

# Chemistry day 2022

Friday, July 1<sup>st</sup> 2022

Campus Sterre, Building S5

Krijgslaan 281, 9000 Gent

The Chemistry day 2022 puts the spotlights on training and research in Chemistry at Ghent University during the academic year 2021-2022. Stakeholders, ranging from internship supervisors to master students are invited to an afternoon in which presentations and posters will give you an update on chemistry training, introduce you to the latest results obtained by master and PhD students in chemistry and outline research highlights by Ghent University professors.

## Programme outline

- |       |  |                        |
|-------|--|------------------------|
| 16u   | <a href="#">Welcome</a> : Chemistry training at Ghent University   | Prof. dr. Z. Hens      |
| 16u15 | <a href="#">Lecture</a> : Exploiting organofluorine chemistry to manipulate properties relevant for drug discovery                                 | Prof. dr. B. Linclau   |
| 16u40 | <a href="#">Lecture</a> : Design your own optical nanothermometer – from core-shell nanoparticles to nanorattles, nanoplatforms and nanocomposites | Prof. dr. A. Kaczmarek |
| 17u10 | <a href="#">Poster session</a> : master and PhD students   |                        |
| 18u30 | Poster award   |                        |

Reception, sponsored by Aji Bio-Pharma Services

Confirm your presence before June 24th via:

<https://eventmanager.ugent.be/Chem>

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contact: [Zeger.Hens@UGent.be](mailto:Zeger.Hens@UGent.be), [Frederic.Lynen@UGent.be](mailto:Frederic.Lynen@UGent.be)

## Welcome | Chemistry training at Ghent University

We begin with a short introduction to the new program in Chemistry as introduced year-by-year at Ghent University since 2017. After briefly highlighting learning goals and teaching formats, we outline where you, as a stakeholder, can contribute to training through supervising research projects or internships, or joining the reflection board.

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Prof. dr. ir. Zeger Hens  
Physics and Chemistry of Nanostructures  
Department of Chemistry  
Ghent University

Zeger Hens graduated from Ghent University in 1995, where he also obtained his PhD in 2000 with Professor W. Gomes. After a postdoctoral stay at Utrecht University in the group of Professor D. Vanmaekelbergh, he returned to Ghent University as an assistant professor in 2002, where he started research on colloidal nanomaterials for opto-electronic applications. In 2014, he became chair of the committee supervising training in Chemistry.

## Lecture | Exploiting organofluorine chemistry to manipulate properties relevant for drug discovery

Selective fluorination of bioactive compounds as part of the drug discovery process has a long history, dating back to the 1950s when the first fluorinated drug was approved. Initially, the traditional application consisted of prevention of oxidative metabolism by replacing vulnerable C–H bonds with a C–F bonds, but over the years this has been extended by a plethora of applications including modification of  $pK_a$ , lipophilicity, hydrogen bond properties and conformational populations, as well as in bioisostere applications, and even for the introduction of non-covalent “multipolar” interactions with protein residues.

Our contributions in this area include methodology to measure the impact of fluorination on the hydrogen bond donating capacity of adjacent alcohol groups, which we are currently extending to investigate polyhydroxylated biomolecules such as carbohydrates, and a  $^{19}\text{F}$  NMR based method to measure the lipophilicity of aliphatic compounds. We have recently been able to exploit this method to achieve the first direct lipophilicity measurements of individual conformers.

In this presentation, an overview of our recent results will be given, and interpreted in a drug discovery context.

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Prof. dr. Bruno Linclau

Organic and Medicinal Chemistry Research Group  
Department of Organic and Macromolecular Chemistry  
Ghent University

Bruno Linclau graduated from Ghent University in 1992, where he also obtained his PhD in 1996 with Professor M. Vandewalle. After a postdoctoral stay at the University of Pittsburgh in the group of Professor DP Curran, he started his academic career in Southampton University, becoming Deputy head of School in 1999. He rejoined Ghent University in 2021 after obtaining a prestigious Odysseus grant, where he started the [Organic and Medicinal Chemistry research group](#). His research interests center around how targeted fluorination influences physical properties that are used in the drug discovery process, involving druglike small molecules, but also typical biomolecules such as carbohydrates, steroids and certain amino acids.

