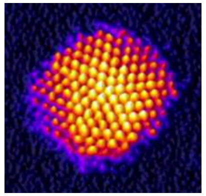

# SEPTEMBER 11 – 14, 2017
# CATALYSIS & NANOPARTICLES SUMMER SCHOOL
# KU Leuven, Belgium

## PROGRAMME

FOUNDATIONS OF CATALYSIS AND NANOSCIENCE
REAL SCIENTIFIC CHALLENGES IN CATALYSIS
SYNTHESIS AND PERFORMANCE OF NANOMATERIALS FOR CATALYSIS
CHARACTERISATION OF NANOMATERIALS FOR CATALYSIS
THEORY OF NANOMATERIALS FOR CATALYSIS
SCALE-UP AND VIABILITY OF NANOMATERIALS FOR CATALYSIS
ENVIRONMENT, SAFETY AND HEALTH OF NANOMATERIALS
THE ROLE OF CATALYSIS IN CLEAN ENERGY AND CLIMATE ACTION

CatSense

**WWW.CATSENSE.EU**

CHAIR: PETER LIEVENS
SCIENTIFIC SECRETARY: DIDIER GRANDJEAN

KU LEUVEN



MEDIA PARTNER

ECOTIPS

Vlaanderen in Actie Pact 2020

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RICHTING MORGEN MET WETENSCHAP, TECHNOLOGIE, CREATIVITEIT & INNOVATIE

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CatSense

Catsense has received funding from the European Union’s Seventh Framework Programme for research, technological development and demonstration under grant agreement number 607417, Marie Curie Actions – International Training Network.

## Programme

**Monday September 11**

09:00 – 09:30 Registration and Welcome at Maria-Theresiacollege

Session 1: Catalysis & Nanoparticles and its challenges

09:30 - 11:00 Kurt W. Kolasinski (West Chester University, USA)

Nanoscience - From curiosity driven research to practical results.

Coffee / Tea Break

Session 2: Theory of nanomaterials for catalysis

11:30 - 12:30 Francesca Baletto (King's College London)

New routes to model metallic nano catalysts

Lunch

Session 3: Environment, Safety & Health of Nanomaterials

14:00 – 15:30 Hilda Witters & Lieve Geerts (VITO, BE)

Exposure & hazard assessment

Risk assessment & management, incl. safe by design

Coffee / Tea Break

16:00 – 17:30 Poster Session



18:00 – 19:00 Welcome Reception

By the Mayor of Leuven, Louis Tobback and

by the Vicerector of KU Leuven, Prof. Peter Lievens

Location: Leuven City Hall

**Tuesday September 12**

Session 4: The role of catalysis in clean energy and climate action

09:00 - 10:30 Ib Chorkendorff (TU Denmark): The use of mass selected clusters for Oxygen reduction, oxygen evolution (water splitting) Hydrogen evolution and for CO2 hydrogenation.

Coffee / Tea Break

10:45 - 12:00 Isotta Cerri (Toyota Motor Europe): Fuel cells for automotive applications

12:00 – 12:30 Katrien Rycken (Leuven 2030): Leuven, European Green Leaf Award 2018

Lunch

Session 5: Scale-up and viability of nanomaterials for catalysis

14:00 – 15:30 Crina Corbos (Johnson Matthey)

Industrial Catalysis

Coffee / Tea Break

Session 6: Synthesis and performance of nanomaterials for catalysis

16:00 – 17:30 Johan Martens (KU Leuven) &

Jolien Dendooven (U Gent)

Tailoring nanoporous materials by atomic layer deposition

19:00 - 22:00 Dinner at Faculty Club

Dinner Speaker: Mohamed Ridouani (City of Leuven): Leuven, carbon neutral by 2030

Winner 2018 - Leuven

EUROPEAN GREEN LEAF

An initiative of the European Commission



**Wednesday September 13**

Session 6 (continued): Synthesis and performance of nanomaterials for catalysis

09:00 - 10:30 Stefan Vajda (Argonne National Lab, USA)

Catalysis and Electrocatalysis by Size and Composition Selected Clusters

Coffee / Tea Break

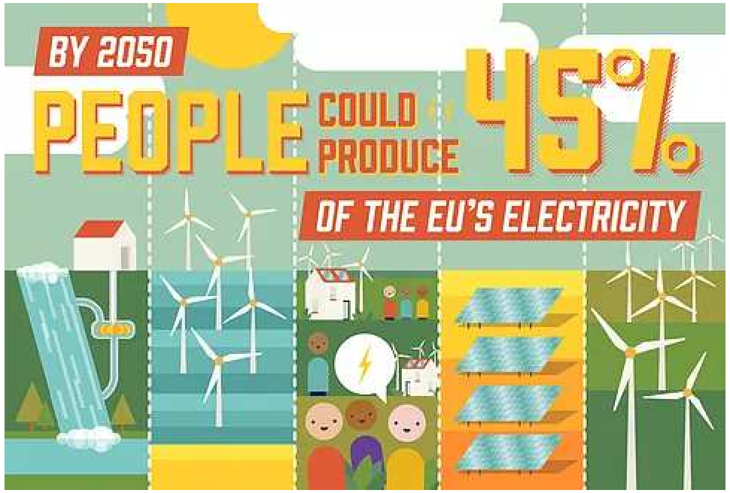
11:00 - 12:30 Maarten Mees (imec, Belgium)

