



**Joint Event**

Scholars International Conference on

# **Catalysis and Chemical Engineering & Scholars**

# **Frontiers in Chemistry Forum**

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**20-21 June 2022**

**NH Potsdam, Berlin, Germany**

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**Hosted By:**

Dileep | Program Manager  
Chemistry frontiers 2022 | CATCHEM 2022  
**SCHOLARS CONFERENCES LIMITED**  
21 Clifton Road, Newcastle Upon Tyne, England,  
United Kingdom, NE4 6XH  
chemistry@scholarscongress.org  
catalysis@scholarscatchem.com  
+447426060443



# SCIENTIFIC PROGRAM

Day 1 | June 20, 2022 | In-Person | Voltaire

08:00-09:00 Registrations

09:00-09:15 Opening Ceremony

## KEYNOTE FORUM

09:15-09:45 Title: Analysis of mechanism of phase separation in aqueous two-phase systems with ATR-FTIR spectroscopy

**Boris Zaslavsky**, Cleveland Diagnostics, Inc., USA

09:45-10:15 Title: There is plenty of room at the bottom

**Abraham Marmor**, Technion - Israel Institute of Technology, Israel

10:15-10:45 Title: Reviving the Coordination Chemistry of Sulfonium Cations

**Yuri Tulchinsky**, The Hebrew University of Jerusalem, Israel

## Networking and Refreshments Break @ Foyer 10:45-11:05

11:05-11:35 Title: Size-Selected Clusters: From Heterogenous Catalysis to Electrocatalysis and Li-O<sub>2</sub> Batteries

**Stefan Vajda**, J. Heyrovsky Institute of Physical Chemistry, Czech Republic

11:35-12:05 Title: Energy and Wild Plants as Renewable Resources for the Production of Biocomposites and Biofuel

**Sandra Bischof**, University of Zagreb, Croatia

## Scientific Sessions

12:05-12:25 Title: The Fermi level dependency on the catalytic activity of a semiconductor: A first-principles study

**Heechae Choi**, University of Cologne, Germany

12:25-12:45 Title: Upstream Development of Microbial Lipid Production

**Dania Awad**, Technical University of Munich, Germany

12:45-13:05 Title: Developing Vibrational Electronic Coupled Cluster (VECC) method: A novel approach for simulations of non-adiabatic vibrational resolved electronic spectra

**Songhao Bao**, University of Waterloo, Canada

## Lunch @ Restaurant 13:05-13:45

13:45-14:05 Title: Bioinspired CPs/AAO Janus Nanochannel Sensor for Effective Detection of HCHO

**Xuanjun Zhang**, University of Macau, China

14:05-14:25 Title: Alkaline oxygen evolution: Exploring Synergy between fcc and hcp Cobalt Nanoparticles Entrapped in N-doped Graphene

**Seulgi Ji**, University of Cologne, Germany

14:25-14:45 Title: Highly dispersed Pd nanoparticles confined in ZSM-5 zeolite crystals for selective hydrogenation of cinnamaldehyde

**Lujain Alfilfil**, Saudi Aramco, KSA

14:45-15:05 Title: Revisiting the identity of  $\delta$ -MgCl<sub>2</sub>: Structure and properties of nano-clusters by DFT, spectroscopy and machine learning. How modelling uncovers the origin of industrial catalysis

**Maddalena D'Amore**, University of Turin, Italy

15:05-15:25 Title: Benzoisothiazolone (BIT): A Fast, Efficient, and Recyclable Redox Reagent for Solid Phase Peptide Synthesis

**Pavan Kumar Reddy**, NSJ Prayog Life Sciences Pvt. Ltd., India

15:25-15:45 Title: Electrocatalytic Refinery for Sustainable Production of Chemicals

**Cheng Tang**, The University of Adelaide, Australia

**Networking and Refreshments Break @ Foyer 15:45-16:05**

### Poster Presentations

16:05-16:20 Title: Novel Visible-Light-Induced Photocatalyst of Hydrophobic Copper doped Titanium Dioxide for Antibacterial Application

**Cheng Yee Leong**, Universiti Teknologi Malaysia, Malaysia

16:20-16:35 Title: Synthesis and Evaluation of C3/C9 Alkoxy Analogues of (-)-Stepholidine as Dopamine Receptor Ligands