## Lecture | Design your own nanothermometer – from core-shell nanoparticles to nanorattles, nanoplatforms and nanocomposites

The field of optical thermometry has advanced tremendously in the last decade. Scientists have been able to develop (nano-)thermometers with appropriate excitation and emission regions, to reach very high sensitivity, and significantly improve the spatial, temporal and temperature resolutions of the thermometers. This is crucial for many advanced applications, such as employing nanothermometers in measuring the temperature inside human cells or for detecting hot spots in microelectronics.

One of the goals which still remains in the field is developing multifunctional materials, ones which can combine thermometry with for example drug delivery and release, magnetism, or even catalytic performance.

In this presentation, we will show our ongoing efforts to develop multifunctional materials, based on purely inorganic nanomaterials, Metal Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), and Periodic Mesoporous Organosilicas (PMOs). Depending on the desired properties and aimed applications we can design and build various architectures - from core-shell nanoparticles to nanorattles with hollow voids, nanoplatforms and nanocomposites. Do we always need such complex materials to achieve the desired goal? And are the possibilities endless and limited only by the scientist's imagination?

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Prof. dr. Anna Kaczmarek  
Department of Chemistry  
Ghent University

Anna Kaczmarek received her master's degree in chemistry from the Adam Mickiewicz University in Poznan, Poland in 2010. In 2015 she defended her PhD in Chemistry at Ghent University. During her post-doctoral research, including several long stays abroad at Cordoba University, Spain and Utrecht University, the Netherlands, she developed her own research line of luminescence thermometry employing inorganic and hybrid organic/inorganic nanomaterials, MOFs, COFs, and PMOs. In 2020 she obtained a permanent position at the Department of Chemistry and started the NanoSensing group. In late 2020 she also obtained a prestigious ERC Starting Grant on the topic of thermometry for theranostic applications. In her work she is especially interested in interdisciplinary research where nanothermometers based on inorganic and hybrid nanomaterials can be combined with other fields e.g. biomedicine, chemical reaction monitoring, nanoelectronics.

## Poster session

### Masterstudents

Title	Authors
X-Ray Fluorescence Based Elemental Analysis of Biological Model Organisms	Carmen Aragon Grau, Laszlo Vincze
Poly(2-oxazoline) based thermoresponsive cell supports via solvent electrospinning.	Jonas De Breuck, R. Merckx, M. Purino, O. Frateur, V. R. de la Rosa, Richard Hoogenboom
Uncovering overinterpretations of NICS using a density perspective	Aaron De Clercq Daria Tolstykh, Sofie Van Damme and Guillaume Acke
Towards the development of antimicrobial hydrogel-based wound dressings for burn wounds	Nicolas Deroose, Manon Minsart, Peter Dubruel
Capturing Electron Correlation by Imposing Average Projected Spin	John De Vos, Xeno De Vriendt, Guillaume Acke, Patrick Bultinck
Simultaneous nanothermometer-catalysis platforms based on Metal Organic Frameworks (MOFs) doped with lanthanide nanoparticles	Jordi Jaenen, Anna Kaczmarek
Exploiting the network architecture of thiol-ene photo-crosslinked PCL for biomedical applications	Astrid Quaak, Quinten Thijssen, Sandra Van Vlierberghe