All-solid-state Li-ion batteries

Lunch

14:00 - 19:00 Excursion to the Hydropower Station of Ecopower on the Dyle River ("Molen van Rotselaar")

Guided tour of the facilities and presentation by Dirk Vansintjan, CEO of Ecopower CVBA



**Thursday September 14**

Session 7: Characterization of Nanomaterials for Catalysis

09:00 - 10:00 Jin Won (Maria) Seo (KU Leuven, Belgium)

Photocatalytic behavior of potassium-doped TiOx nanostructures produced by wet-corrosion process

10:00 - 11:00 Olga Safonova (Paul Scherrer Institut, Switzerland)

How in situ X-ray spectroscopy can help rational design of better catalysts.

Coffee / Tea Break

11:30 - 12:00 Closing Remarks

12:00 - 13:00 Lunch

End of Summer School

**Monday September 11**

Session 1: Catalysis & Nanoparticles and its challenges

09:30 - 11:00 Kurt W. Kolasinski (West Chester University, USA)

**Nanoscience - From curiosity driven research to practical results.**

The routine attainment of ultra-high vacuum, invention of pulsed lasers, development of scanning probe techniques and advances in high-speed electronics lead to a golden age of discovery in surface science. Key facets of surface structure (geometrical and electronic) and their response to reactive environments have been elucidated. The dynamics of energy transfer between molecules and surfaces, electrons and phonons have been mapped out to allow insights into chemical bond breaking and formation in real time. Advances in surface science with its inherently multidisciplinary perspective spawned nanoscience, which shares with it a blurring of the boundaries of between scientific and engineering disciplines that is heightened by a sharpened focus on the interfaces between materials, synthesis and characterization. The challenge of nanoscience is to transform the discovery of new phenomena, techniques and materials into understanding that leads to more efficient and sustainable industrial process and products. Examples from heterogeneous catalysis (ammonia synthesis), charge transfer dynamics (electron transfer at the liquid/solid interface) and materials synthesis (formation of nanowires, porous and pillared silicon) will be discussed.



**Kurt W Kolasinski** has been Professor of physical chemistry at West Chester University since 2014 having joined the faculty in 2006.

He received his BS in Chemistry from the University of Pittsburgh, where he performed undergraduate research with John T. Yates, Jr. Richard N. Zare was his PhD thesis advisor at Stanford University, where they used laser spectroscopy to investigate the dynamics of molecules scattered and thermally desorbed from solid surfaces.

He assumed an Alexander von Humboldt Fellowship to work in Gerhard Ertl's division of the Fritz-Haber-Institut in Berlin (1991–1994). Under the direct supervision of Eckart Hasselbrink, he studied laser induced desorption, thermal desorption and catalytic reactions on surfaces with the aid of laser and electron energy loss spectroscopy. He returned to the US as a National Research Council Resident Research Associate at the National Institute of Standards and Technology in Gaithersburg, MD then held faculty positions at the University of Birmingham (UK) (1995–2001), Queen Mary University of London (2001–2004), and the University of Virginia (2004–2006). His research focuses on surface science, laser/surface interactions and nanoscience. A particular area of expertise is the formation of semiconductor nanostructures and porous silicon using a variety of chemical and laser-based techniques. Instrumental in establishing an initiative at UVA concerning sustainability and energy issues, he continues to be active in this area at WCU.

He is the author of over 100 scholarly publications as well as the textbooks *Surface Science: Foundations of Catalysis and Nanoscience* and *Physical Chemistry: How Chemistry Works*.

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**Monday September 11**

Session 2: Theory of nanomaterials for catalysis

11:30 - 12:30 Francesca Baletto (King's College London)

**New routes to model metallic nano catalysts:**

**Searching and selecting the best metallic nanocatalyst for target applications**

Keywords: nanocatalysis, Pt-alloy, nanoparticles

Nanoclusters are today of widespread use in various applications, ranging from nanomedicine, to memory storage, nanooptics, nanoplasmonics, and nanocatalysis. Such a wide range of applications is possible because of a large variety of their peculiar chemo-physical properties can be tuned by playing with size, shape, and chemical composition of the nanoparticle itself. Indeed, the properties of a cluster depend on their geometry, although the structure-activity relationship is not fully understood yet. In this talk, I will try to elucidate this link with examples taken from nanomagnetism [1] and nanocatalysis [2]. I will show how geometrical quantities can be used to predict the qualitative behaviour of a metallic nano catalyst in a wide size range, up to a diameter of 11 nm, and to propose optimal structures. The effect of thermal stability and the role of structural transitions [3] is discussed.