**Hari Krishna Namballa**, City University of New York, USA

**Day 01 Ends**

**Day 2 | June 21, 2022 | Virtual | GMT+2**

11:00-11:15 Opening Ceremony

### Keynote Forum

11:15-11:45 Title: China's small-scale production and its change through the reform and opening-up policy

**Takeshi Mine**, University of Toyo, Japan

11:45-12:15 Title: Cobalt-based Carbon Monoxide Releasing Molecules (CORMs): Design, synthesis and anti-inflammatory activity

**Simone Carradori**, D'Annunzio University of Chieti - Pescara, Italy

12:15-12:45 Title: Advances in Compact NMR for Analysis of Complex Samples

**Alina Adams**, RWTH Aachen University, Germany

**Networking and Refreshments Break @ 12:45-13:00**

13:00-13:30 Title: Structure-based drug discovery enabled for membrane protein targets

**Michael Hennig**, leadXpro, Switzerland

13:30-14:00 Title: New Perspectives and Insights into Silver Catalyzed Direct Propylene Epoxidation

**Anne Gaffney**, Idaho National Laboratory/University of South Carolina, USA

### Scientific Sessions

14:00-14:20 Title: Creation of core-shell TiC-TiO<sub>2</sub> nanoparticles for visible-NIR-driven photocatalysis

**Sujun Guan**, Toyo University, Japan

14:20-14:40 Title: Ferroelectric Engineered Electrode-Composite Polymer Electrolyte Interfaces for All-Solid-State Sodium Metal Battery

**Yumei WANG**, National University of Singapore (Chongqing) Research Institute, China

14:40-15:00 Title: Synthesis and Properties of a Tetrahedral Fe Complex with Metal-Centered Chirality

**Koichi Nagata**, Tohoku University, Japan

15:00-15:20 Title: The Role of N and Pt co-dopants in Sequential and Vice-versa Mode Preparations on TiO<sub>2</sub> Photocatalyst for Photocatalytic Degradation of Methylene Blue Dye characteristics and dosage form designs

**Wan Izhan Nawawi Bin Ismail**, UiTM Cawangan Perlis Kampus Arau, Malaysia

**Networking and Refreshments Break @ 15:20-15:35**

- 15:35-15:55 Title: Efficacy assessment of natural zeolite containing wastewater on the adsorption behaviour of Direct Yellow 50 from; equilibrium, kinetics and thermodynamic studies  
**Eman Alabbad**, Imam Abdulrahman bin Faisal University, KSA
- 15:55-16:15 Title: DNA-scaffolded synthetic enzymes for tunable high performance catalysis  
**Valerie Welborn**, Virginia Tech, USA
- 16:15-16:35 Title: Engineered ACE2 Decoy Mitigates Lung Injury and Death Induced by SARS-CoV-2 Variants  
**Lianghui Zhang**, The University of Illinois at Chicago, USA
- 16:35-16:55 Title: The cancer target ribonucleotide reductase and its allosteric regulation  
**Chris Dealwis**, Case Western Reserve University, USA
- 16:55-17:15 Title: Catalysis in Nano- and Microreactors  
**Raed Abu-Reziq**, The Hebrew University of Jerusalem, Israel

### Poster Presentations

- 17:15-17:25 Title: Transition-Metal (Pt, Pd, Rh, Ru) Single-Atom Catalysts based on the ZnO(0001̄)-2x2 vacancy reconstructed surface: An ab-initio study  
**Jimena Magdalena Jacob**, Ensenada Center for Scientific Research and Higher Education, Mexico
- 17:25-17:35 Title: Examining the Degrading Effects of Acid Rain on Solar Panels and Its Reflectors  
**Leah Kim**, Regis University, USA
- 17:35-17:45 Title: Enhanced arsenic(V) removal by commercially available ion exchanger modified with La(III) ions  
**Sebastian Dudek**, Maria Curie-Sklodowska University, Poland
- 17:45-17:55 Title: Using of Chemically Modified Chitosan for the Sorption of some Toxic Metal Ions in Aqueous Systems  
**Huda Alghamdi**, Imam Abdulrahman bin Faisal University, KSA
- 17:55-18:05 Title: Studies spectroscopy FTIR of copolymers used as viscosity improvers for SAE 10W mineral oil  
**Ioana Stanciu**, University of Bucharest, Romania