### Phd students and post-docs

Title	Authors
Trace-element analysis of mineral grains in Ryugu rock fragment sections by synchrotron-based confocal X-ray fluorescence	Benjamin Bazi, Laszlo Vincze
Nucleation and morphology variations in a UiO-66 MOF family	Marek Belis, Kristof Van Hecke
Turning 3D-COFs into luminescent ratiometric thermometers	Laurens Bourda, S. Mohanty, M. Peng, H. Rijckaert, P. Van Der Voort, A. M. Kaczmarek, Kristof Van Hecke
The aqueous surface chemistry of metal oxide nanocrystals: from fundamental insights to CT imaging	Loren De Block, E. Goossens, J. De Roo, Klaartje De Buysser
'Fully Conjugated Donor-Acceptor Covalent Organic Frameworks for Photocatalysis	Yoran De Smet, Gilles Matthys, Pascal Van der Voort
Molecular Dynamics Simulations on an InP Quantum Dot Model System Reconstructed from STEM Images	Kim Dümbgen, Zeger Hens
Amphiphilic poly(2-oxazoline)s : a promising material for conventional and Pickering emulsion stabilization	Valentin Bardoula, Richard Hoogenboom
Molecular Engineering of Light-Stabilized Dynamic Materials	Alyssa Ghielmetti, Filip Du Prez
Eco-friendly catalysts for cross-coupling reactions	Yaxu Liu, Catherine Cazin
A simple synthetic entryway into new families of NHC-gold-amido complexes and their in vitro antitumor activity	Ekaterina Martynova , Thomas Scattolin, Enrico Cavarzerani, Min Peng, Kristof Van Hecke, Flavio Rizzolio and Steven P. Nolan
Improving green Yb <sup>3+</sup> /Er <sup>3+</sup> upconversion luminescence by co-doping metal ions into an oxyfluoride matrix	Sonali Mohanty , Anna Kaczmarek
Investigating the stereochemistry of Entolysin A and B to gain insight into their mode of action.	Penthip Muangkaew, Annemieke Madder
Colloidal III-V Quantum Dot Photodiodes for SWIR Photodetection	Jari Leemans, Zeger Hens
The self-oriented La <sub>2</sub> O <sub>3</sub> layer: an integration tool for thin films	Ewout Picavet, Hannes Rijckaert, Dries van Thourhout, Jeroen Beeckman, Klaartje De Buysser
Mechanosynthesis of transition-metal catalysts.	Gianmarco Pisani, Catherine Cazin

Biocompatible upconverting Yb <sup>3+</sup> -Er <sup>3+</sup> -Co-doped inorganic Na <sub>3</sub> ZrF <sub>7</sub> nanoparticles, and hybrid PMO@Na <sub>3</sub> ZrF <sub>7</sub> nanoparticles for temperature sensing in the physiological range	Simona Premcheska , Anna Kaczmarek
Novel building block towards highly functionalized cyclopentanoid scaffold	Bram Ryckaert, Johan Winne
Towards intestinal tissue engineering exploiting gelatin-based inks - influence of stiffness and 3D morphology on cell response	Anna Szabo, Sandra Van Vlierberghe
Covalent ligands on the rise: Discovering new furan-equipped peptide and protein ligands for crosslinking onto cell surface receptors	Laure Tack, Annemieke Madder
New Cysteine-analogue Strategies for Bioengineered Peptide Stapling and Helical Stabilization	Atiruj Theppawong, Annemieke Madder
Application-Grade InP-Based Quantum Dots'	Hannes Van Avermaet, Zeger Hens
Biomaterials Unraveled: At the Interface of Materials Science and Molecular Modeling	J. V. Meerssche, J. Vekeman, J. V. Hoorick, R. Aerts, T. Verstraelen and S. Van Vlierberghe
Circular Thermoset Materials: New Generation of Sustainable Materials	Filip Van Lijsebetten , Filip Du Prez
Raman Spectroscopy as a tool for archaeometric research	Eva Vermeersch, Peter Vandenaabeele
Energy transfer photocatalysis enabled by Gold N-heterocyclic carbene complexes	Vladislav Voloshkin , Ekaterina A. Martynova, Sebastien G. Guillet, Francis Bru, Marek Beliš, Kristof Van Hecke, Catherine S. J. Cazin and Steven P. Nolan
Supramolecular peptide hydrogels for delivery of therapeutic agents	Hue Vu , Annemieke Madder

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