**References**:

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**Francesca Baletto**

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Senior Lecturer in Physics

Education and previous appointments:
Feb. 1999: M.Sc. degree cum laude in Physics at Univ. of Genova, Italy
June 2003: Ph.D. in Physics at Univ. of Genova, Italy
Aug. 2003- May 2006: UNESCO fellow at ICTP, Trieste, Italy
May 2006 – Jul 2007: Research Assistant at DMSE, MIT, USA
August 2007 – March 2013: Lecturer in Physics, KCL, UK

My research focuses on the development and application of numerical simulations, both ab-initio and classical, for the investigation and the design of nanomaterials for target applications, with a focus to nanocatalysis. My work includes the modelling of the growth and nucleation; structural transitions; molecule adsorption, magnetic, and optical properties, and electron transfer processes in metallic nanoalloys, metallic surfaces and water systems. My research is funded by different research bodies, including EPSRC, EU COST-Action, FAPESP-KCL, CNPq. She is author of more than 40 publications with a h-index of 20; a book chapter for the Encyclopedia of Nanoscience (ed. Nalwa, 2004), and a chapter on "Modelling Janus Nanoalloys" for "Metal Clusters and Nanoalloys: From Modeling to applications" (ed. Springer, 2013).

**Monday September 11**

Session 3: Environment, Safety & Health of Nanomaterials

14:00 – 14:45 Hilda Witters (VITO, BE)

**Exposure & hazard assessment**

Innovative nanotechnology with the production of engineered nanomaterials and design of new processes is a scientific breakthrough in material design and the development of new consumer products. The successful implementation of nanotechnology will be illustrated and examples are given of the diversity of applications or products. In this respect, there is potential exposure to nanomaterials and the possible environmental health and safety (EHS) impact needs to be considered. Specific physicochemical properties of nanomaterials offer technological advantages, but can also generate hazardous biological outcomes. In order to assess the risks of nanomaterials, exposure and hazard assessment is needed. Based on a case study, a measurement strategy for workplace exposure will be demonstrated. During development of nanomaterials or nano-based processes, possible exposure scenarios at each life cycle stage are identified and monitoring is required to define hot spots. Furthermore, some methods for reliable testing of toxicity of nanomaterials for environmental organisms, or evaluation of human health endpoints are described. In this way, data on exposure and hazardous effects of nanomaterials are generated and together with physic-chemical characteristics, these are the input for an integrated risk assessment.



**Dr. Hilda Witters** has a Master degree in Biology and obtained her PhD at the University of Antwerp (Belgium) in 1990. She is project manager in the ABS team (Applied Bio & molecular Sciences) of the department Environmental Risk and Health at VITO (Mol, Belgium).

With a background in ecotoxicological research, and main expertise in the field of endocrine disruption and neurodevelopmental toxicity, she is dedicated to the development, validation and standardization of alternative methods for human and environmental hazard assessment. She is study director for toxicological studies which are run according to GLP qualifications (Good Laboratory Practice).

She is currently involved in several projects related to the safety of emerging compounds (neurotoxicity of chemicals and drugs, EFSA), new biobased chemicals or nanomaterials (H2020 project EC4SafeNano: http://www.ec4safenano.eu/ ).

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**Monday September 11**

Session 3: Environment, Safety & Health of Nanomaterials

14:45 –15:30 Lieve Geerts (VITO, BE)

**Risk assessment & management, incl. safe by design**

Risk assessment means comparing hazard and exposure data. Exposure concentrations below the toxicological limit mean that the risk is negligible. Exposures exceeding the safe value however pose a potential risk to human health or the environment; consequently the exposure has to be reduced by risk management measures. Such measures are by preference structural (e.g. closed process) or general (e.g. box-in-box packaging) and may be combined with personal protective equipment (e.g. respiration mask, gloves) suitable to reduce the exposure. The Safe-by-design approach is a risk assessment that identifies potential risks early on during the design of products or processes. So potential risks are identified before they occur; hence adequate risk mitigation for safe use can be implemented before the nanomaterials are actually manufactured or used. We will illustrate the theory with real examples from research projects on nanomaterials and with a computational risk banding tool.

In order to protect staff and keep them alert, each laboratory or industry working with nanoparticles should regularly train staff to use nanomaterials in a safe way. We will present a short overview of the nanosafety procedures implemented at VITO.



**MSc. Lieve Geerts** has a Master degree in biochemistry from the University of Leuven (Belgium), and a postgraduate degree in REACH and GHS from the University of Ghent (Belgium).

At VITO she is leader and scientific researcher in risk assessment projects. Her specialties are hazard and exposure assessment (including computational toxicology and exposure modelling), and risk characterisation and mitigation for workers, consumers and the environment.

She is involved in research projects based on the Safe-by-Design concept where product/process design and safety go hand in hand.