**Day 02 Ends**

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## Joint Event

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# CATALYSIS AND CHEMICAL ENGINEERING & SCHOLARS FRONTIERS IN CHEMISTRY FORUM

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Keynote  
Speakers  
Day 1



**Boris Zaslavsky**

Cleveland Diagnostics, USA

**Analysis of mechanism of phase separation in aqueous two-phase systems with ATR-FTIR spectroscopy**

The mechanism behind liquid-liquid phase separation emergence in aqueous mixtures of two polymers remains poorly understood. We reported recently that analysis of the OH-stretch band by Attenuated Total Reflection-Fourier Transfer Infrared (ATR-FTIR) spectroscopy shows that the arrangements of H-bonds in coexisting phases of aqueous two-phase systems (ATPSs) formed by various pairs of polymers are different. In our previous study of the interfacial tensions of various ATPSs, we suggested that aqueous mixture

of two polymers at concentrations close to that of the phase separation threshold may be considered as a microheterogeneous system. We proposed that these systems form microdomains which differ in regard to the solvent features of water within them. Here, we examine the arrangement of H-bonds in different ATPSs formed by various polymers at a given composition (above binodal line) and of non-phase forming mixtures below the binodal line. We used ATR-FTIR spectroscopy to analyze the OH-stretch band and the model describing water as composed of four subpopulations characterized by Gaussian fractions representing subpopulations of water molecules with various H-bond strengths, geometry, and molecular arrangements. We now show experimentally that the phase transition in terms of H-bond rearrangement in aqueous mixtures of two polymers occur below the binodal line. These data strongly support our previous hypothesis that dissimilar microdomains appear prior to observed phase separation with their dissimilarity increasing with the concentration of the two polymers. Similar effects are observed in a single polymer-salt aqueous mixtures. We conclude that the formation of these microdomains, specifically their increase in size and dissimilarity, initiate phase separation in ATPS.



**Abraham (Avi) Marmur**

Technion – Israel Institute of Technology, Israel

**Biography**

Abraham (Avi) Marmur is a professor emeritus of chemical engineering at Technion – Israel Institute of Technology. He has worked and published in the field of interfacial phenomena for about forty-five years, has published extensively in this field and relat-

ed research areas, and has been consulting for major companies. He has also participated in many international conferences and has been active in lecturing in universities and industrial sites in many countries. At Technion, professor Marmur received awards for excellence in research and in teaching. In addition, he was an editor of Reviews in Chemical Engineering, and was on the advisory committee of Journal of Colloid and Interface Science and Journal.

**There is plenty of room at the bottom**

This lecture discusses new insights concerning phenomena in Nano-systems that have been either only partially understood for a long time or not recognized at all. Example of such systems to be discussed include the interfacial region between a liquid and a fluid, nano-particles nucleation during phase change, and nano-roughness-induced non-wettability. The lecture will show how relatively simple theories may still give much insight into complex phenomena.



### Yuri Tulchinsky

The Hebrew University of Jerusalem, Israel

### Biography

Yuri Tulchinsky has completed his PhD at the Technion – Israeli Institute of Technology in the field of organometallic chemistry with Prof. M. Gandelman in 2014. He then joined the group of Prof. M. Dinca at MIT where he worked on metal organic frameworks (MOF). Since 2018 Dr. Tulchinsky has been appointed as an Assisting Professor at the Hebrew University of Jerusalem. His research interests span different areas of organic, organometallic and supramolecular chemistry, in particular, development of unusual ligand frameworks for future applications in homogeneous catalysis.

