at nanometer scale. He has been IEEE Fellow since 2014. He received the Médaille BLONDEL 2015, the SOI Consortium Award 2016, the European SEMI Award 2017, the Médaille AMPERE 2019, the Georges Vanderlinden Prize 2021 and the IET Achievement Medal in Electronics 2022, in recognition in his vision and pioneering work for RF SOI. He has been managing a Chair in eco-innovation at CEA-Leti since January 2024.

SOLID-STATE PIEZOIONIC SENSORS BASED ON IONIC LIQUID MONOMERS

J. Guerrero[1], V. Shevtsov[2], J.-M. Raquez[1], A. Shaplov[2], J. Odent[1]

.1) Laboratory of Polymeric and Composite Materials (LPCM), Center of Innovation and Research in Materials and Polymers (CIRMAP), University of Mons (UMONS), Place du Parc 20, Mons, 7000
2) Luxembourg Institute of Science and Technology, L-4362 Esch-sur-Alzette, 5 rue Bommel, ZAE Robert Steichen, LIST Luxembourg, 4940

Email: JuanAlejandro.GUERREROTERAN@umons.ac.be

Piezoionic sensors are a novel type of stress sensor that has brought interest in the last few years. The piezoionic effect is based on an ion gradient generated by a pressure applied to an ionically conductive gel. The latter could be a hydrogel with electrolytes (salt), ionogels (hydrogel containing an ionic liquid), or polyelectrolytes with fixed macroions and mobile counterions [1-3]. One of the major drawbacks of most current hydrogel piezoionic sensors is the presence of water. This limits their stability over time due to evaporation of water [1]. On top of that, systems such as ionogels or hydrogels swollen with an aqueous electrolyte solution consists of two mobile ions [1]. Consequently, this type of piezoionic sensor exhibit a decay of potential when the mechanical stimulus applied is steady due to a re-equilibrium in the material [1,3]. Therefore, ionic liquid monomers (ILM) are a promising candidate to develop solid-state piezoionic sensor that can discriminate transient and steady mechanical stimulus and are stable at environmental conditions [4]. This work proposes to develop solid-state piezoionic sensor based on crosslinked Polyionic liquid copolymerized with two different neutral monomers. Two types of ILM cationic and anionic type were studied, as well as, two types of neutral monomers with different length of pendant chain, in order to enhance the piezoionic response.

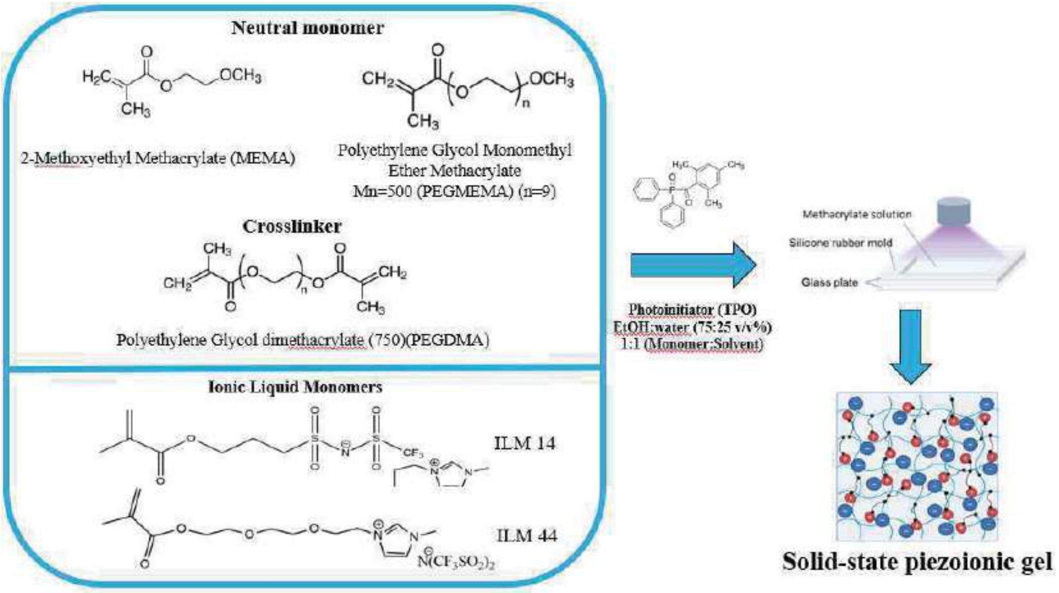

Figure 1. Illustrative Scheme of photopolymerization of solid-state piezoionic sensor based on ionic liquid monomer (ILM)

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Numerical simulation of an inverse opal photonic crystal using the RCWA method

O. Habli, O. Deparis
Laboratoire de Physique de Solide
University of Namur, 5000, Belgium
Email of Omayma.habli@unamur.be

Photonic crystals (PCs) have been extensively investigated for light manipulation. Among the vast diversity of photonic crystals [1], inverse opal (IO) photonic structures possess numerous advantages due to their promising optical and structural properties in addition to their relative ease of design and synthesis [2-3].

In this work, we have studied by numerical simulation the optical response of an inverse opal photonic crystal. It was calculated and illustrated using the rigorous coupled wave analysis (RCWA) method.

Indeed, we have varied different parameters such as the plane wave number, the incidence angle, pore diameter, etc.

The results show a shift in the reflectance spectrum at the electronic absorption edge of the used material which makes the studied IO structure suitable for use in photocatalysis applications.

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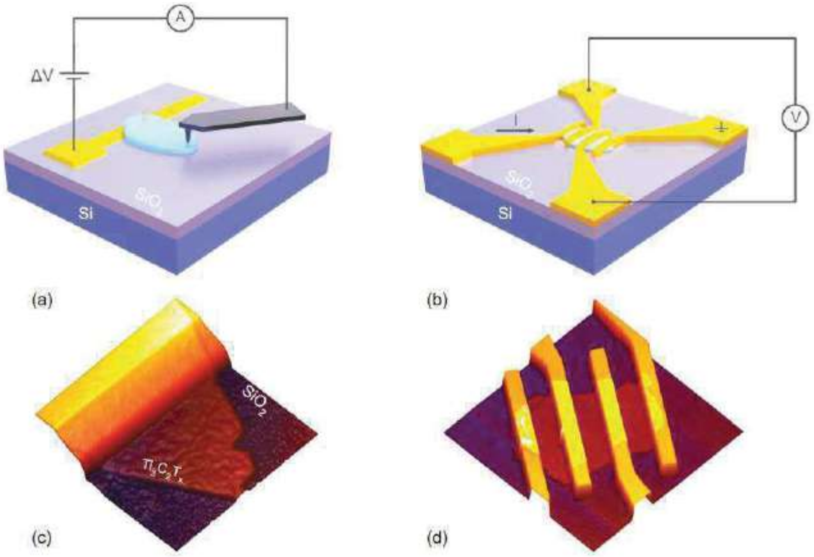
Charge transport in few-layer 2D crystals at micro and nanoscale: the case of $Ti_3C_2T_x$ MXenes

O. de Leuze[1] , F. Massa[1], H. Pazniak[2], T. Ouisse[2], B. Nysten[1], S. Hermans[1], B. Hackens[1]
[1]IMCN, Université catholique de Louvain, Louvain-La-Neuve, Belgique
[2]LMGP, Université Grenoble-Alpes, Grenoble, France
oriane.deleuze@uclouvain.be

Over the past few years, 2D materials have garnered significant interest in various fields such as electronics, energy storage, and catalysis. Among them, MXenes – 2D transition metal carbides and nitrides – offer tunable electronic properties and surface engineering possibilities, making them prime candidates in sensing and optoelectronics, among others [1][2]. In the vast majority of applications using MXenes, devices are fabricated with randomly stacked monocrystalline flakes of different thicknesses, forming a thin film. To date, electronic transport in MXenes has been mostly studied in such films, but it becomes clear that intra-flake and inter-flake charge transport should be studied separately [3]. In this context, the present work investigates charge transport in individual flakes of $Ti_3C_2T_x$, the most studied MXene. A common practice to perform electrical measurements on 2D individual flakes is to drive current and measure voltage drop across lithographically-patterned top metallic contacts, as illustrated in Fig. 1 (b) and (d). While this technique is reliable for extracting quantitative resistivity values averaged at flake-scale, it does not allow advanced characterization at the nanoscale. This is why we also perform conductive atomic force microscopy (C-AFM) on individual flakes, as illustrated in Fig. 1 (a) and (c), showing the topography of a flake overlapping a metallic electrode and an insulating substrate. In C-AFM, a bias is applied between the tip and the sample, and the current is measured as the tip scans the sample surface, in contact mode. Hence, a flake conductivity map is obtained along with the topography. The specific configuration used here makes it possible to extract both in-plane and out-of-plane resistivity components and therefore the resistivity anisotropy of $Ti_3C_2T_x$. The challenges of bringing together C-AFM and four-contact measurements to study charge transport in few-layer flakes will be discussed.



(a) Illustration of the C-AFM measurement on an individual flake deposited on an Au electrode, on a Si/SiO_2 substrate. (b) Illustration of a conventional four-contact measurement setup. (c) 3D view of the AFM topography of a $Ti_3C_2T_x$ flake deposited partially on an electrode, obtained in tapping mode. (d) 3D view of the AFM topography of patterned contacts on a $Ti_3C_2T_x$ flake, obtained in tapping mode.

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Exploitation of *Canarium Schweinfurthii* core shells as carbon source for the case hardening of steels

Eugenie Louta F., Jérôme Tchuindjang T., Dieunedort Ndapeu and Anne Mertens
Aerospace and Mechanic department (Metallic Materials Science), University of Liege, 4000 Liege
e.louta@doct.uliege.be

The objective of solid carburizing thermochemical treatment is to enrich with carbon the surface layer of the substrate subjected to this treatment. This enrichment improves the mechanical (hardness), tribological (wear) and microstructural properties of the treated substrate. The solid carburizer is a carbon material that can release its carbon to diffuse into steel at high temperature, with or without a catalyst. In this study, we have made solid carburizers from vegetable shells (bio-carburizers) from Cameroon. These shells were first collected, crushed, washed, dried, ground and sieved at a grain size of 300/500 µm and then carbonized at 450°C for periods of 10 to 60 minutes to obtain bio-carburizers. These bio-carburizers were then used for the case-hardening of cylindrical samples of two different substrates (C35 and 42CrMo4 steel alloys) at 950°C for 3 hours. The samples were cut radially and transversally, embedded in resin, polished and etched with nitric acid. The microstructural analysis was done by optical microscopy. The measured Vickers hardness and the hardness profile were obtained using a FALCON 500G204 durometer. Vickers hardness measurements show an increase in hardness associated with the increase in carbon content in the surface layer. The hardness profile allows to show a cemented thickness of up to 2 mm depending on the bio-cement used. The microstructure observed by optical microscopy reveals a variation in the present phases depending on the process for bio-carburizers production.

Investigation of the Au nanorods synthesis parameters tunability by statistical methods

A. Engel[1,2]*, C. Rasse,[3] F. Drault[1,2], S. Demoustier-Champagne[2], S. Hermans[1]
[1]IMCN (MOST division), UCLouvain, 1 Place Louis Pasteur, B-1348 Louvain-la- Neuve, Belgium.
[2]IMCN (BSMA division), UCLouvain, 1 Place Louis Pasteur, B-1348, Louvain-la-Neuve, Belgium.
[3]SMCS, UCLouvain, Voie du Roman Pays, B-1348, Louvain-la-Neuve, Belgium.
**antonin.engel@uclouvain.be*

Gold nanorods (NRs) are notable for their localized surface plasmon resonance (LSPR) properties, which are sensitive to their aspect ratio (AR), i.e. the ratio between the longitudinal and transversal dimensions. More precisely, their second plasmonic peak position (λ_2, linked to the longitudinal dimension) is linearly proportional to their AR, making them highly applicable in various fields such as photocatalysis, photovoltaics, biosensing, and medical imaging [1].

The seed-mediated synthesis method, commonly employed for gold NRs, traditionally involves the use of ascorbic acid as a mild reducing agent, leading to relatively poor yield not exceeding ~15% [1]. Here, hydroquinone (HQ) was used as alternative mild reducing agent to achieve nearly quantitative yield, surpassing the conventional use of ascorbic acid. In this study, the high-yield synthesis of gold nanorods was investigated, focusing on the tunability and underlying mechanisms of the process using a design of experiment (DOE) approach.