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16:00 – 17:30 Poster Session

**Spectroscopic characterization of copper clusters for catalytic CO2 fixation**
OLGA LUSHCHIKOVA (RADBOUD UNIVERSITY, THE NETHERLANDS)

**Rapid prototyping of integrated microfluidic electrochemical Organophosphate Pesticide biosensors**
WONDIMU ALEMU GEBREYES (UNIVERSITÀ DEGLI STUDI DI MILANO, ITALY)

**Composition dependent self-organization in $Au_xAg_{1-x}$ phase segregated nanostructures.**
TING-WEI LIAO (KU LEUVEN, BELGIUM)

**Reducibility of ZrO2-Based Catalysts: Role of Nanostructuring and Metal-Oxide Interface in Oxidation Reactions**
ANTONIO RUIZ PUIGDOLLERS (UNIVERSITY OF MILANO – BICOCCA, ITALY)

**Adsorption of propene on bare and yttrium doped gold clusters**
JÚLIA BARABÁS (Budapest University of Technology & Economics, Hungary)

**Adsorption of CO on neutral and cationic palladium doped gold clusters**
PIERO FERRARI (KU LEUVEN, BELGIUM)

β - **bismuth oxide nanocrystals / multi-wall carbon nanotubes nanocomposites**
ARVIND K. BHAKTA (UNIVERSITY OF NAMUR, BELGIUM)

**NiFe Clusters produced in Gas-phase by Laser Ablation as Model Electrode for the Oxygen Evolution Reaction in Water Splitting**
LISA GEERTS (KU LEUVEN, BELGIUM)

**Sintering study on Au and AuTi clusters**
YUBIAO NIU (UNIVERSITY OF BIRMINGHAM, UK)





18:00 – 19:00 Welcome Reception

By the Mayor of Leuven,
Mr. Louis Tobback and

by the Vicerector of
KU Leuven,
Prof. Peter Lievens

Location: Leuven City Hall

*Louis Tobback, Mayor*

*Leuven City Hall (Brabantine Late Gothic style, built 1448 - 1469)*

**Tuesday September 12**

Session 4: The role of catalysis in clean energy and climate action

09:00 - 10:30 Ib Chorkendorff (Technical University of Denmark)

**Catalysis for Sustainable Fuels and Chemicals: The use of mass selected clusters for Oxygen reduction, oxygen evolution (water splitting) Hydrogen evolution and for CO2 hydrogenation.**

In this presentation, we shall first emphasize the importance of energy and the size of the problem we are facing in such a transition. We expect that when becoming fossil free most of the energy will come in the form of electricity mainly from sun and wind, while biomass will also contribute. It shall be illustrated that there are plenty of such resources, but the challenge is to make them cheaper and in particular use them efficiently. We must learn how to store energy in another scale than what we know today so we have energy available when the primary sources such as sun and wind are not contributing.

A substantial part of our energy system can be electrified, but we must also make fuels for areas which cannot such as aviation and long transport haul. Chemical production is today also based on fossil fuels and must be revised. We shall discus new routes for chemical production and ideas of delocalization since the energy production will be delocalized. We shall touch briefly on our major research directions in relation to finding new and efficient catalysts for conversion of sustainable energy: We will describe the current limitations which will define our route forward[1]. We shall describe our approaches to water splitting both directly[2] and by coupling it to Photo-Electro-Catalysis[3] using earth abundant elements [4]. How we can find new catalysts for fuel cell converting the chemical energy back to electricity using Fuel cells[5,6]? In both cases the focus is on the Oxygen Evolution/Reduction Reactions since that is the most challenging. Concerning making chemical and fuels we shall discuss recent advances in $CO_2$ and CO hydrogenation[7,8,9] including the even more ambitious goal of making ammonia by hydrogenation $N_2$ electrochemically. We shall demonstrate our surface science approach for finding new and efficient catalysts and how we can make very well-defined nanoparticle by a mass-selected method[2,5] and hopefully help us designing new catalysts that can break the scaling relations.




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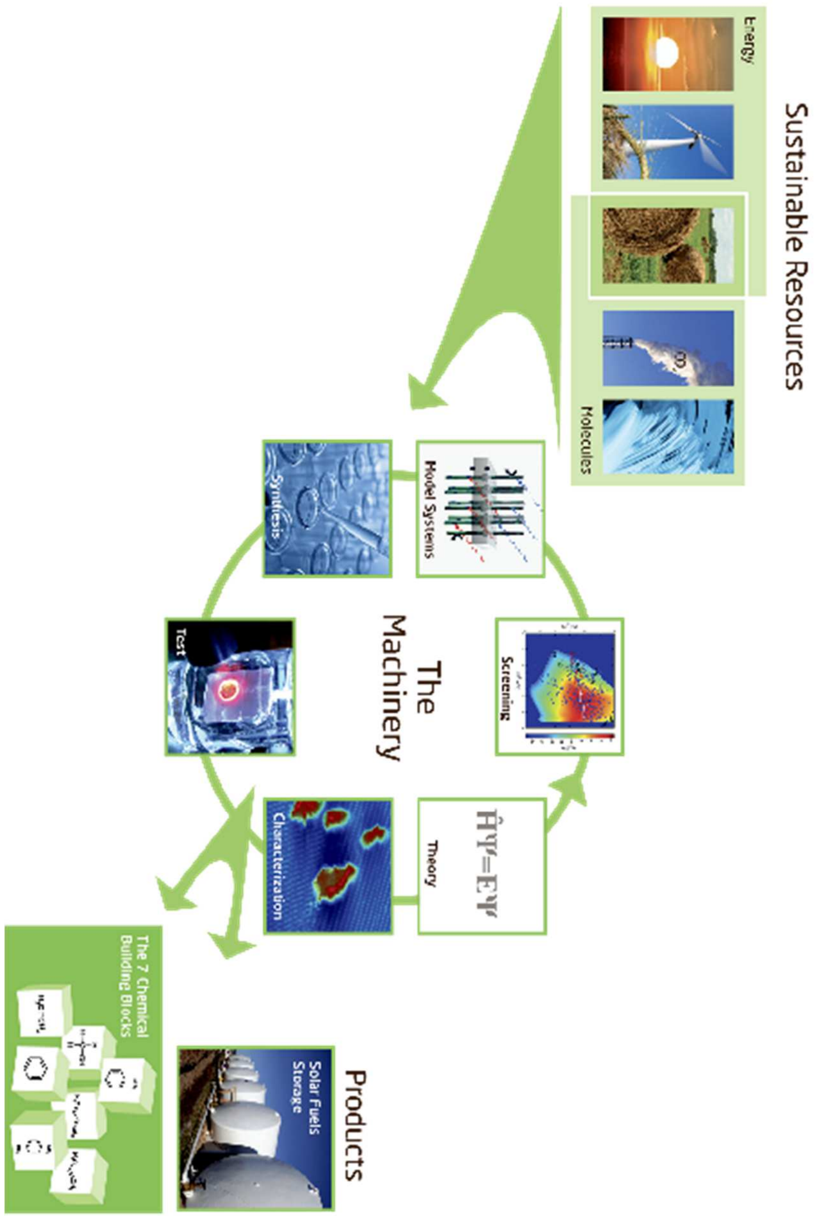