### Reviving the Coordination Chemistry of Sulfonium Cations

More than a century old, sulfonium ions are still intriguing species in the landscape of organic chemistry. On one hand they have found broad applications in organic synthesis and material science, but on the other hand, while isoelectronic to the ubiquitous tertiary phosphine ligands, their own coordination chemistry has been neglected for the last three decades. Only a handful of crystallographically char-

acterized sulfonium complexes of Mo(0), W(0), and Mn(I) were reported, where these ligands exhibited strongly  $\pi$ -acidic character. Similar with phosphine ligands, sulfonium ligands also have low lying  $\sigma^*$ -orbitals, which can accept electron density. However, because of the positive charge, there may be repulsion between sulfonium and the metal center. This repulsion can be overcome by introducing supporting donor arms, so we designed the pincer ligands with two phosphine supporting donors and tripodal ligand with three supporting phosphine donors. Here we present the synthesis and full characterization of the first Rh(I) and Pt(II) complexes of pincer and tripodal sulfonium ligands. Moreover, for the first time, the coordinating ability of an aromatic sulfonium has been established. A thorough computational analysis of the exceptionally short S-Rh bonds obtained attests for the strongly  $\pi$ -accepting nature of sulfonium cations and places them among the best  $\pi$ -acceptor ligands available today. Our calculations also show that when embedded within a pincer framework their  $\pi$ -acidity is enhanced. Therefore, in addition to the stability and modularity that these frameworks offer, our pincer complexes might open the way for sulfonium cations to become powerful tools in  $\pi$ -acid catalysis.

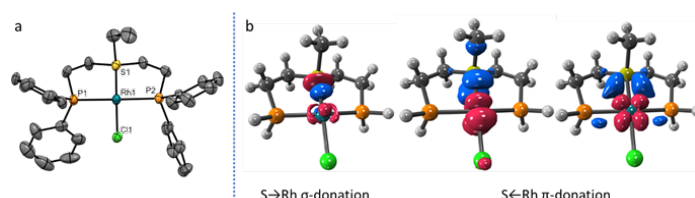


Figure 1: Representative example of RhCl complex of aliphatic sulfonium pincer (a) and deformation density plots of  $\sigma$ - and  $\pi$ -interactions between the S and Rh atoms (b).

**Stefan Vajda**

J. Heyrovsky Institute of Physical Chemistry, Czech Republic

**Biography**

Stefan Vajda is currently the head of the recently established Department of Nanocatalysis of the J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Science located in Prague. He is also the ERA Chair holder at the Institute. Stefan pioneered the studies of atomically precise size- and composition selected subnanometer size cluster-based catalyst under realistic reaction conditions of temperature and pressure in industrially relevant processes. Stefan received his Diploma (MSc) degree in Physical Chemistry and his PhD in Chemistry from Charles University in Prague, and habilitated from Experimental Physics

at the Freie Universität Berlin. His awards include a Fulbright Fellowship spent at the University of Chicago. Before returning to Prague in 2019, Stefan was active at the Freie Universität Berlin and Argonne National Laboratory US. During his career, Stefan published over 120 peer-reviewed articles and book chapters, has 7 issued US patents and presented over 80 invited talks at international conferences.

**Size-Selected Clusters: From Heterogeneous Catalysis to Electrocatalysis and Li-O<sub>2</sub> Batteries**

In this presentation, we will provide an overview of recent results which emerged from the studies of the performance of supported size-selected clusters in a variety of reactions, from heterogeneous to electrochemical and batteries, discussing the effect of cluster size and composition along the role of the support and reaction conditions.

While the main focus of the paper will be on (electro) catalysts made of monodisperse subnanometer clusters, unexpected propensities of under reaction conditions dynamically formed nanoassemblies will be discussed as well. In the last part of the paper, as time shall allow, we will highlight the opportunities provided by atomic precision design of bimetallic clusters in fine-tuning their performance and their bifunctionality in industrially relevant reactions.

**Sandra Bischof**

University of Zagreb, Croatia

**Biography**

Sandra Bischof is Professor of Textile Technology at the University of Zagreb Faculty of Textile Technology (TTF), Department of Textile Chemistry & Ecology and Head of the Textile Science Research Center (TSRC) at TTF. Within the period 2012-2018 she was Dean of the TTF. Her research area is chemical modifications of cellulose (textiles, wood and paper), functionalization of textiles for advanced and protective purposes (Durable Press, flame retardant, antimicrobial, UV, microwave, hydro/oleophobic protection), advanced technologies (plasma, UV, MW treatments), nanotechnology & nanosafety, biofibers and nano-bio composites. She has received several awards for the scientific excellence from Croatian Ministry of Science, Educa-

tion and Sports (2009), University of Zagreb (2009), City of Zagreb (2012) and Annual State award for 2019 in the category Scientific Achievements in the Technical Field (2020). She has published more than 140 research articles of which 30 in SCI(E) journals.