The influence of various synthesis parameters, including the concentrations of seed solution, silver nitrate, cetyltrimethylammonium bromide (CTAB), HQ, and gold precursor, on the second plasmonic peak position (λ_2) of gold NRs obtained was studied. A customized DOE was developed to evaluate these parameters and their interactions, and the impact on the LSPR wavelength (λ_2) linked to the anisotropic growth of the rod. The study revealed significant quadratic effects and interactions, particularly involving CTAB and silver nitrate, pointing towards the formation of a complex between these two components that drives anisotropic growth (**Figure 1**A-E).

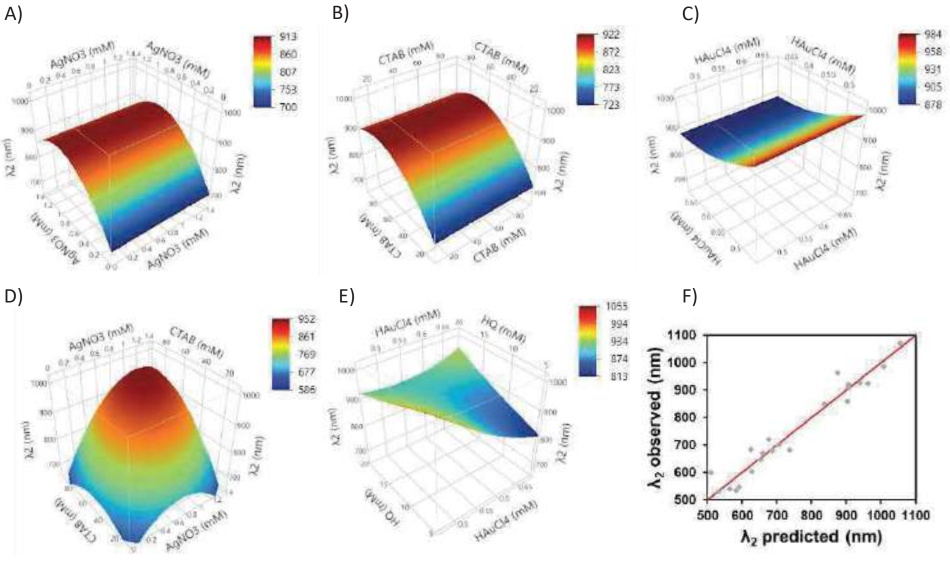

Figure 1. Prediction profilers of λ_2. position as function of (A) $AgNO_3$, (B) CTAB, (C) $HAuCl_4$, (D) $AgNO_3$ * CTAB and (E) $HAuCl_4$ * HQ concentrations. (F) Observed by predicted plot for the λ_2 position.

The statistical model developed through DOE successfully predicts the plasmonic properties of the synthesized gold NRs with well-controlled AR (**Figure 1**F), validated by its accuracy in forecasting outcomes for conditions not explicitly tested. This comprehensive understanding of the synthesis parameters and their interactions allows to optimize the production of gold NRs with desired properties, tuned as function of the desired application.

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Calixarene-Coated Gold Nanorods as Robust Photothermal Agents

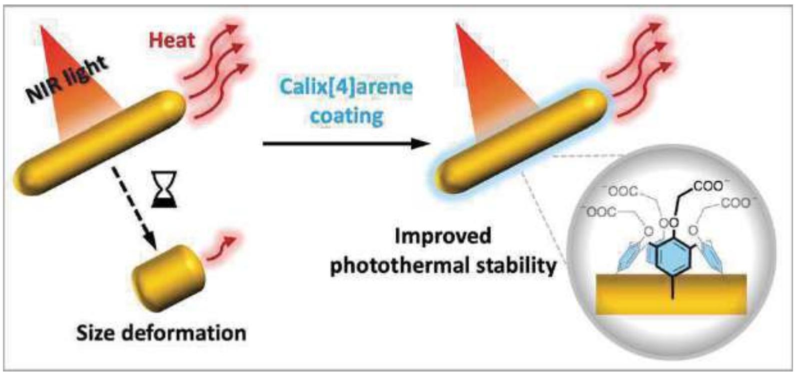
V. Lepeintre[1,2], F. Camerel[3], C. Lagrost[3,4], M. Retout[1], G. Bruylants[1], I. Jabin[2]

[1] Engineering of Molecular NanoSystems (EMNS), Ecole Polytechnique de Bruxelles, Université libre de Bruxelles (ULB), avenue F. D. Roosevelt 50, CP165/64, B-1050, Brussels, Belgium
[2] Laboratoire de Chimie Organique (LCO), Université libre de Bruxelles (ULB), avenue F. D. Roosevelt 50, CP160/06, B-1050, Brussels, Belgium
[3] Institut des Sciences Chimiques de Rennes (ISCR) – CNRS UMR 6226, Université de Rennes, F-35000 Rennes, France
[4] ScanMAT – CNRS UAR 2025, Université de Rennes, F-35000 Rennes, France

Contact: victor.lepeintre@ulb.be

Gold nanorods (AuNRs) have emerged as highly promising materials for advancing biomedical *in vivo* applications.[1] They exhibit two distinctive Localized Surface Plasmon Resonance (LSPR) bands: transverse and longitudinal. The maximum absorption wavelength of the latter can be tuned by altering the aspect ratio of the rods. For high aspect ratios, it falls within the near-infrared (NIR) region where minimal absorption by endogenous molecules enhances light penetration into tissues.[1]

Photothermal therapy (PTT) is a promising non-invasive cancer treatment strategy exploiting the conversion of light to heat by photothermal agents for thermal ablation of cancer cells.[2] AuNRs possess several qualities that make them excellent photothermal agents: high biocompatibility, long circulation times, ease in functionalization, and intense optical extinction coefficients in the NIR region.[2] However, one limitation is their anisotropic structure that is prone to deformation under laser irradiation, leading to changes in their optical and photothermal properties over time.[3] To overcome this challenge, an efficient strategy involving the use of calix[4]arene-tetradiazonium salts for stabilizing AuNRs has been implemented. These molecular platforms are capable of irreversible grafting onto surfaces through the reduction of their diazonium groups, thereby resulting in the formation of extremely robust organic monolayers.[4–6] This innovative coating strategy not only ensures enduring stability but also facilitates conjugation of AuNRs. This work showcases the superiority of these fortified AuNRs over conventional counterparts, notably exhibiting exceptional resilience even under sustained laser exposure in the context of PTT.[7] By bolstering the stability and reliability of AuNRs in PTT, our approach holds the potential to drive significant advancements in the field.



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Poster presentations

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A Compendium of Methodically Determined Ground- and Excited-State Properties of Homoleptic Osmium(II)Photosensitizers

Felix Glaser,[a] Simon De Kreijger,[a] **Katerina Achilleos,[a]** Lakshmi Narayan Satheesh,[a] Alexia Ripak,[a] Noémie Chantry,[a] Céline Bourgois,[a] Sophie Quiquempoix,[a] Joffrey Scriven,[a] Julien Rubens,[a] Milan Vander Wee-Léonard,[a] Martin Daenen,[a] Martin Gillard,[a] Benjamin Elias[a] and Ludovic Troian-Gautier[a],[b]*

Institut de la Matière Condensée et des Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis (MOST), Université catholique de Louvain (UCLouvain),

Place Louis Pasteur 1 box L4.01.02, B-1348 Louvain-la-Neuve, Belgium

Wel Research Institute, Avenue Pasteur 6, 1300 Wavre, Belgium

In here, we report on the synthesis of 16 osmium (II) homoleptic photosensitizers bearing substituted 2,2’- bipyridines, 1,10- phenanthrolines and diaza ligands, in overall high yields and straight forward purification processes. This investigation reports a widespread dataset of their ground and excited state properties, including UV-Visible Absorption (UV-Vis), Time Resolved and Steady State Photoluminescence, variable temperature measurements using Time- Correlates Single Photon Counting technique and Cyclic Voltammetry. The Osmium (II) complexes absorbed intensely in the blue range of the solar spectrum and their absorption further extended in the red region. Osmium (II) complexes exhibited excited state lifetime that ranged from 5 ns to 470 ns and photoluminescence quantum yield that spanned 0.00017-0.0551, in agreement with the energy gap law. Variable temperature measurements highlighted that these Os(II) photosensitizers do not deactivate via the metal-centered (MC) state but rather via a 4th 3MLCT. This observation would lead to increased photostability of these Os(II) photosensitizers, leading to some fascinating routes for various envisioned future applications such as photoredox catalysis.

A Co(II) Dinuclear complex as a Robust Inhibitor of *Fusarium oxysporum* f. sp. *Albedinis*

Yousra Bahjou[1,2], Smaail Radi [*,1], Yann Garcia[*,2]

[1] LCAE, Department of Chemistry, Faculty of Science, University Mohamed I , P.O. Box 524, Oujda 60 000, Morocco.
[2] Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis (IMCN/MOST), Université catholique de Louvain, Belgium.

E-mail: yousra.bahjou@uclouvain.be

C-N junctional tetrazole and bi-pyrazole motif ligands can easily form various types of coordination networks (CCs/CPs), which have piqued the interest of researchers due to their diverse architectures and topologies, as well as their broad potential applications in fields such as molecular magnetism, medicinal chemistry, photoluminescence, and catalysis [1,2]. A series of new tetrazole and C,N-bipyrazole ligands, 2-(3,5,5'-trimethyl-1'H-[1,3'-bipyrazol]-1'- yl)acetonitrile (**L1**) and 1'-((1H-tetrazol-5-yl)methyl)-3,5,5'-trimethyl-1'H-1,3'-bipyrazole (**HL2**), were prepared and identified by different spectroscopic methods, including ^{1}H-NMR, ^{13}C-NMR, FT-IR and HRMS. The reaction of the two new ligands (**L1**) and (**L2**) with several metals, Ni (II), Cu (II) , Co (II) and Cd (II) leads to the formation of a new group of mononuclear coordination complexes, namely: [Ni(**L1**)$_3$](ClO$_4$)$_2$ (**1**), [Cd(**L1**)$_2$Cl$_2$] (**2**), [Cu(**HL2**)(**L2**)]ClO$_4$ (**3**), [Cu(**L2**)$_2$] (**4**) and a dinuclear complex [Co$_2$(**HL2**)(**L2**)Cl$_3$] (**5**). These different coordination complexes were characterized by single crystal X-ray diffraction and show completely different architectural structures due to the nature of the metal ion coordination and the structural features of the organic ligands as well as the effect of the counter anion. These compounds demonstrate noticeable bacteriostatic activity against both Gram(+) and Gram (–) bacteria, as well as antifungal properties against a range of fungi. Particularly impressive is the remarkable 97% inhibition achieved by **5** at a concentration of only 81.1 μmol/L against *Fusarium oxysporum* f. sp. *albedinis*, the causing agent of Bayoud disease in palm trees [3].

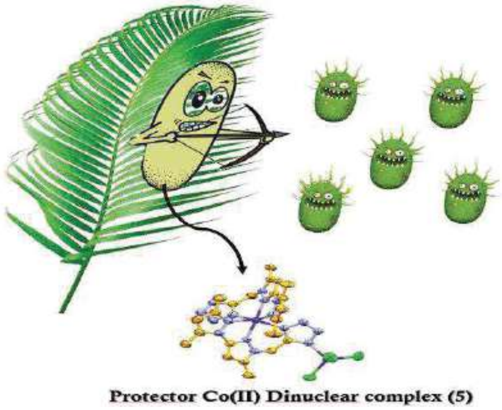

Figure 1 : Graphical abstract

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Development and characterization of 3D photoactive ZnO nanotubes membranes.