**Professor Ib Chorkendorff**

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Ib Chorkendorff is Professor in Heterogeneous Catalysis at the Technical University of Denmark.
He is also Director of The Villum Center for Science of Sustainable Fuels and Chemicals. He has been author and coauthor of more than 300 scientific papers and 17 patents. His teaching activities include experimental surface physics, nanomaterials, sustainable energy systems and further special courses in physics, while his research activities focus on investigating fundamental aspects of surface reactions and finding new and smart materials to improve energy production/conversion and environmental protection. He is co-founder of three start-up companies RENCAT APS, HPNOW APS, and Spetroinlets APS. He has collaborations with a number of industrial companies in Denmark like: Haldor Topsøe A/S, EEWI A/S, Danish Power Systems DPS, and Dinex A/S, DTI A/S.

Education and Professional Career:

1985 Ph.D. in Physics, Department Physics, Odense University
1986 - 87 Post-doc with Professor John T. Yates Jr., Surface Science Center, Univ. of Pittsburgh, USA.
1987 - 99 Associate Professor at the Department of Physics, Technical University of Denmark
1999 - Professor in Heterogeneous Catalysis, Dept. of Physics
2005-2015 Director of Center for Individual Nanoparticle Functionality
2013- Consulting Professor, SUNCAT, SLAC, Stanford University, Palo Alto, USA
2015- Co-founder of “HPNow APS”, “RenCat APS”, and "Spetroinlets APS”
2016- Director of the Villum Center for the Science of sustainable Fuels and Chemicals
2017 ERC-ADV grantee

**Tuesday September 12**

Session 4: The role of catalysis in clean energy and climate action

10:45 - 12:00 Isotta Cerri (Toyota Motor Europe)

**Fuel cells for automotive applications**

Hydrogen Fuel Cell Vehicles are zero-emissions vehicles that represent a viable solution to energy and climate change issues; hydrogen can be in fact generated by different energy sources. Toyota started the development of fuel cell technologies in 1992; after several model changes and 'limited market' introduction experience, in December 2014 Toyota launched a hydrogen fuel cell vehicle (Mirai) that in addition to a very attractive drivability features a cruising range of more than 500km, a cold-start capability at -30degC and about 3 minutes refuelling time.

The system uses in-house made components such as the fuel cell stack, the fuel cell boost converter, and the high-pressure hydrogen tanks. With a maximum power of 114 kW the Toyota fuel cell stack achieves a volumetric power density of 3.1 kW/L thanks to the design and manufacturing of a unique separator consisting of 3D fine mesh flow channels and an internal water circulation system that eliminate the use of any external humidifiers.

A new more compact, high-efficiency, high-capacity converter has been developed to boost the generated power to 650 volts, thereby downsizing the fuel cell stack and reducing the system costs. High pressure Hydrogen vessels with a three-layer structure made of carbon fibre-reinforced plastic are used to store hydrogen at 70 MPa at a world-leading 5.7 wt% hydrogen storage capacity (mass of stored hydrogen / mass of empty tank).

Toyota is now looking at the future planning to increase the production of the fuel cell vehicle in line with the high vehicle demand and solve the next technology challenges to be able to enter a mass scale production market at the advancement of a widespread hydrogen infrastructure.



**Dr. Isotta Cerri**

**Toyota Motor Europe, Belgium**

Dr. Isotta Cerri worked as scientific researcher on catalytic processes at Politecnico di Torino after receiving a PhD in Chemical Engineering on catalytic combustions.