**Energy and Wild Plants as Renewable Resources for the Production of Biocomposites and Biofuel**

The research involved four different feedstocks derived from annually renewable resources (Virginia mallow, Arundo donax and Gigant Miscanthus) and from abundant waste (Spanish Broom). Applied biomass was used to produce fibers and biofuels. Solid waste from the fibres production which amounts up to 50%, presents valuable resource to be used to produce biofuel. According to the principles of green chemistry to design safer products and to use safer solvents and reaction conditions, harsh alkali solvents were substituted with environmentally friendlier solutions. Reaction conditions and energy efficiency were improved in a way that instead of high consumption of electric energy, microwave energy was used for the pretreatment of biomass in the production of textile fibres. Excellent energy properties were confirmed with the results of high values of carbon and hydrogen. The results revealed that 2.2-2.6 kg of plants is required for the production of 1 kg of fuel, confirming our assumption of acceptability of chosen ligno-cellulosic biomass for the production of high-quality fuel.

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Speakers  
Day 1

**Heechae Choi**

University of Cologne, Germany

**Biography**

Heechae Choi received his Ph.D degree in 2012 in Hanyang University (Seoul, Korea). After 4-year postdoctoral researcher period at Korea Institute of Science & Technology (KIST), he founded two companies, Virtual Lab Inc. and Materials Data Corp., which provide materials simulation software and materials processing consulting service, respectively. From September of 2018, Dr. Choi works in University of Cologne as a research group leader.

**The Fermi level dependency on the catalytic activity of a semiconductor: A first-principles study**

Adsorption energy is the most important factor to de-

termine the catalytic activity of a material. In chemical adsorption (chemisorption) process, charge carriers can move through a created localization electronic state by charge transfer between adsorbates and a catalyst. The catalytic reaction on a metallic catalyst surface, changes in carrier concentration due to charge transfer are negligible because of the sufficient free electron carriers in metal catalysts. On the contrary, in a semiconductor, the possibilities of charge transfer between adsorbates and a semiconducting catalyst surface can be changed depending on the position of the Fermi level, which is manipulatable via doping/defect engineering, external control and so on. However, the influence of the changeable Fermi level on the adsorption energies has been mostly ignored so far. We motivated by the inevitable discrepancies of catalytic activity predictions using a conventional theoretical method to calculate the adsorption energies using Density Functional Theory (DFT). Herein, we introduce a simple way to predict catalytic activities with consideration of the varying Fermi level in a semiconductor and the variation of charge states of intermediates due to charge transfer during chemisorption process. For a prototype study, we computed the adsorption energies of  $\text{CH}_4$  dissociation on a  $\text{CeO}_2(111)$  surface, which is an n-type semiconductor with a band gap (3.2 eV) using ab-initio calculations. Our pioneering work suggests the simple way to optimize doping condition and the cocatalyst metals for improved catalytic reactivities.



**Dania Awad**

Technical University of Munich, Germany

**Biography**

Dania Awad (born in 1988) is a postdoc and team leader at the Werner Siemens Chair of Synthetic Biotechnology (WSSB) at the Faculty of Chemistry of the Technische Universität Munich (TUM). Dr. Awad received her doctorate degree in 2020 with Summa cum laude. Named as a Franz Effenberger fellow in 2021 by Clariant and the German Chemical Society (GDCh), her research activities are concerned with the application of multiomics techniques and analyses (genomics, transcriptomics, proteomics and metabolomics) to elucidate biocatalytic and metabolic processes that influence the conversion of various carbon and energy sources by microorganisms (yeast, bacteria and algae) into high-value products (e.g., biofuels, oleochemicals, bioplastics). Under the direction of Prof. Dr. Thomas Brück, Dr. Awad complements the WSSB's goals of producing sustainable products for the chemical, construction and pharmaceutical industries.