L. Barremaecker[1,2], S. Demoustier-Champagne[2], S. Hermans[1]
[1]*IMCN (MOST division), UCLouvain, 1 Place Louis Pasteur, B-1348, Louvain-la-Neuve, Belgium.*
[2]*IMCN (BSMA division), UCLouvain, 1 Place Louis Paster, B-1348, Louvain-la-Neuve, Belgium.*
lauraleen.barremaecker@uclouvain.be

Developing zinc oxide (ZnO) nanostructures from one-dimensional (1D) to three-dimensional (3D) nanotube (NT) networks is appealing as it could be useful for several applications, such as heterogeneous catalysis involving flow chemistry and continuous processes. ZnO is widely recognized as a photocatalyst of choice and can be used for water depollution without needing to be doped or functionalized.[1] A key benefit of the proposed nanotube synthesis method resides in its ability to allow precise control of nanotube dimensions, through the selection of template pores, tube arrangement (1D or 3D) and wall thickness.[2]

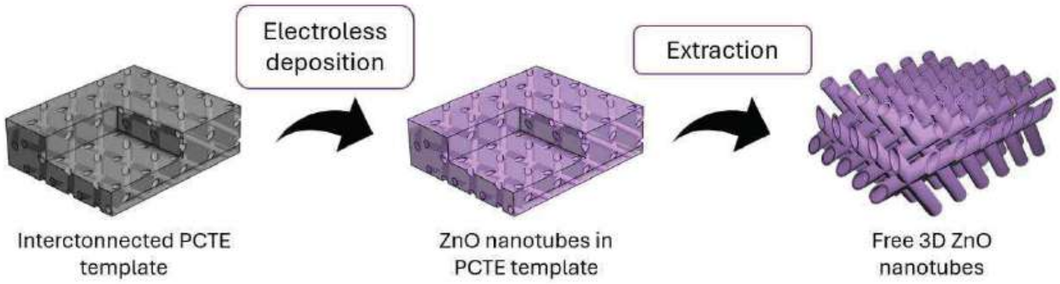

***Figure 1**: Schematic representation of the production of free 3D ZnO NTs using interconnected PTCE membrane.*

To this aim, polycarbonate track-etched (PCTE) membranes (from it4ip) with an interconnected cylindrical nanopores system have been used as template[3]. The current synthesis of 3D ZnO NTs (Figure 1) is an adaptation of a method from the literature[4]. Initially used for the deposition of ZnO on flax fibers, this approach has been optimized to suit a PCTE template with interconnected pores, enabling the formation of ZnO NTs. The synthesis consists in an electroless deposition followed by the removal of the template. The obtained materials were characterized by multiple techniques such as Scanning Electron Microscopy (SEM) (Figure 2), X-Ray Diffraction (XRD), Diffuse Reflectance UV-vis Spectroscopy (DRUS) and X-ray Photoelectron Spectroscopy (XPS) at each step of their elaboration and key parameters to control zinc oxide deposition were identified. The successful formation of interconnected nanotubes membranes composed of the desired photoactive phase was confirmed.

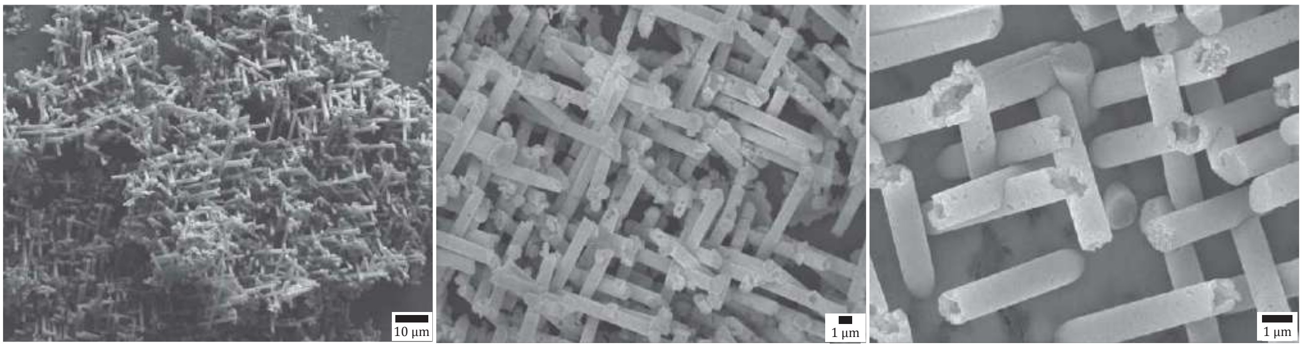

***Figure 2:** SEM images of ZnO 3D-NTs formed by electroless deposition.*

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1D Piezoelectric Zinc Oxide: Materials Optimization and Multi-scale Characterizations

Imen Benkhaled[a,b], Pierre Nickmilder[a], Denis Remiens[b], Elhadj Dogheche[b], Philippe Leclère[a]
[a] Laboratory for Physics of Nanomaterials and Energy (LPNE)
Research Institute in Materials Science and Engineering
University of Mons (UMONS), B-7000 Mons, Belgium.
[b]Université Polytechnique Hauts de France (UPHF)
IEMN UMR CNRS 8520 (IEMN), F – 59300 Valenciennes, France.

Email: Imen.Benkhaled@umons.ac.be

For several decades, Zinc oxide (ZnO) has been one of the most promising lead-free piezoelectric materials known for its piezoelectric properties for energy harvesting. This green material can be a substitute for materials containing toxic elements such as lead.

One-dimensional (1D) ZnO nanostructures, such as nanowires (NWs), have been widely studied by many teams around the world in recent years, as they can be synthesized using a variety of methods, including hydrothermal synthesis. This method has the advantage of having a low carbon footprint, is more environmentally friendly as it is realized at low temperature (<100°C) and it is simple and inexpensive.

In this research activity, the ultimate aim is to manufacture materials on several scales, namely thin films and ZnO NWs with a strong crystal structure and vertically oriented microstructure. We have studied the contribution of ZnO seed layer, deposited by sputtering, on the growth of NWs.

To optimize the seed layer required for vertical nanowire growth, several parameters were studied, including the Argon/O_2 ratio.

The resulting seed layers and NWs were studied by environmental Scanning Electron Microscopy (eSEM), X-ray diffraction (XRD) and Atomic Force Microscopy (AFM). The eSEM analysis shows the columnar structure by the section and the grain structure by the surface of ZnO seed layers as well as the hexagonal structure of the NWs . The topography of ZnO seed layers and NWs was observed by AFM.

The electrical performance of the resulting structure was also studied: The I-V curves show non-linear electrical characteristics, confirming the formation of Schottky contacts. The piezoelectric coefficient d33 was also studied.

In fine, a ferroelectric behavior observed for ZnO, known as a non-ferroelectric material, was studied by ss-PFM (switching spectroscopy Piezoresponse Force Microscopy) and cKPFM (contact mode Kelvin Probe Force Microscopy) illustrating the great attention to pay to the data acquisition avoiding measurement artifacts and leading to misinterpretation of the materials properties.

Photoinduced electron transfer processes at metal oxide interfaces

C. Bourgois,[a] B. Elias,[a] L. Troian-Gautier[a], [b]

[a] Institut de la Matière Condensée et des Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis (MOST), Université catholique de Louvain (UCLouvain),Place Louis Pasteur 1 box L4.01.02, B-1348 Louvain-la-Neuve, Belgium

[b] Wel Research Institute,Avenue Pasteur 6, 1300 Wavre, Belgium

Photocatalytic energy conversion has long been proposed as a sustainable alternative to fossil fuels. The breakthrough of Dye-Sensitized Solar Cells (DSSC) in this domain, evolving into **Dye-Sensitized Photoelectrochemical Cells (DSPEC)**, which integrate photocurrent generation with chemical transformations as for example hydrogen production (Figure 1-a) represent real solutions.[1] In this project, we synthesized heteroleptic Ruthenium(II) terpyridine complexes (Figure 1-b) for use as photosensitizers in the DSPEC anodic compartment. These complexes were anchored onto metal oxide surfaces, including TiO_2, SnO_2, and nanoITO, via phosphonic acid groups, and their photophysical properties were characterized.

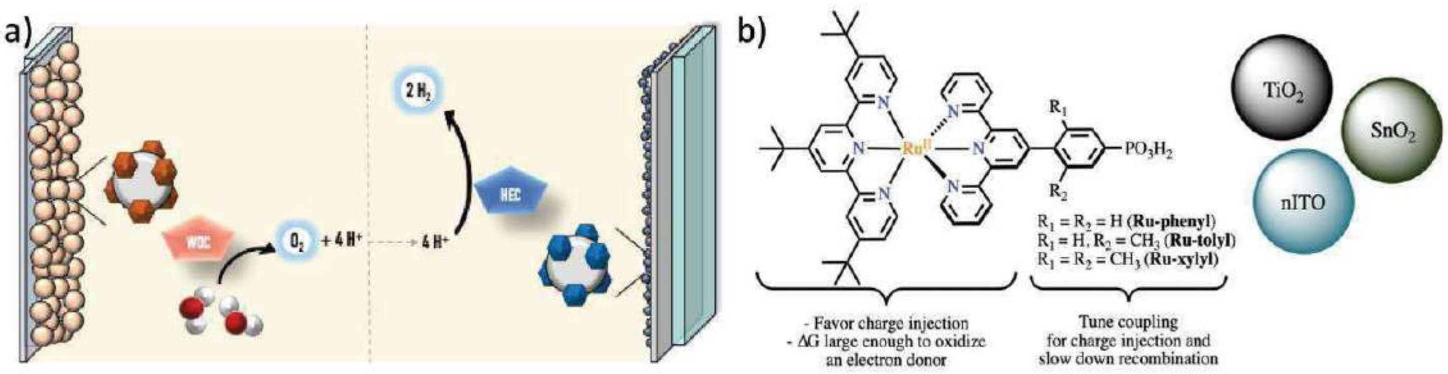

Figure 1. a) Simplified view of the DSPEC components and the hydrogen production reaction. b) Structure of ruthenium terpyridines with a phenyl, tolyl or xylyl bridge. On the right are represented the types of metal oxides used as semiconductors.

A key focus was the impact of different molecular bridges (phenyl, tolyl, and xylyl) separating the metal center from the semiconductor on the electron transfer dynamics. Time-resolved UV-Visible spectroscopy revealed that electron transfer rates and charge recombination processes are heavily influenced by the nature of these bridges. Our findings demonstrated that recombination rates are slower with the tolyl and xylyl bridges compared to phenyl, suggesting that bridge structure plays a crucial role in modulating electron coupling, which is in agreement with results obtained in a similar study.[2] Additionally, we explored the regeneration of the oxidized photosensitizer using tri-p-tolylamine (TTA) as an electron donor, further extending the lifetimes of charge-separated states. The results confirm the viability of these photosensitizers for improving DSPEC performance by slowing recombination and increasing charge separation efficiency.

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Impact of the conformers and of the solvent on the two-photon absorption of highly conjugated systems

Robin Crits,* Marilu Grace Maraldi, Marc de Wergifosse

Theoretical Chemistry Group, MOST Division, Institute of Condensed Matter and Nanosciences, UCLouvain, Place Louis Pasteur 1, 1348 Louvain-la-Neuve, Belgium

*e-mail: robin.crits@uclouvain.be

In the late 90's, Brédas and coworkers[1] studied the 2PA responses of a set of trans-stilbene derivatives functionalized by electron donating/withdrawing groups using semi-empirical methods with the aim of designing organic molecules with large two-photon absorption cross sections. As it was usual at the time, they considered only one single geometry in gas phase for each system to compute 2PA. Thus, dynamic structural effects and the impact of the solvent were totally neglected in their comparisons to experiment. In this work, we aim at providing the most realistic description for the 2PA of this set of molecules by assessing dynamic structural effects and the (explicit) impact of the solvent on the 2PA response. For this, two methodologies are proposed: first, by studying the conformer ensemble for each molecule in gas phase or in implicit solvation and second, by explicitly accounting for solvent molecules and performing molecular dynamic (MD) simulations.

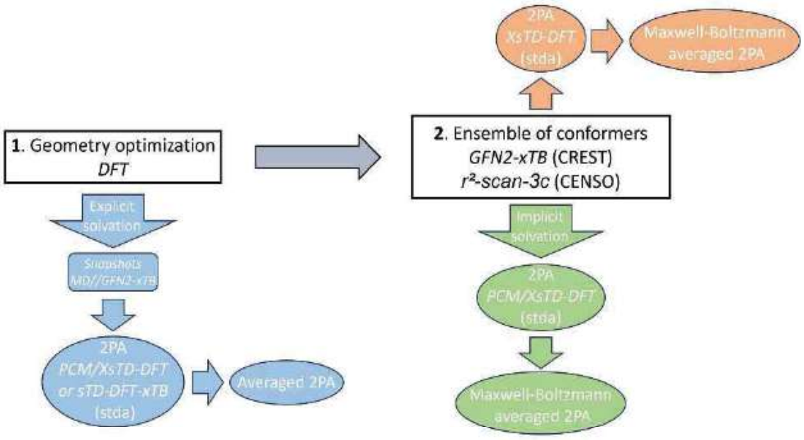

Figure 1: Computational workflow of this study.