She has been actively working in the field of fuel cell technologies for Toyota as from 2004 in the advanced technology department where currently she is leading the fuel cell, battery and robotics teams.

In the area of fuel cells she has been developing innovative electrode membrane assemblies based on newly developed material, structures and manufacturing processes.

For Toyota she has been involved in several bilateral cooperations in order to develop improved materials and production processes of the different components of the automotive fuel cell stack and high pressure hydrogen tanks to enable the commercialization of reliable and affordable fuel cell vehicles. She is the author of several publications and inventor of patents.

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**Tuesday September 12**

Session 4: The role of catalysis in clean energy and climate action

12:00 – 12:30 Katrien Rycken (Leuven 2030): **Leuven, European Green Leaf Award 2018**

Leuven has placed a strong focus on climate change, introducing a number of actions to achieve its goal of being carbon neutral by 2030. One example of this is the reinvestment of gains made from energy efficiency into new measures for green energy. Public participation features strongly in its climate and energy projects.

Rycken facilitated the establishment of the ngo 'Leuven 2030' with 60 partners of the Leuven community and helped it grow to more than 300 companies, organizations and citizens. She inspired many partners to collaborate on specific urban climate related challenges and focusses on building bridges whitin society. She's in charge of the professional development of the scientific, communicative, participatory, operational, financial aspects of the Leuven climate transition.



Since 4 years, **Katrien Rycken** is the coordinator of the citywide project 'Leuven 2030', previously known as 'Leuven Climate neutral 2030'. She graduated as a master in engineering architecture and studied urban geography in Toulouse, France. Rycken worked as a unit leader on integrated building projects at Grontmij (now Sweco), until 2013 when she started as the coordinator of 'Leuven 2030' at AGSL, the autonomous city department on urban development.

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**Tuesday September 12**

Session 5: Scale-up and viability of nanomaterials for catalysis

14:00 – 15:30 Crina Corbos (Johnson Matthey)

**Industrial Catalysis**

## Nanoparticles in Catalysis

Heterogeneous catalysis and nanotechnologies are very closely related fields. The ongoing demand for faster, more efficient and greener catalysts drive research into the synthesis of nanoparticles with well-defined sizes, shapes and compositions. Precise control of the nanoparticles is crucial to understand the structure-performance relationships in catalysis, which is critical to the design new NPs with optimized catalytic performances for practical applications. Advances in the characterization contributed to a great extent in understanding the synthesis and the properties of nanomaterials allowing for better materials design.



## Crina Corbos

I graduated from the department of Catalysis and Materials at Poitiers University, France, in 2007 in the field of Environmental Catalysis. My research was focused on NOx removal from automotive exhaust gas using NOX traps, understanding and improving their sulfur resistance. Shortly after my PhD, I joined Advanced Industrial Science and Technology center in Tsukuba, Japan (AIST) as invited researcher, where I continued to study other aspects of Emission control Technologies (Selective Catalytic Reduction and Three way catalysts). After 2 years in Japan, I come to Johnson Matthey as a Marie Curie fellow, based at Johnson Matthey Technological Center in Sonning Common, UK. My research during that time focused on the synthesis of nanoparticles with controlled morphology and their application in liquid phase catalysis. Since 2012, I'm working at Johnson Matthey technology center in Sonning common Uk as a scientist. I continue working in the heterogeneous catalysis field, with applications in pharma and fine chemical industry. My interests are in the development and characterization of new materials, in particular the preparation of nano-sized particles and nanostructured solids with application in the area of catalysis, biotechnologies and renewable energy.

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**Tuesday September 12**

Session 6: Synthesis and performance of nanomaterials for catalysis

16:00 – 17:30

Johan Martens (KU Leuven) & Jolien Dendooven (U Gent)

**Tailoring nanoporous materials by atomic layer deposition**

Atomic layer deposition (ALD) is a self-limited growth method which relies on sequential reactions of gas phase precursor molecules with a solid surface to deposit oxides, metals and other materials in an atomic layer-by-layer fashion. Owing to the unique surface-controlled chemistry of ALD, the technique offers means to precisely tune the pore size and chemical surface composition of nanoporous materials, and to produce replica materials. In addition, the nucleation controlled growth mode observed for noble metal ALD processes can be used advantageously to design spatial arrangements of metal nanoparticles deposits. ALD is therefore an enabling technology for the controlled atomic-scale design of supported model catalysts.

In this presentation, we will present examples of ALD strategies for the incorporation of Al and Ga acid sites and Pt nanoparticles in zeolites, the synthesis of Pt nanoparticles with tunable particle size and areal density, and the creation of Pt replicas of 3D porous materials with special pore architectures. Secondly, we will show how these materials offer unique and interesting properties for hydroisomerization and hydrocracking catalysis, and electrocatalysis. Our work demonstrates that the high control over material synthesis offered by ALD can enable an improved understanding of the relation between the structural properties and the catalytic performance.