**Upstream Development of Microbial Lipid Production**

The use of Single Cell Oils (SCOs) as platforms for biofuels and oleochemicals production have garnered great interest. Commercialization of SCOs-based pro-

cesses remains hindered by its relatively high production cost and low overall yield. Hence, any significant improvement in raw materials cost and space-time yields is central to the accelerated industrial deployment of this promising technology. *Cutaneotrichosporon oleaginosus* is a prominent oleaginous yeast due to its wide substrate spectrum, high lipid titers and resistance to fermentative inhibitory compounds. In order to develop *C. oleaginosus* into an SCO production platform, we carried out a concerted approach encompassing: 1) Computational-based media optimization, whereby a Response Surface Methodology to guide and streamline the experimental media optimization matrix with 12 nitrogen and 10 carbon sources was employed. The resulting data provided new insights into *C. oleaginosus* physiology under variable nutritional states. 2) A systematic analysis of carbohydrate intake and metabolism, whereby a bottom-up proteomic approach allowed efficient matching of possible biomass feedstock. Relative quantification of spectral intensities from crude proteomic datasets enabled the identification of new enzymes and provided new insights into protein secretion and carbohydrases activities. 3) Valorization of algal waste biomass: whereby a single-step enzymatic hydrolysis to generate *Scenedesmus obtusiusculus* hydrolysate was developed, bypassing energy-intensive thermo-chemical pretreatment. The resulting hydrolysate was utilized as the sole carbon source for fermentative production of SCOs by *C. oleaginosus*, greatly decreasing the bioprocess production costs. 4) High-throughput strain development, whereby fast neutron irradiation was applied unprecedentedly for the rapid genetic enhancement of oleaginous yeasts, in conjunction with high-throughput selection- (cerulenin) and screening (miniaturized absolute lipid quantitation). Enhanced mutants displayed higher biomass and total lipid yield. 5) Currently, a multiomics approach to elucidate lipogenesis and identify metabolic bottlenecks, feedback regulation, and competing biosynthetic pathways, as well as targets for genetic engineering of this yeast, is in development.



**Songhao Bao**

University of Waterloo, Canada

**Biography**

Songhao Bao, currently a PhD student at University of Waterloo studying theoretical / computational chemistry which is an interdisciplinary subject that combines knowledge of chemistry, quantum physics and computer science to develop software and algorithms for molecular modeling. I pursue an academia career. I believe that the behavior of microscopic world (atom / molecule) could be understood at a fundamental level via first principles with the resort of computer simulations. This could be both beneficial for industry applications and metaphysically manifest my ultimate goal to seek the timeless truth of the world. However, I am also interested in some state of the art technology that have positive impact on humanity. I am especially interested in the application of artificial intelligence and believe that it is a game changer on many fields for both fundamental science and conventional industry

**Developing Vibrational Electronic Coupled Cluster (VECC) method: A novel approach for simulations of non-adiabatic vibrational resolved electronic spectra**

Non-adiabatic dynamics is associated with many photo-electron chemical processes where the nuclear motion of the molecule is strongly coupled with its electronic structure and the Born-Oppenheimer approximation becomes invalid. To simulate such dynamical process, vibronic coupling models need to be introduced. The construction of vibronic models is non-trivial. To avoid the divergence of the gradient at the conical intersection, diabaticization procedure need to be introduced to transform from adiabatic basis to diabatic basis.

In this talk, we introduce an efficient algorithm that could simulate the wave packet dynamics of the non-adiabatic vibronic models in diabatic basis. This approach parameterized the time-dependent wavefunction using coupled cluster-like exponential ansatz without introducing basis set. In this way, unlike conventional basis set based method to simulate the wave packet dynamics, our approach avoids exponential scaling over the size of the system. As a result, in our approach, the propagation is conducted by time integrations over coupled cluster residue equations, which involves a few tensor products and has classical-like (polynomial) scaling over size of the system.

As an application of our computational method, we simulate gas phase absorption electronic spectra of large organic compounds. This application would provide reference for characterizations for experimental chemists and what is more, it could potentially provide insights to photo-electron based chemical processes.