To achieve these goals, starting geometries were optimized at the DFT level (Fig. 1, **step 1**). Conformers were generated at the semi-empirical GFN2-xTB level of theory using the *CREST* algorithm.[2] Subsequently, the conformer ensemble was resorted out and re-optimized at the DFT level (i.e. r^2-scan-3c) using *CENSO* (Fig. 1, **step 2**).[2] 2PA cross-sections were evaluated at the XsTD-DFT[3] level of theory for every structures. Finally, Maxwell-Boltzmann weighted 2PA spectra were computed to account for the most relevant conformers at room temperature. This methodology was applied both in gas phase (Fig. 1 **orange**) and in solution using the polarizable continuum model (Fig. 1 **green**).

Alternatively, explicit solvent molecules are added around the targeted systems to account for both the solvent and the dynamic structural effects (Fig. 1 **blue**). Snapshots are generated from MD simulations at the GFN2-xTB level of theory. 2PA is then computed for each snapshot using simplified quantum chemistry methods considering the dual-threshold approach.[4] Averaged 2PA spectra are finally obtained by combining 2PA spectra from different snapshots.

This poster will only present results for the first methodology because for the following part, most of the calculations are still running.

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Efficient and Selective Removal of Heavy Metals Using MCM-41-Based Hybrid Materials Modified with Triazole Molecules

Youssef Draoui[1,*], Smaail Radi[2], Aurelian Rotaru[3], M. Amparo F. Faustino[4], M. Graça P. M. S. Neves[4], Nuno M. M. Moura [4], Yann Garcia[1]
[1]Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis (IMCN/MOST), Université Catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium.
[2] LCAE, Department of Chemistry, Faculty of Science, University Mohamed I , P.O. Box 524, Oujda 60 000, Morocco.
[3] Department of Electrical Engineering and Computer Science & Research Center MANSiD, “Stefan cel Mare” University, University Street, No. 13, Suceava 720229, Romania.
[4] LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

* Corresponding authors: youssefx7draoui@gmail.com

Water is fundamental to life and vital to many sectors of the global economy. However, pollution from heavy metals like cadmium and lead poses serious threats to both human health and the environment While various water treatment technologies exist, issues with performance, cost, and selectivity persist. Recent research has focused on developing effective materials for water purification, with hybrid materials—combining organic and inorganic components—showing promise. Among these, silica-based materials are notable for their ability to adsorb heavy metals, offering improved capacity, speed, selectivity, and reusability, making them ideal for large-scale water treatment. [1,2]

In this study, two new hybrid materials, M1 and M2, were synthesized using silica gel and MCM-41, respectively, as the inorganic components, and 3-(3,5-dimethyl-1H-pyrazol-1-yl)-1H-1,2,4-triazole (L) as the organic component. The ligand introduced, revealed remarkable complexation ability against various set of transition metals as reported by our previous work,[3] making it a good candidate for developing reliable hybrid materials for heavy metals extraction. These materials were extensively characterized using various physical and spectroscopic techniques, including attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, elemental analysis, thermogravimetric analysis (TGA), solid-state 13C NMR, scanning electron microscopy (SEM), and Brunauer-Emmett-Teller (BET) surface area analysis combined with Barrett-Joyner-Halenda (BJH) methods. Parameters such as adsorbate concentration, shaking time, temperature, and solution pH were systematically investigated. The reusability and selectivity of the materials were also assessed. To understand the adsorption mechanism and facilitate data analysis, various models, including Langmuir, Freundlich, Temkin, and Sips adsorption isotherms, as well as pseudo-first-order, pseudo-second-order, and intraparticle diffusion models, were applied and discussed.

The adsorbent M1 and M2 demonstrated highly dependable performances for industrial-scale heavy metal extraction in aqueous solutions due to their ease of use, high cadmium extraction capacity, rapid metal elimination, and exceptional cost-effectiveness. The performance of these adsorbents against real contaminated sample further validates their practical utility.

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Embedding $[Ru(bpy)_3]^{2+}$ on SiO_2 nanotubes for future multi-catalytic applications

S. Eeckhout, F. Drault, J Long, S. Demoustier, S. Hermans, O. Riant
UCLouvain – IMCN - Pôle MOST, Place Louis Pasteur 1, 1348 Louvain-la-Neuve, Belgium
sarah.eeckhout@uclouvain.be

As scientists strive to make their research more innovative and efficient whilst environmentally relevant, a profusion of greener strategies have emerged. For our part, implementing reusable muti-catalytic systems has caught our attention. To do so, we intend on developing hollow nanotubes with a different type of catalyst on the inside and outside surfaces in order to, for one part, allow different reactions with just one system and, for the other, allow simple recycling of otherwise difficult to recover catalyst.

Our first aim is to graft photocatalysts on the outer surface. $Ru(bpy)_3^{2+}$ is one of the most prominent photo-redox catalysts in the field. Its versatility and efficiency have made it a common choice for photocatalytic applications. However, this metal-based catalyst's relatively elevated cost and potential toxicity raises concerns. Thus, there is a significant interest for developing methods to recover and recycle such compounds. A strategy that has raised interest is the one proposed by J. Wang *et al.*[1], which consists in embedding $Ru(bpy)_3^{2+}$ into silica nanospheres. Not only has the method proven beneficial for the photostability of the complex, it has also shown good photoactivity and recyclability. With these prospects, we intended on extending this strategy to our project by ingraining the aforementioned hybrid $Ru(bpy)_3^{2+}$-SiO_2 nanoparticles onto SiO_2 nanotubes. Through this method we hoped to reach the first step toward our multicatalytical goals by functionalizing the outer walls of our nanotubes.

The modified nanotubes were characterized through SEM and diffuse reflectance spectroscopy. The techniques seemed to confirm that the nanostructures were indeed decorated with Ru complex. The obtained solid was then tested using a similar reaction to the one described by the Wang group [1,2]. After some optimization (as shown in the figure below) we found that quantitative yields could be reached within 6h of irradiation. We, therefore, set out to verify the recyclability of the system. The first 2 runs both provided 100% of product. While more runs are to be conducted, this activity suggests a rather promising future for the developed solid.

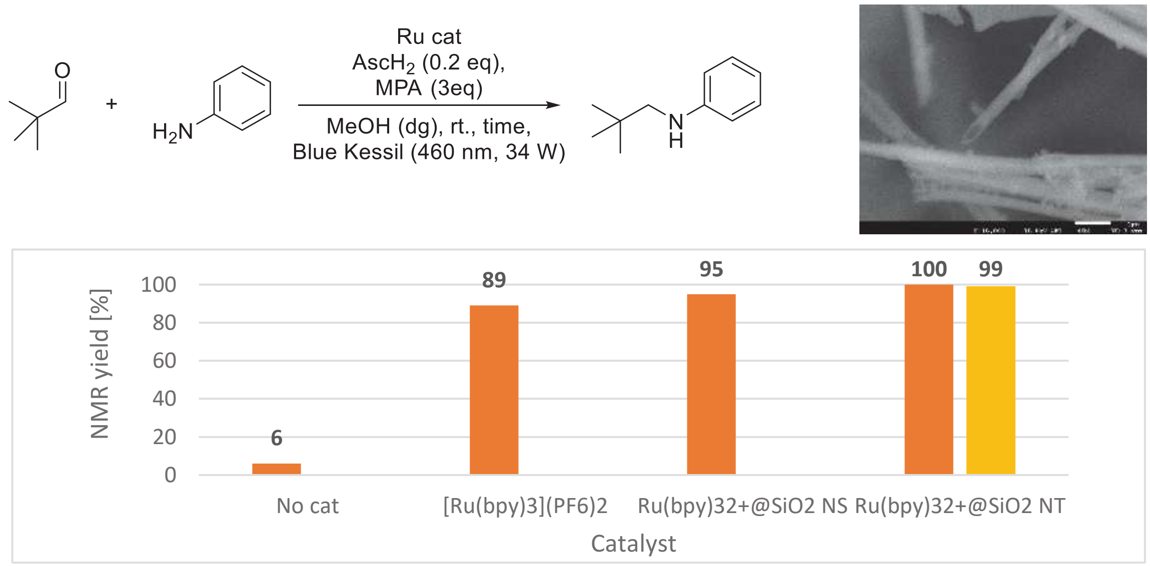

Figure 1 Reductive amination reaction (upper left), SEM image of $Ru(bpy)_3$ embedded onto silica nanotubes (upper right), bar chart of the photocatalytic reductive amination tests (bottom).

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Sustainable extraction of chitin and chitosan from Hermetia illucens breeding waste: Controlled properties and Eco-friendly approach

Samia Elouali[a,b], Samira Benali[a], Mohammed Rhazi[b], Jean-Marie Raquez[a]
[a]Laboratory of Polymeric and Composite Materials, University of Mons, Mons, 7000, Belgium.
[b]Interdisciplinary Laboratory in Bio-Resources, Environment and Materials, Higher Normal School, Cadi Ayyad University, 4000, Marrakech, Morocco.
Email: samia.ELOUALI@umons.ac.be

Sustainably exploiting the waste of the black soldier fly (BSF) to produce chitin and chitosan remains a challenge. This work valorizes the pupal cases of BSF for chitin and chitosan extraction. Four chemical extraction processes have been employed. Process 1, the standard method for this source, served as a control. Processes 2 and 3 were designed to assess and select the most effective delipidation method, while the optimized Process 4 involved autoclave conditions (121°C-2.2 Bar). All chitin derivatives obtained were characterized by FTIR, SEM, XRD, ^{1}H-NMR, TGA, potentiometry, viscosimetry, and ICP-OES. Extraction using Process 4 (P4) proved to be the most efficient, demonstrating a deproteinization efficiency of 94.25 ± 0.6% in a total reaction time of 1.15 ± 0.08 h and water consumption of 250 ± 26.86 L/kg, significantly lower than in other processes. In terms of yield, this process resulted in chitin and chitosan with respective yields of 34.74 ± 1.15% and 83.33 ± 1.28%, outperforming the other methods. Regarding physicochemical properties, P4 produced chitin and chitosan with improved thermal stability, with DTG_{max} values of 421°C and 345°C, respectively. Additionally, the crystallinity of chitin was reduced by 25.68%. For chitosan, the degree of acetylation (DA) was the lowest, while maintaining a high molecular weight of 220 378 g/mol. These results confirm that P4 is efficient and environmentally friendly, making it well-suited for industrial applications.

Keywords: Black Soldier Fly, breeding waste, edible insects, sustainable extraction.

Novel borohydride zeolite solid state electrolytes for alkali batteries

Yuqin Fan, Igor E. Golub, Heiwei Xu, Alexandru Vlad, Yaroslav Filinchuk*
Institute of Condensed Matter and Nanosciences, Université catholique de Louvain, Place Louis Pasteur 1, 1348 Louvain-la-Neuve, Belgium

Yuqin.fan@uclouvain.be

Complex metal borohydrides have received significant interest as solid-state ionic conductors. Lithium borohydride, $LiBH_4$, exhibits a wide electrochemical stability window (0~5 V vs Li/Li^+) and is compatible with most electrodes. Its main drawback, however, is its low room-temperature electrical conductivity ($<10^{-7}$ S cm^{-1}). Zeolites are micro or mesoporous structures composed of aluminosilicate minerals linked by oxygen atoms. However, even though the porous framework of zeolites can be used to construct an 3D interconnected pathway for ion transport and achieve fast ion conduction as a potential open-framework electrolyte for solid batteries, the related studies are still lacking. Herein, we investigated the confinement of $LiBH_4$ in porous zeolite and its effect on the Li-ion conductivity. We studied two kinds of commercial zeolite CVB720 and CVB760, which has different space area. For $LiBH_4$-zeolite system, we found that $LiBH_4$/CVB720 with a weight ratio of 2:1 has the highest ionic conductivity. And at 30°C, the ionic conductivity of $LiBH_4$-CVB720(2:1) reached 1.29×10^{-5} S cm^{-1}, which was three order magnitude than pure $LiBH_4$ ($\approx10^{-8}$ S cm^{-1}). When the temperature increased to 80℃, the ion conductivity of $LiBH_4$/CVB720 is 1.34×10^{-4} S cm^{-1}. These attempts not only pave a way for the design of a new borohydride composite but also achieve a potential and suitable solid electrolyte for Li-ion batteries.