**Johan Martens**

Johan A. Martens is professor of Physical Chemistry at the University of Leuven in Belgium. He is head of the Catalysis Division and affiliated with the Centre for Surface Chemistry and Catalysis. Prof. Martens is renowned for design of zeolites, ordered mesoporous and hybrid organic-inorganic materials for catalysis, molecular separation and controlled release. His research spans a wide application rage including environmental protection, solar fuels, pharmaceutical formulation and food science and technology. Prof. Martens embodies innovation with over 100 patent applications and foundation of 3 active spin off companies. He is recipient of Methusalem funding, the Highest level of structural funding by the Flemish Government granted to individuals in regard to proven excellence in research. Prof. Martens is an active member of the Royal Flemish Academy of Belgium for Sciences and the Arts.

**Jolien Dendooven**

Dr. Jolien Dendooven is affiliated with the CoCooN Research Group at the Department of Solid State Sciences of Ghent University, Belgium (UGent). She received her PhD in Physics from the UGent in 2012. Her PhD work focused on the modelling and characterization of atomic layer deposition (ALD) in nanoporous materials, especially for applications in catalysis. She introduced x-ray fluorescence (XRF) and grazing incidence small angle x-ray scattering (GISAXS) as novel approaches for synchrotron-based in situ characterization during conformal ALD and is currently exploiting these techniques to study ALD of noble metal nanoparticles through a FWO postdoctoral scholarship. Dr. Dendooven has co-authored 60 papers in the field of ALD.

19:00 - 22:00 **Dinner at Faculty Club**

Groot Begijnhof 14, Leuven




Dinner Speaker:

**Mohamed Ridouani** (Deputy Mayor, City of Leuven)

**Leuven, carbon neutral by 2030**

Since 10 years, Mohamed Ridouani is deputy mayor of the city of Leuven, responsible for Education, Economy, Sustainability and Urban Development. He graduated as a Master in economics and completed a post graduate in international relations. Ridouani worked as a business consultant at Deloitte, until 2007 when he exchanged the business world for local politics.

As deputy mayor, Ridouani succeeded in bringing people and organizations together, within the different fields of his office. He's the inspirer of Leuven 2030, in which more than 300 companies, organizations and citizens are united to turn Leuven into a sustainable city. Ridouani is also the founder of the education council which includes everyone in the educational field, and Leuven MindGate, a collaboration of different companies and institutions, to brand and boost Leuven's image as the world's hotspot for health, technology and creativity.

**Wednesday September 13**

Session 6 (continued): Synthesis and performance of nanomaterials

09:00 - 10:30 Stefan Vajda (Argonne National Lab, USA)

**Catalysis and Electrocatalysis by Size and Composition Selected Clusters -** Supported clusters made of a handful of atoms can be considered as tailorable models of the catalytic active site, and changes in the size and composition of the clusters by a single (ad)atom or changing the support can often dramatically alter their activity and selectivity.[1-2] The ligand-free clusters discussed in this talk are synthesized in the gas phase and, after mass selection deposited on oxide and carbon based supports. The primary focus of this presentation is on their size and composition uniform subnanometer clusters in heterogeneous catalytic and electrocatalytic reactions, while also providing select examples of comparison of performance with their nanometer size cousins. The first part of the lecture will aim on model catalysts interrogated under realistic reaction conditions of pressure and temperature using *in situ* X-ray characterization (scattering and absorption) combined with the monitoring of the reaction products, to correlate particle size/shape and oxidation state with catalytic performance, illustrated on the example of propylene epoxidation with molecular oxygen by subnanometer to nanometer size silver clusters/cluster assemblies[3,4] and on the example of low-temperature oxidative dehydrogenation of cyclohexane by subnanometer Cu, Pd and $Cu_xPd_y$ clusters.[5] In the second part of the presentation, the performance of Ag and other clusters in Li-Air batteries will be discussed.[6,7]

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**STEFAN VAJDA** E-mail: vajda@anl.gov

Stefan Vajda received his MS degree in Physical Chemistry and PhD in Chemistry at the Charles University in Prague. After receiving his PhD, he spent a year with Fulbright Fellowship at the University of Chicago. He completed his Habilitation in Experimental Physics at the Free University Berlin, before moving to the Argonne National Laboratory in 2002. Currently, he is a Senior Scientist at the Materials Science Division of the Argonne National Laboratory and Fellow of the Institute of Molecular Engineering of the University of Chicago. His current research interests include:

- Atomic clusters and cluster based materials.
- Nanocatalysis: Study of the cluster size/composition & function relationship at the sub-nanometer and nanometer scale, support effects in catalysis.
- Combined *in situ* synchrotron X-ray scattering, X-ray absorption and mass-spectroscopy studies of nanocatalysts under realistic reaction conditions.
- $CO_2$ and CO conversion; selective catalysis under low pressure and at low temperature.
- Oxidative dehydrogenation reactions, selective oxidation reactions.
- Electrocatalysis by clusters (water oxidation, $CO_2$ conversion).
- Clusters and cluster-based assemblies in Li-$O_2$ electrochemistry / Li-Air batteries.