Towards in vivo Bioconjugation using Calix[4]arenes-coated Gold Nanomaterials

J. Janssens[1,2], V. Lepeintre[1,2], G. Bruylants[1], I. Jabin[2]

1 Engineering of Molecular NanoSystems, Ecole Polytechnique de Bruxelles, Université libre de Bruxelles (ULB), avenue F. D. Roosevelt 50, CP165/64, B-1050 Brussels, Belgium
2 Laboratoire de Chimie Organique, Université libre de Bruxelles (ULB), Avenue F. D. Roosevelt 50, CP160/06, B-1050 Brussels, Belgium
julie.janssens@ulb.be

Due to their numerous exceptional properties, gold nanomaterials are attracting growing attention in biomedical applications. However, the functionalization of gold nanomaterials is crucial for their downstream applications, as this step aims to confer them sufficient stability in complex media, such as biological samples or plasma. Recently, the grafting of calix[4]arenes derivatives onto gold surfaces has demonstrated a significant enhancement of the stability of gold suspensions under various conditions.1 Furthermore, the bioconjugation of gold nanomaterials holds significant potential, as attaching biomolecules to gold nanomaterials enables specific recognition of receptors on targeted cell surfaces. Conducting this bioconjugation in vivo is considered a promising yet challenging strategy to enhance current imaging techniques and therapeutic systems. The complexity of the biological environment however necessitates highly selective and efficient reactions. To this end, biorthogonal reactions, defined as reactions that occur without interacting or interfering with biological components, have been developed.2 These reactions are based on the reaction between functional groups which are not naturally present in living systems and thereby, require the specific modification of molecules (e.g. probes, biomolecules), rendering them highly selective. Combining the advantages of both bioorthogonal reactions and gold nanomaterials could open new perspectives in in vivo diagnostics and therapy.

In this context, we will show how the calix[4]arene-based coating strategy can be extremely efficient for the development of gold nanomaterials able to undergo biorthogonal reactions in the context of in vivo bioconjugation. Our results provide new insights into designing efficient nanosystems that can be (bio)-functionalized in complex biological media.

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Two-step spin crossover behavior of a 3D iron(II) framework based on triazole-ligand

Xiaochun LI, Yann GARCIA
IMCN-MOST, Université catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la- Neuve, Belgium
xiaochun.li@uclouvain.be

Some transition metal complexes, particularly those of the first transition series with configurations $3d^4$ to $3d^7$, can undergo a spin crossover (SCO) between a low-spin (LS) and a high-spin (HS) state when induced by an external stimulus such as light, temperature, pressure, electric field, or guest molecules [1]. SCO compounds are a promising way of attaining bistability at the molecular level and have been studied extensively over the last few decades for potential applications in high-density information storage devices, quantum computers and spintronics [2].

In this work, a new three-dimensional iron(II) spin crossover framework based on tris(4,4'-bis-1,2,4-triazole), hereafter abbreviated as ***btr***, has been synthesized with the formula $[Fe(\textbf{\textit{btr}})_3](anion)_2$.

The crystal structures of this new iron(II) complex was determined by Single-crystal X-ray diffraction and it showed that the complex crystallized in the *R3* space group, and the structure is three-dimensional [3]. Two crystallographically independent iron sites were revealed, denoted as Fe1 and Fe2, respectively. Single-crystal data were collected at three different temperatures, that is, 80 K, 160 K and 250 K, to assess the structural changes associated with the spin transition. The magnetic properties were studied using SQUID (Superconducting Quantum Interference Device). This compound exhibits SCO behavior. The low-spin to high-spin transition occurs in two steps with an unprecedented ca. 67 K plateau, each involving around 50% of Fe^{2+} ions. The low-temperature step is abrupt and undergoes a thermal hysteresis with a width of 12 K from 116 K to 128 K. The high-temperature step is centered on 187 K without thermal hysteresis. Differential scanning calorimetry (DSC) data were collected on a bulk crystalline sample. The heat capacity curve of the sample shows obvious peaks associated with the spin transition. Two endothermic peaks are observed at 119 K and 184 K, which correspond to the spin transition in the heating mode measured by SQUID. The associated enthalpy and entropy variations of the two endothermic peaks in heating mode are evaluated as ΔH = 16.24 KJ mol^{-1} and ΔS = 112.11 J mol^{-1} K^{-1}, respectively. These values are within the experimental range for Fe(II) SCO systems. The band intensity ratio of variable temperature Raman spectrum verified the two-step SCO with hysteresis effect. In addition, ^{57}Fe Mössbauer spectra were obtained at selected temperatures, which allowed us to follow the temperature dependence of the HS and LS molar fractions in an accurate fashion.

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Keggin polyoxometalates: a novel versatile platform for deoxydehydration catalysis

A. Magerat, S. Hermans, E.M. Gaigneaux
Institute of Condensed Matter and Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis
(MOST), Université catholique de Louvain (UCLouvain), Place Louis Pasteur, 1 – 1348 Louvain-la-Neuve
alixandre.magerat@uclouvain.be

Keggin polyoxometalates are $[ZM_{12-x}M'_xO_{40}]^{n-}$ heteropolyanions (HPAs) where Z is a heteroatom (e.g. P or Si) and M is a transition metal (e.g. Mo or W) (fig. 1a) [1]. Sometimes, one (or more) M metals can be substituted by (an) other(s) (M') in order to tune the redox properties of the anion. The acidity and the hydrophobicity can be controlled as well by varying the counter-cation (e.g. H^+, Cs^+, etc.). These different possible chemical compositions provide Keggin HPAs high tunability and versatility.

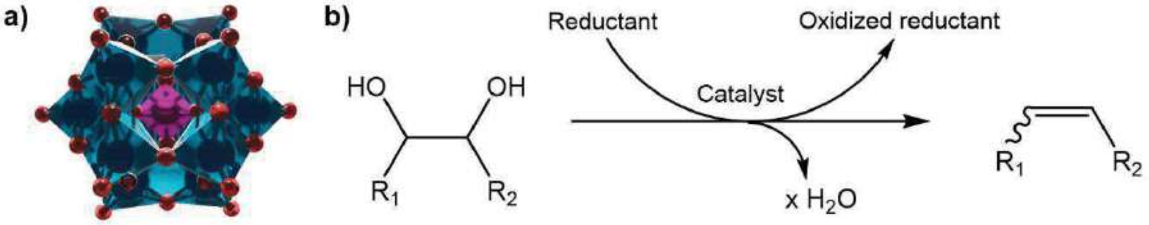

Figure 1. a) Keggin heteropolyanion structure. Pink: heteroatom tetrahedron (ZO_4). Blue: transition metal octahedra (MO_6). Red: oxygen atoms. The counter-cations have been omitted for clarity. b) Catalytic deoxydehydration; depending on the nature of the reductant, x = 1 or 2.

To our knowledge, these compounds have never been used to catalyze deoxydehydration (DODH), a promising reaction that transforms vicinal diols, a common chemical motif in biomass-derived molecules, into alkenes (fig. 1b) [2]. In this contribution, we report the interesting catalytic performances of $PMo_{12}O_{40}^{3-}$ with tetrabutylammonium as counter-cation ($TBAPMo_{12}$) in the DODH of 1,2-hexanediol (as model substrate). Additionally, we show that the poor catalytic performances of $TBAPW_{12}$ can be greatly improved by replacing one W by a Re atom, yielding the very active $TBAPW_{11}Re$ (fig. 2).

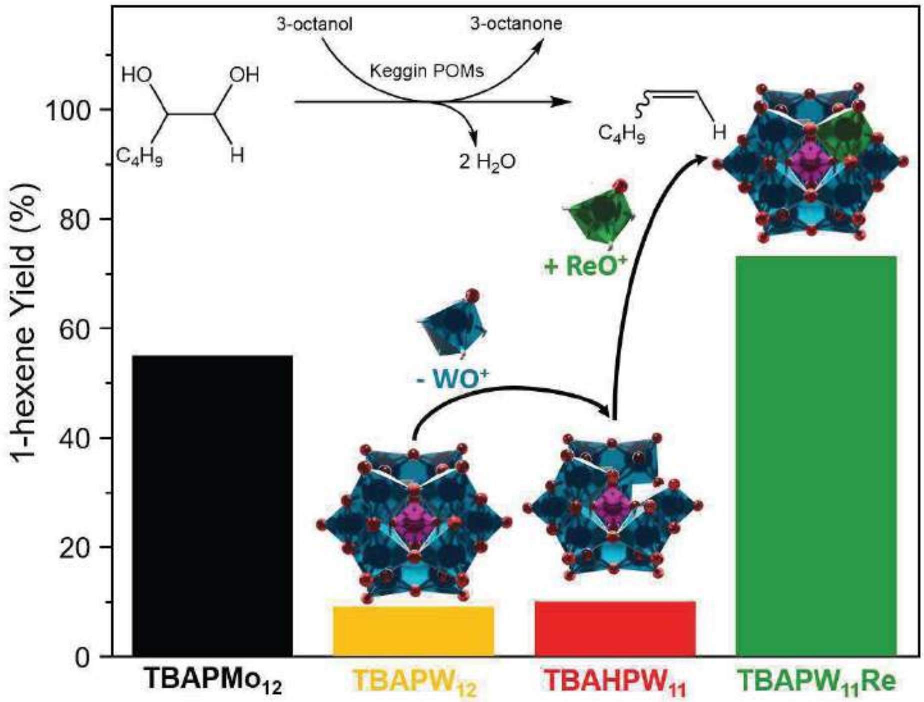

Figure 2. Catalytic performances of different Keggin phosphometalates. Conditions: 18h, 210°C, 5% mol. metal (for Mo and W) and 2% mol Re. The model reaction studied is depicted in the figure.

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Make it simple: benchmarking the performances of XsTD-DFT to compute one- and two-photon absorption

Marilù G. Maraldi, Marc de Wergifosse
Theoretical Chemistry Group, Institute of Condensed Matter and Nanoscience, Catholic University of Louvain,
1348 Louvain-la-Neuve, Belgium
marilu.maraldi@uclouvain.be

Multiscale methods allow the computation of one- and two-photon absorption (1PA and 2PA) of large systems by partitioning them into layers. They rely on the assumption that the optical response mostly originates from a small portion of the system, that is treated at a quantum mechanical (QM) level. Despite their computational efficiency, multiscale methods do not fully capture the response of the surroundings. This motivates a full-QM treatment of the entire system for realistic comparisons with experiments. A full-QM treatment is nevertheless out of the reach of current ab initio methods. Grimme and co-workers[1] proposed the simplified TD-DFT (sTD-DFT) method[2] as an alternative scheme to compute excited states. This was extended to nonlinear optical (NLO) properties by de Wergifosse. It was the opportunity to compute, with this “all-atom QM” scheme, NLO properties of systems as large as fluorescent proteins or nanoparticles. These works showed the importance to explicitly account for the impact of surroundings. Recently, de Wergifosse[3] introduced the eXact integral sTD-DFT (XsTD-DFT) scheme which removes the semi-empiricism of the sTD-DFT scheme.

The present work evaluates the performances of the XsTD-DFT method to compute 1PA and 2PA, with respect to reference RI-CC2/aug-cc-pVDZ calculations. We selected three different molecular sets: the first one (from QUEST database) is composed of 29 small molecules with excited states of valence, charge transfer (CT) and Rydberg character, for which theoretical best estimates are available. The second set includes 48 π-conjugated medium size molecules exhibiting CT excited states with large 2PA strengths. We also included an ensemble of micro-hydrated molecules to study how local environmental effects are treated by the XsTD-DFT scheme. We first assessed the performance of the XsTD-DFT method for different global and range-separated hybrid exchange-correlation (XC) functionals (TPSSh, B3LYP, PEB0, M06, BHandHLYP, M06-2X, CAM-B3LYP, ωB97X-D3, ωB97M-V), comparing trends to full TD-DFT and RI-CC2. Second, we studied basis set effects, testing different double-ζ basis sets (3-21G, 6-31G*, cc-pVDZ, 6-31+G*, def2-SVP, aug-cc-pVDZ). We observed that the XsTD-DFT scheme closely reproduces trends in excitation energies, oscillator strengths, and 2PA strengths (δ2PA) with respect to the full scheme. For excitation energies, of 1PA and 2PA active states, we report MADs of 0.10 eV (TD-DFT), 0.63 eV (sTD-DFT), and 0.14 eV (XsTD-DFT) at M06-2X/aug-cc-pVDZ level. For oscillator strengths larger than 0.1, we observed mean absolute deviations (MADs) from RI-CC2 of 0.08 (TD-DFT), 0.23 (sTD-DFT), and 0.10 (XsTD-DFT) at the same level of theory. Hybrid XC functionals with low amount of exact exchange better reproduce magnitudes of δ_{2PA}: at PBE0/aug-cc-pVDZ level, MADs of log(δ2PA) (within a range of 103 and 106 a.u. strengths) are 0.17 (TD-DFT), 0.16 (sTD-DFT), and 0.15 (XsTD-DFT), while MADs of excitation energies (of these 2PA active states) are 0.46 eV (TD-DFT), 0.73 eV (sTD-DFT), and 0.38 eV (XsTD-DFT).The advantage of simplified QC methods is their general computational speed up: XsTD-DFT (sTD-DFT) overall runs 69 (135) times faster than TD-DFT on the same 16 Intel Xeon E5-2650 v2 CPUs (2.60 GHz).

In conclusion, we showed that XsTD-DFT is a computationally efficient and robust alternative to TD-DFT to compute 1PA and 2PA trends. The parameter-free XsTD-DFT improves results with respect to sTD-DFT scheme, making it a flexible and general method for excited states calculations. As emerging applications, XsTD-DFT can be used to simulate realistic systems accounting for dynamic structural effects and impact of the surroundings, going beyond the single molecule approach.

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Strain effects on GeV centers by means of density functional theory

T. G. I. van Wijk,[1,2] E. A. Melan,[1] E. Y. Guillaume,[1,2,3] D. E. P. Vanpoucke[1,2]
[1] Hasselt University, IMO, QuATOMs, Martelarenlaan 42, B-3500 Hasselt, Belgium
[2] imec, imo-imomec, Wetenschapspark 1, B-3590 Diepenbeek, Belgium
[3] NISM, University of Namur, Rue de Bruxelles 61, 5000 Namur, Belgium
esinaylin.melan@uhasselt.be

Color centers in diamond have suitable properties for a variety of high-end quantum applications. Previously, it has been demonstrated that the GeV center has an intense zero-phonon line (ZPL) and a small phonon sideband due to the highly symmetric D_{3d} symmetry of the color center.[1, 2, 3] Strains, however, have an impact on these properties. In nanocrystalline diamond, these effects are not negligible, and characterization is needed. This work aims to unravel the impact of strains on the electronic structure and the ZPL of the GeV center in diamond using group theory and first principles calculation.[4]

The GeV center is modeled using density functional theory for defect concentrations of 1.61 % down to 0.10 %. Structure optimization confirms the expected D_{3d} symmetry. Next, the hydrostatic compressive and tensile strain is modeled by altering the volume of the relaxed structure by ±1 % and ±2 % while keeping the cubic shape. Both blue- and red-shifts are obtained for compressive and tensile strains, respectively. It shows a linear relation between the shift in ZPL and the pressure with a decreasing shift of the ZPL for lower GeV concentrations (see Figure 1a). Extrapolation to experimentally relevant concentrations shows a shift of 0.17 nm/GPa for both compressive and tensile strains. On the other hand, a linear strain is applied by changing the lattice parameter in the $< 100 >$ direction by ±1 % and ±2 % while the others are fixed. This alteration causes a structural change in the color center. The symmetry is broken and reduces to the C_{2v} symmetry group. The ZPL shifts result in only red-shifts for both strain types (see Figure 1b). A change of 4.7 nm/GPa and 3.2 nm/GPa is found for compressive and tensile linear strain, respectively, at experimentally relevant concentrations. These obtained results are in line with experimental research on similar GeV color centers.[5]

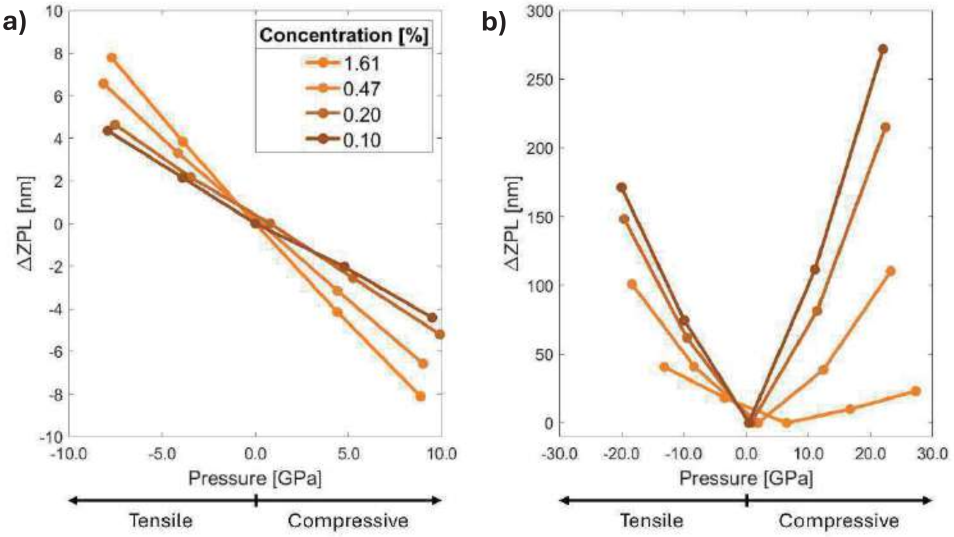

Figure 1. ZPL shift (ΔZPL) as a function of pressure under a) hydrostatic strain and b) linear strain in the $< 100 >$ direction for different GeV defect concentrations modeled with the PBE functional.

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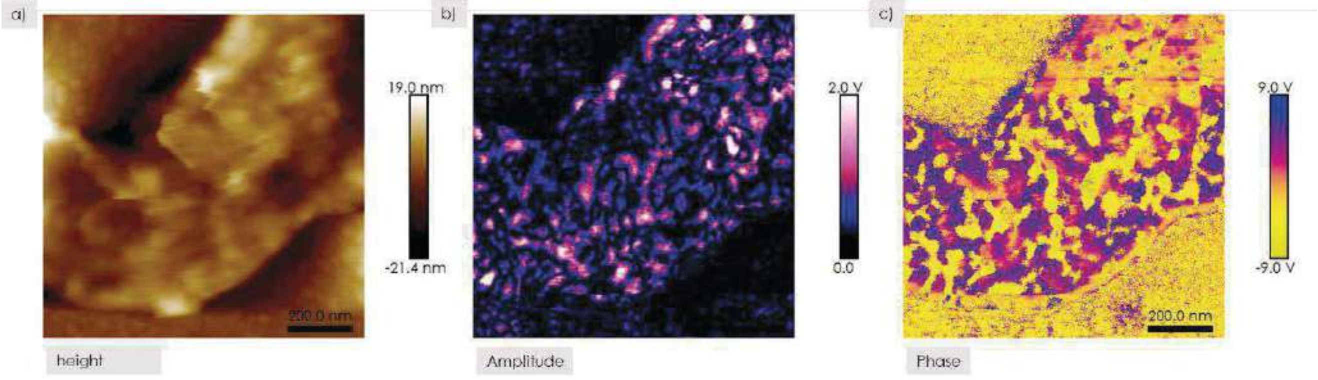
On the characterization of electromechanically organic-inorganic hybrid active materials

Pierre Nickmilder, Imen Ben Khaled, Philippe Leclère
Laboratory of Physics of Nanomaterials and Energy (LPNE)
Research Institute for Materials Science and Engineering
University of Mons (UMONS), 7000 Mons
pierre.nickmilder@umons.ac.be

The energy crisis demands urgent exploration of new methods for electricity production and storage. A promising approach involves the development of systems made of materials exhibiting piezoelectric properties for charge generation. Although some materials such as PZT exhibit excellent piezoelectric properties, the presence of toxic lead hinders their applicability, necessitating the exploration of alternative materials.

This study focuses on developing a hybrid composite system that combines the flexibility of the organic Poly(vinylidene fluoride-co-trifluoroethylene), (PVDF-TrFE) copolymer with the enhanced piezoelectric sensitivity of Bismuth ferrite (BiFeO3 or BFO) nanoparticles. The piezoelectric and ferroelectric properties of these systems were analyzed using Piezoresponse Force Microscopy (PFM). PFM, which utilizes the inverse piezoelectric effect, allows for the localized investigation of electromechanical behavior. However, artifacts, especially due to electrostatic interactions, can interfere with accurate measurements. To reduce those effects, we employed techniques like identifying the Electrostatic Blind Spot (ESBS), optimizing the laser positioning on the cantilever [1]. In addition to conventional PFM, we used advanced techniques such as switching spectroscopy PFM (ssPFM) to monitor electromechanical responses and extract ferroelectric hysteresis [2]. We also verified the true ferroelectric nature of our materials response through contact Kelvin Probe Force Microscopy (cKPFM) experiments, highlighting the importance of double-checking results by comparing them with known non-ferroelectric samples like ZnO. Furthermore, we also explored spectroscopy modes coupled with contact resonance measurement methods to quantify weak piezoelectric displacements.

Through these research efforts, we aim to contribute to the development of piezoelectric hybrid materials with improved electromechanical properties. These materials hold significant potential for addressing the energy crisis and driving advancements in electricity generation.



PFM measurement on the PVDF-TrFE and BFO particles nanocomposite. a) topography, b) amplitude and c) phase

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TiOxCy organometallic coatings: The role of carbon in promoting hydrophilicity for dental implants

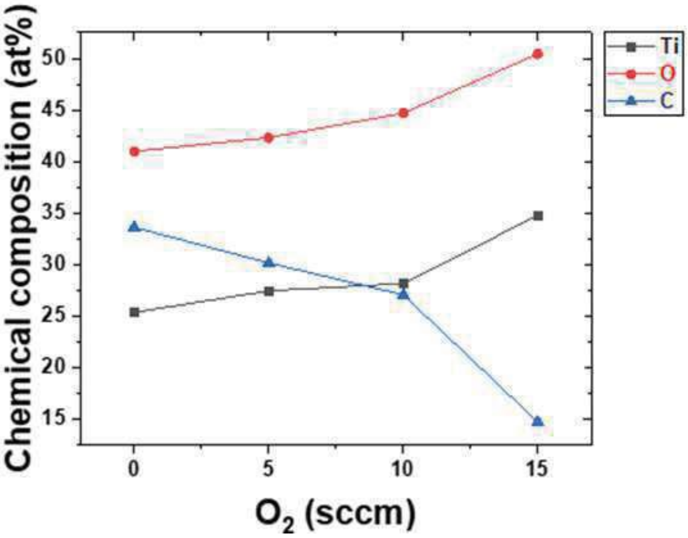
S. Rubio, A , L. Houssiau
Laboratoire Interdisciplinaire de
Spectroscopie Electronique,
University of Namur,
Namur, 5000, Belgium
Email of sandra.rubioaguado@unamur.be

Titanium, along with its alloys, is a biocompatible material and widely employed in biomedical applications. Specifically, its use in dental implants is very promising due to their mechanical, chemical and biological properties [1]. The wettability of the implant is crucial for accelerate osseointegration mechanisms, due to the external surfaces of the implant with low hydrophilicity do not promote contact between the metal part of the implant and the cells, leading to poor osseointegration and, therefore, implant failure [2].

The implant body, or screw, is the part of the dental implant that is inserted into the jawbone, and the metal must integrate with the bone, making the creation of hydrophilic surfaces necessary for optimal bonding. From this perspective, the development of TiOxCy organometallic coating with different composition, varying from mineral (low C) to organic (high C) is proposed.