**Wednesday September 13**

Session 6 (continued): Synthesis and performance of nanomaterials

11:00 - 12:30 Maarten Mees (imec, Belgium)

**All-solid-state Li-ion batteries**

Lithium ion batteries capture about 70% of the portable electronics market and replaced most of the nickel-metal hydride battery technology in hybrid electric vehicles and Plug-in electric vehicles. The energy and power density of the existing battery technology is however still not sufficient to cope with the future demands. Also, as personal electronic devices become smarter and smaller at the same time, the demand for more powerful batteries with smaller volumes grows. In many devices, the battery already takes up most of the available space. The issue is even larger for microsystems where battery power is needed for autonomous operations in e.g. wireless sensor networks (WSN), body area networks (BAN) and medical implants. Therefore, innovations in battery technology are desperately needed and the inclination towards disruptive technologies increases.

Together with world leading Li-ion cell developers/manufactures, imec is developing next generation battery technologies. In the past 7 years, we have made strong progress in the research and development of the all-solid-state Li-ion battery. In the all-solid-state cell, the (flammable) liquid electrolyte is replaced by solid electrolytes. Next to solving the issues with safety, the transition to a solid-state electrolyte can lead to significant improvements in the battery performance as well. We target higher energy densities, longer battery lifetime and wider temperature range of operation.



**Maarten J. Mees** received his PhD degree in Physics – titled 'First-principles Modeling of Nanostructured Materials for Energy Storage Applications' – from the University of Leuven, Belgium, in 2014.

From 2014 to 2015, he was a postdoctoral researcher at the Technical University of Eindhoven, working on atomic layer deposition of a solid-state Li-ion electrolyte.

In 2015 he started at imec, first as a project leader, and later as the R&D team leader of the energy storage activities. His current focus is on the development of solid-state Li-ion batteries.

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**Thursday September 14**

Session 7: Characterization of Nanomaterials for Catalysis

09:00 - 10:00 Jin Won (Maria) Seo (KU Leuven, Belgium)

**Photocatalytic behavior of potassium-doped TiOx nanostructures produced by wet-corrosion process**

Titanium oxide nanostructures doped with potassium (KTiOx) were prepared by the wet corrosion process (WCP) and systematically characterized. WCP is a simple, one-step process, which is based on the KOH treatment of Ti materials. Depending on the precise concentration of the KOH solution, the surface morphology and K-content of KTiOx can be controlled with high reproducibility. Variables such as surface area, pH of the treating solution and structural properties were evaluated, especially with respect to the photocatalytic behaviour of KTiOx in the decomposition of methylene blue (MB) and other dyes. The results demonstrate that the effect of the structural properties, the increased surface area and the negatively charged surface strongly affect the photocatalytic activity.



**Prof. Jin Won (Maria) Seo** is currently professor at the Dept. Materials Engineering (MTM) of KU Leuven. She joined KU Leuven in 2007 coming from EPFL in Switzerland where she was postdoctoral researcher and later scientific staff member at the Institute of Physics of Complex Matter IPMC. She graduated from RWTH Aachen and did her PhD at the Research Centre Jülich in Germany. She also worked at the Electron Microscopy Center EMAT of University of Antwerp in Belgium as well as at the IBM Zurich Research Laboratory in Switzerland.

Her research interest focuses on the synthesis, functionalization and application of nanoscale materials, mainly carbon-based nanomaterials, oxide nanomaterials and thin films. She is also interested in nanoscale characterization, especially by means of electron microscopy. She has published more than 150 publications in peer reviewed journals, 25 papers in reviewed proceedings and one book chapter. She is also co-inventor of 5 different patents.

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**Thursday September 14**

Session 7: Characterization of Nanomaterials for Catalysis

10:00 - 11:00 Olga Safonova (Paul Scherrer Institut, Switzerland)

**How in situ X-ray spectroscopy can help rational design of better catalysts.**

In the first part of the talk I will explain the basics of X-ray absorption fine structure (XAFS) methods and show how they can be used to probe electronic and geometric structure of nanoparticles as well as structure-activity relationships in catalysis.

Then I will present example studies illustrating how these spectroscopic methods helped to uncover the nature of active sites in catalysis and electro-catalysis allowing rational design of advanced materials.



**Dr. Olga Safonova** studied and obtained her PhD in Inorganic chemistry at the Lomonosov Moscow State University. Then she moved to Grenoble, where she did a postdoc and became a staff scientist at the European Synchrotron Radiation Facility working in the field of heterogeneous catalysis and X-ray absorption and diffraction methods.

Since 2010, she is a senior scientist at the Energy and environment division at the Paul Scherrer Institute in Switzerland. Her scientific interests are focused on the understanding of structure-activity relationships in heterogeneous catalysts involving metal and oxide nanoparticles, and isolated metal sites. Research projects of Dr. Safonova are focused on the development of time-resolved approaches and methods to access the structure of active sites in heterogeneous catalysts on the atomic scale. Her main expertise lies between chemical kinetics and in situ X-ray absorption fine structure (XAFS) techniques based of hard X-rays. Recently the work of Dr. Safonova was focused on the mechanistic studies of low temperature CO oxidation of ceria-based catalysts. During this period novel time-resolved XAFS methods and experimental approaches were developed, which allowed deciphering the structure of active sites, the nature of the rate determining step and the rational design of more active catalysts for low-temperature CO oxidation.

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