In this work, TiOxCy films are deposited on Ti90Al6V4 foils using Plasma Enhanced Chemical Vapor Deposition (PECVD) technique. The thin films have been prepared under the same conditions except for the flow and proportion of the reactive gas, producing changes in the chemical composition of the films and consequently in their hydrophilicity. The characterization of the coatings was conducted using X-ray photoelectron spectroscopy (XPS), contact angle and profilometry analyses to study the chemical composition, the hydrophilic character of the surface and the thickness.

The results indicate that carbon-rich TiOxCy thin films promote the hydrophilicity, and they could induce favorable cell adhesion and improve the osseointegration.



Chemical composition of TiOxCy thin films as a function of oxygen flow

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A Compendium of Methodically Determined Ground and Excited State Properties of Homoleptic Ruthenium (II) Photosensitizers

Felix Glaser,[a] Simon De Kreijger,[a] Katerina Achilleos,[a] **Lakshmi Narayan Satheesh**,[a] Alexia Ripak,[a] Noémie Chantry,[a] Céline Bourgois,[a] Sophie Quiquempoix,[a] Joffrey Scriven,[a] Julien Rubens,[a] Milan Vander Wee-Léonard,[a] Martin Daenen,[a] Martin Gillard,[a] Benjamin Elias[a] and Ludovic Troian-Gautier[a],[b]

[a] Institut de la Matière Condensée et des Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis (MOST), Université catholique de Louvain (UCLouvain),Place Louis Pasteur 1 box L4.01.02, B-1348 Louvain-la-Neuve, Belgium

[b] Wel Research Institute,Avenue Pasteur 6, 1300 Wavre, Belgium

Photoredox catalysis has gained significant attention in recent years. This approach primarily involves photosensitizers with metal centers based on transition metals like Ru(II), Os(II) and Ir(III) due to their favorable electronic and photophysical properties. Typically, versatile chelating ligands such as polypyridine, which can coordinate with various metal centers, are used. In particular Ru(II) and Os(II) based polypyridyl complexes have been prominent since the 1950s as they strongly absorb visible light. This makes them excellent photosensitizers as they can efficiently harvest light energy which is crucial for driving photoredox transformations.

This study focuses on Ruthenium photosensitizers, detailing the synthesis of 16 homoleptic ruthenium (II) photosensitizers with substitute 2,2’-bipyridine, 1,10-phenanthroline and diaza ligands. While most of these compounds are already known, this study provides comprehensive datasets on their ground and excite state properties. The synthesis yielded high amounts of products with relatively simple purification steps. These photosensitizers exhibit strong light absorption in the visible spectrum (400-480 nm) with molar absorption coefficient that ranged from 12,000 to 30,000$M^{-1}cm^{-1}$. Excited-state lifetime, steady-state photoluminescence and photoluminescence quantum yields, as well as the radiative and non-radiative rate constants, were measured in acetonitrile at 20°C, both in air and under argon. The steady state photoluminescence was also recorded at 77 K in butyronitrile glasses which resulted in a hypsochromic shift of the photoluminescence spectra and the observation of well resolved vibronic structures. The cyclic voltammetry in acetonitrile allowed to determine the ground state redox properties of this series of Ru(II) photosensitizers and to estimate excited-state redox potentials.

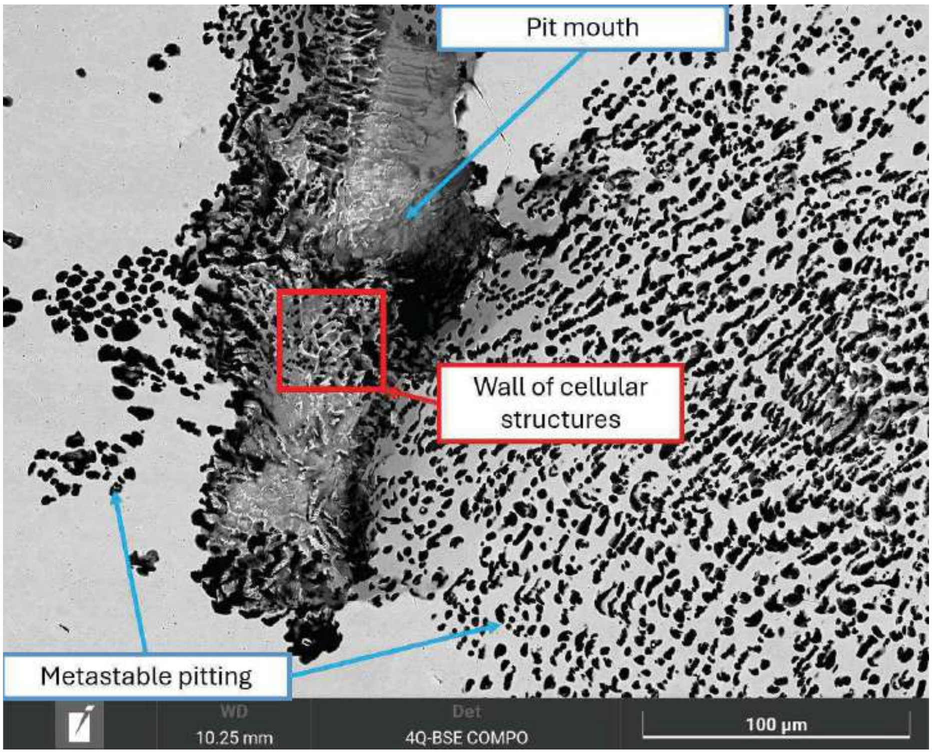
Evaluation of Corrosion Resistance of 316L stainless steel with or without SiC additions produced via Directed Energy Deposition

A.H. Seidou[1], O. Dedry[1], J.T. Tchuindjang[1], A. Mertens[1]
[1] Metallic Materials Science (MMS), Aerospace and Mechanical Engineering Dpt., University of Liège.
Email: AHB.Seidou@uliege.be

Metal additive manufacturing technologies, such as the Directed Energy Deposition (DED) process, offer promising flexibility to develop novel metallic alloys through the mixing of different powders, and to produce monolithic or functionally graded coatings [1]. Both the manufacturing process and material composition are known to significantly impact the microstructure of such AM metals.

This study investigates the microstructure and corrosion characteristics of 316L stainless steel and 316L combined with silicon carbide (SiC), both produced by DED, in comparison to a wrought reference material. The electrochemical corrosion behavior in a 0.5M NaCl solution was correlated to observed microstructural features of the various materials. Electrochemical testing, performed using potentiostatic and potentiodynamic polarization methods at room temperature, revealed that 316L stainless steel exhibits excellent corrosion resistance. This was observed both in the homogeneous wrought reference and in cellular structures formed due to elemental segregation induced by DED technique.

Microstructural and pitting development were examined using light microscopy and scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS). The findings indicate that the presence of SiC influences surface properties, potentially preventing the occurrence of pitting corrosion depending on its concentration.



SEM micrograph of 316L DED after potentiodynamic polarization in 0.5M NaCl solution

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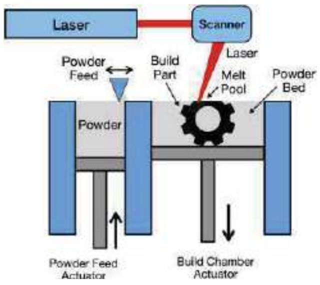
Repair of complex aluminum parts processed by additive manufacturing

G. Snoeck, J.T. Tchuindjang, A. Mertens
Metallic Materials for Additive Manufacturing (MMS), *Aerospace and Mechanical Engineering Dpt., University of Liège*, Place du 20-Août 7 4000 LIÈGE
Gauthier.Snoeck@uliege.be

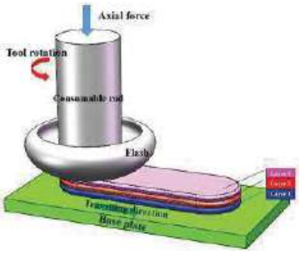
In order to escape the atmosphere of Earth and reach space, launchers are needed. In this context, Space4ReLaunch, a Belgian academic collaborative project, aims to improve reusable launchers. Damage can occur during the production step as well as during handling, but also in service, as these launchers are subjected to multiple cycles. Damaged parts often have to be replaced, which is costly, time-consuming and generates waste. Repair would then be an interesting alternative to alleviate these issues.

In this work, Additive Manufacturing (AM) of aluminium alloys (4xxxx series: Al-Si) will be used to attempt to repair aluminium parts. Different processes will be tested, each having its own advantages and disadvantages. Laser Powder Bed Fusion (LPBF) will be used to perform a metallurgical study and obtain a better understanding of the impact of the process on the material. This process involving the fusion of the material, some defects such as porosity, cracking, oxidation and evaporation of alloying elements are likely to occur. Solid state processes, such as Multi-Layer Friction Surfacing (MLFS) will also be tested, as they can reduce the occurrence of defects.

Some post-processing, such as the heat treatments T5 (direct aging) and T6 (solution treatment followed by an artificial aging), will also be applied in order to increase the quality of repair.



The powder bed fusion process [1]



Schematic of friction surfacing additive manufacturing process [2]

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Probing magnetic domains and thermoelectric effects in Co_2MnGa Weyl ferromagnets via localized heating

M. Razeghi[1], J. Spièce[1], V. Fonck[1], Y. Zhang[3,4], M. Rohde[1], R. Joris[2], P. S. Dobson[5], J. M. R. Weaver[5], L. da Costa Pereira[2], S. Granville[3,4], P. Gehring[1]
[1]IMCN/NAPS, Université Catholique de Louvain (UCLouvain), Louvain-la-Neuve, 1348, Belgium.
[2]QSP, KU Leuven, Leuven, 1587, Belgium.
[3]Robinson Research Institute, Victoria University of Wellington, Wellington, PO Box 600, New Zealand.
[4]MacDiarmid for Advanced Materials and Nanotechnology, Wellington, PO Box 600, New Zealand.
[5]James Watt School of Engineering, University of Glasgow, Glasgow, G12 8LT, United Kingdom.
jean.spiece@uclouvain.be

Weyl ferromagnets are of particular interest due to their topological electronic structure that are predicted to exhibit unique magneto-transport properties. Among Weyl semimetals, Co_2MnGa has demonstrated high transverse thermoelectric properties, generating significant interest for potential energy harvesting and heat pumping applications. However, the magnetic domain configuration in micropatterned devices remains largely unexplored, despite its critical influence on device performance.

By applying heat locally using a hot atomic force microscope tip, we generate temperature gradients across the device, leading to measurable longitudinal and transverse thermoelectric responses. Under a variable magnetic field, we observe the transition between the Seebeck and Nernst effects, as well as the magnetic domain structure in the microfabricated device. Additionally, we examine the magneto-Seebeck effect, which reveals the modulation of the Seebeck coefficient by the magnetic field.

Visualizing magnetic domains in Co_2MnGa provides deeper insights into the interaction between magnetic and thermoelectric phenomena in Weyl ferromagnets. This study combines advanced microscopy techniques with precise thermal manipulation, enabling high-resolution spatial mapping of the magnetic domain structure in response to temperature variations. Ultimately, the research will enhance understanding of topologically driven magneto-thermoelectric effects and their potential applications in spintronics and energy harvesting technologies.

Key factors influencing cage escape in photoinduced electron transfer.

Ana Karem Vega Salgado‡ and Ludovic Troian-Gautier‡,ϕ

‡ UCLouvain, Institut de la Matière Condensée et des Nanosciences (IMCN), Molecular Chemistry, Materials and Catalysis (MOST), Place Louis Pasteur 1/L4.01.02, B-1348 Louvain-la-Neuve, Belgium

ϕWel Research Institute, Avenue Pasteur 6, 1300 Wavre, Belgium

The interaction between an excited-state photosensitizer and a quencher within an encounter complex can give rise to bimolecular electron transfer, leading to the formation of the corresponding geminate radical pair. The cage escape yield, i.e. the separation of the geminate radical pair is key for many light induced transformation. Many factors have been proposed to affect the cage escape process, such as the spin, the driving force for forward or reverse electron transfer, viscosity, etc. One of the parameters that has been proposed to influence the cage escape is the driving force, which governs the ability of the excited photosensitizer to donate or accept an electron from the quencher, facilitating the separation of charges within the radical pair.

In here, we investigated the effect of spin and driving force for forward and reverse electron transfer using 12 Ruthenium and Osmium photosensitizers and phenothiazine as electron donor. Quenching rate constants, determined by steady-state and time-resolved spectroscopic techniques, ranged from $2x10^7$ to $1.5x10^{10} M^{-1}s^{-1}$ in acetonitrile. These values were usually an order or magnitude larger in dichloromethane. Finally, the cage escape yields were determined through comparative actinometry methods using changes of molar absorption coefficients that were determined by spectroelectrochemistry. The trend in cage escape yields between Ru(II) and Os(II) photosensitizers will be further discussed in relationship to spin and driving force for forward and reverse electron transfer.

Solid-state modification of poly(butylene terephthalate) with a photoreactive Cinnamamide monomer

Jacques Kevin Wandji[1], Rosica Mincheva[1], Jean-Marie Raquez[1]
[1]*Laboratory of Polymeric and Composites Materials (LPCM), University of Mons (UMONS), Avenue Victor Maistriau 14,7000 Mons, Belgium*
Jacques.WANDJI@umons.ac.be

ABSTRACT

For the past 70 years, the ubiquity of plastics have revolutionized modern life. However, the wastes associated with these materials pose a persistent pressing energy and environmental challenge to science and industry [1]. To date, recycling and reuse is currently the most efficient approach to reduce plastic wastes but encounters significant drawbacks such as degradation, energy-intensive, selectivity and cost [1]–[3]. In this project, we propose to redesign post-consumer polyesters wastes and give them a second life with enhanced properties through an innovative and alternative upcycling approach implemented via solid-state modification (SSM). At first, the feasibility of the SSM between poly(butylene terephthalate) (PBT), a polyester and N,N-Bis(2-hydroxyethyl) Cinnamamide (BHECA) was demonstrated via differential scanning calorimetry (DSC) at a small scale. At the second step, the reaction conditions were then transferred to a gram-scale batch reactor with inherent enhanced mass and heat transfer processes compared to DSC, in order to further improve material properties. Interestingly, DSC and ^{1}H NMR of the synthesized copolyester via batch reactor revealed increased glass transition temperature (T_g) and demonstrated that exchange reactions between PBT and BHECA occurs and takes places with both the trans and cis conformation of BHECA but in majority with the cis moiety (61%).

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Aromatic Substitution Modulated Spin Crossover Behavior in the Model $[Fe(H_2Bpz_2)_2(bipy)]$ Complex

Mengmeng Wang[1], Koen Robeyns[1], Aurelian Rotaru[2], Yann Garcia[1]

[1]Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis (IMCN/MOST), Université catholique de Louvain, Place L. Pasteur 1, 1348, Louvain-la- Neuve, Belgium.
[2]Department of Electrical Engineering and Computer Science and MANSiD Research Center, "Stefan cel Mare" University, University Street, 13, Suceava 720229, Romania.
mengmeng.wang@uclouvain.be

The spin crossover (SCO) phenomenon refers to that the spin of a complex can shift between two states of high spin and low spin in response to external stimuli, including temperature, light, pressure, *etc*., which endows this kind of material potential applications in high-density information storage, sensors, display devices and molecular electronics. Fine-tuning of the ligand filed around the central metal ion and supramolecular interactions in the crystal packing contribute to influence the SCO property and bring us value information about the magneto-structural correlation. Complex $[Fe(H_2Bpz_2)_2(bipy)]$[1] exhibits thermal, pressure and light induced SCO is one of the classic representing SCO complexes. Modifying the structures can not only adjust the spin-transition temperature but also add new physicochemical properties. Our group have studied the effect of alkyl, ester and halogen substitutions on the SCO property of $[Fe(H_2Bpz_2)_2(bipy)]$ (H_2Bpz_2 = dihydrobis(1-pyrazolyl)borate; bipy = 2,2′-bipyridine) before.[2-4] Here, we introduced different aromatic substitutions, 1-phenylmethanimine (**1**), 1-(naphthalen-1-yl)methanimine (**2**), 1-(naphthalen-2-yl)methanimine (**3**), and 1-(anthracen-9-yl)methanimine (**4**) in the C_5 and C_5' position of the bipy ligand and synthesized four H_2Bpz_2-containing Fe^{II} complexes (Figure 1, left). Variable-temperature direct current magnetic susceptibility measurements on polycrystalline samples under 1000 Oe reveal diversiform incomplete SCO behavior (Figure 1, right). Complex **3** shows the most abrupt transition at around 150 K, complex **2** exhibits two steps slow spin transition at around 250 K and 130 K while complex **4** shows the slowest spin transition as the change of temperature. Small hysteresis loops were observed in complexes **1-3** at around 70 K, but no hysteresis loop appears at around the spin transition temperatures. Single crystal structure analysis and Mössbauer spectra were used to help explain the magnetic performance.

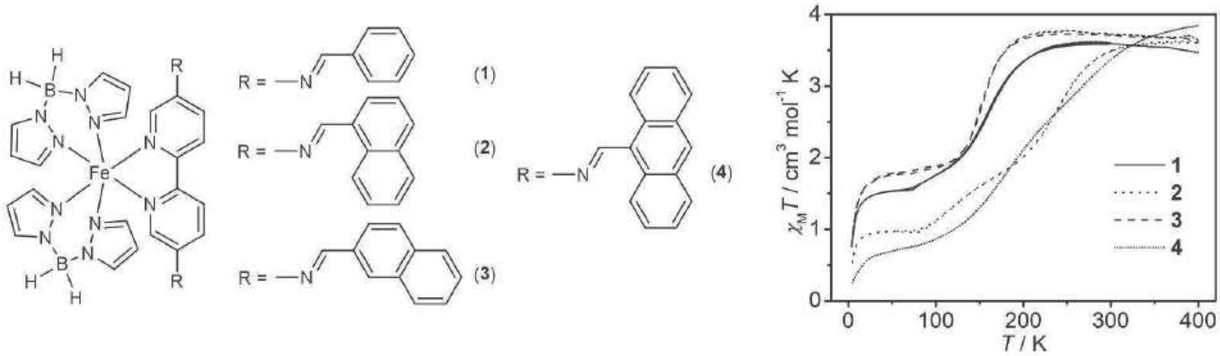

Figure 1. Schematic structure of Fe^{II} complexes with different aromatic substitutions at the C_5 and C_5' position of the bipy ligand (left); and their temperature-dependent $\chi_M T$ plots (right).

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Light Responsive PNIPAM/Gold Nanoparticles Hydrogel Composites for Biomedical Applications

Yalcinkaya E.[a,b], Cassignol M.[a,b], Raquez J-M.[a], Lambert P.[b], Odent J.[a]
[a] Laboratory of Polymeric and Composite Materials (LPCM), Center of Innovation and Research in Materials and Polymers (CIRMAP), University of Mons (UMONS), Place du Parc 20, Mons 7000, Belgium
[b] Transfers, Interfaces & Processes (TIPs), Université Libre de Bruxelles (ULB), Av. Franklin Roosevelt 50, 1000 Bruxelles, Belgium
esra.yalcinkaya@umons.ac.be

Light-driven hydrogels are a safe option for in vivo applications due to their ability to provide non-contact, rapid, precise, and remote spatial light control [1]. Light triggers movement by either changing the structure of light-absorbing molecules or heating light-absorbing molecules or nanoparticles in responsive materials[2]. For responsive materials, Poly (N-isopropylacrylamide) (PNIPAM) is a typical temperature-responsive polymeric hydrogel, which exhibits outstanding volume phase transition characteristics around its LCST at ca. 32°C in aqueous solutions [3,4] and has great potential in biomedical applications [3]. Thus, combining PNIPAM as a polymer matrix and plasmonic nanoparticles specifically gold nanoparticles will make the system light-responsive. However, the presence of nanoparticles in the light-responsive photoresist can increase temperature, making it unsuitable for the consistent temperature requirements of cell culture and tissue regeneration, thus the photothermal effect should not be overlooked. Hence, limiting the nanoparticle concentration in the light-sensitive photoresists to an appropriate level is important [5]. As a result, creating light responsiveness using less than 0.5 mol% AuNPs was aimed in this work.

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Aerosol synthesis of Al_2O_3-CeO_2 as catalyst support for ethanol dry reforming: effect of CeO_2 over coke gasification

Feilong Yang[1], Damien P. Debecker[1]

[1]Institute of Condensed Matter and Nanoscience (IMCN), UCLouvain, Louvain-La-Neuve, Belgium

feilong.yang@uclouvain.be

Ethanol dry reforming (EDR) has garnered wide interest for the upgrading of renewable bioethanol to syngas accompanied by the utilization of CO_2. Ni/Al_2O_3 is one of the most typical reforming catalysts for its economical effect and remarkable cracking activity. However, the susceptibility to coke-induced deactivation has hindered its further development in industry. However, the stability and coke resistance of Ni/Al_2O_3 could be optimized by doping some reducible oxide including CeO_2, La_2O_3, ZrO_2, owing to their oxygen storage capacities[1,2]. The aerosol-assisted sol-gel (AASG) method is well-suited for synthesizing multifunctional heterogeneous catalysts with tailored properties (texture, size, surface functionalities, composition etc.)[3]. This work focused on the synthesis of Al_2O_3 support using AASG approach, with the concomitant incorporation of CeO_2 as coke scavenger, followed by Ni loading through wetness impregnation. The effect of Ce addition over catalytic performance and coke gasification were also investigated. The characterization revealed that the synthesized Al_2O_3 and Al_2O_3-CeO_2 had a characteristic microsphere morphology, with homogeneous composition and remarkable texture. The EDR test showed that unlike 20Ni/Al_2O_3-AASG, which deactivated after 6 h, the Ce-promoted catalysts demonstrated enhanced stability and 20Ni/Al_2O_3-20CeO_2-AASG catalyst maintained stable activity throughout 15 h test under 700 °C. Moreover, TGA-MS analysis of spent catalysts displayed that Ce addition effectively reduced carbon deposition. Kinetic studies of coke gasification via CO_2-TPO further confirmed that Ce significantly accelerated carbon gasification in EDR reaction, despite a higher energy barrier, underscoring CeO_2's role in improving carbon resistance.

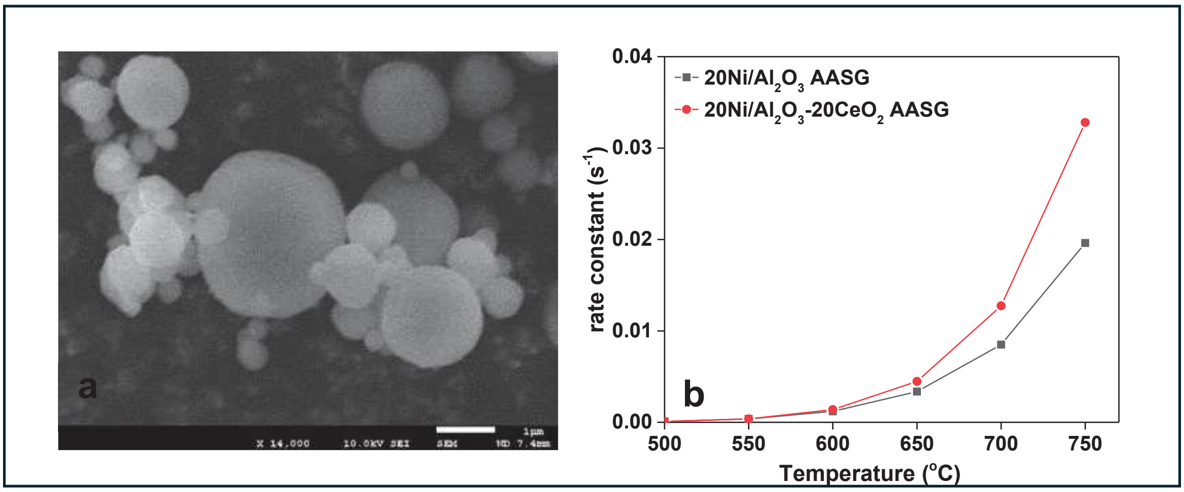

FIGURE 1. (a) SEM image of Al_2O_3-CeO_2-AASG, (b) rate constant of coke gasification under different temperature.

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