**Xuanjun Zhang**

University of Macau, China

**Biography**

Xuanjun Zhang is an associate professor at Faculty of Health Sciences, University of Macau. He obtained his PhD degree from University of Science & Technology of China. After working as postdoctoral fellow and visiting scientist at Shantou University, National University of Singapore, Linköping University, University of Washington, he started assistant professor position at Linköping University in 2011 and promoted to Decent in 2014. He moved to University of Macau in 2015. Dr. Zhang's research focuses on molecular probes and nanosensors for imaging/sensing and theranostics. He has published more than 140 SCI papers in international recognized journals such as *Angew. Chem.*; *J. Am. Chem. Soc.*; *Chem. Sci.*; *ACS Nano.*; *Coord. Chem. Rev.*; etc. with H-index 41.

**Bioinspired CPs/AAO Janus Nanochannel Sensor for Effective Detection of HCHO**

Probe reactivity has long been considered to play a key role in artificial nanochannel sensors, but systematic studies of membrane wettability on detection

performance are currently lacking. Inspired by biological aquaporins, we developed an effective strategy to regulate the hydrophilic/hydrophobic balance by the controllable in situ assembly of coordination polymers (CPs) using BDC-NH<sub>2</sub> on anodic aluminum oxide (AAO) nanochannels to promote HCHO detection. We found that the hydrophobic/hydrophilic balance in CP/AAO heterosomes plays significant roles in the effective detection of HCHO. The hydrophobic AAO barrier layer is necessary to support the confinement effect, while the hydrophilic CP surface is favorable for HCHO to access the channels and then condense with the responsive amine to generate a new imine. The optimized CP/AAO Janus device shows excellent performance in the quantitative analysis of HCHO over a wide range from 100 pM to 1 mM by monitoring the rectified ionic current.

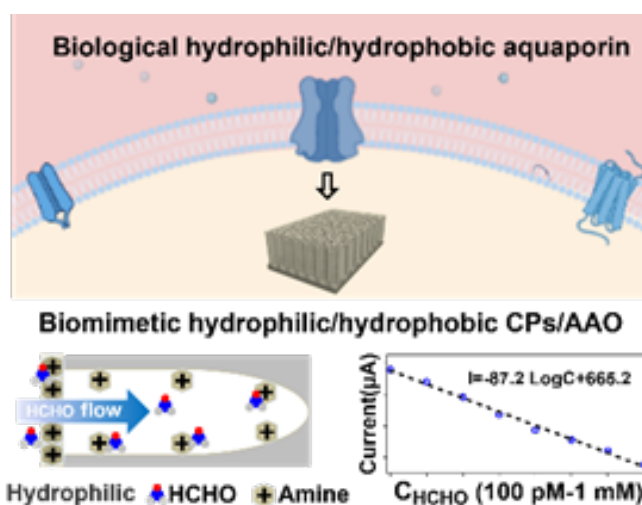


Figure 1. Schematic showing of bioinspired CP/AAO Janus nanochannel sensors for effective detection of HCHO over wide range from 100pM to 1mM.

**Seulgi Ji**

University of Cologne, Germany

**Biography**

Seulgi Ji studied Chemistry at the Chungbuk National University, South Korea and undergraduated as BS in 2014. Then, she received her MS in Chemistry at the University of Cologne, Germany in 2021. She joined the research group of Prof. Sanjay Mathur in 2021 and is currently working on her PhD program in the research group of Prof. Sanjay Mathur and Dr. Heechae Choi. Her research focuses on the electrocatalysis study using DFT calculations.

**Alkaline Oxygen Evolution: Exploring Synergy between fcc and hcp Cobalt Nanoparticles Entrapped in N-doped Graphene**

We synthesized a Mott-Schottky catalyst by entrapping cobalt nanoparticles inside the ultrathin N-doped graphene shell (Co@NC) with outstanding catalytic activity and long-term stability for oxygen evolution reaction (OER). Further, we theoretically demonstrated how the synergistic effect between hcp and fcc Co enhances the catalytic activity using Density Functional Theory (DFT) calculations. The hcp Co dominantly controls the surface reaction of electrocatalytic oxygen evolution, on the other hand, fcc Co involves in the formation of the built-in electric field at the interface with N-doped graphene. Especially, the built-in electric field between fcc phase of Co and N-doped graphene provides an additional driving force to prompts  $H^+$  ions transport away from the carbon surface to prevent the local pH reduction near catalytic surface. Our work can potentially provide a new strategy to design of heterogeneous catalysts for water electrolysis, oxygen reduction reaction, and so on.

**Lujain Alfifil**

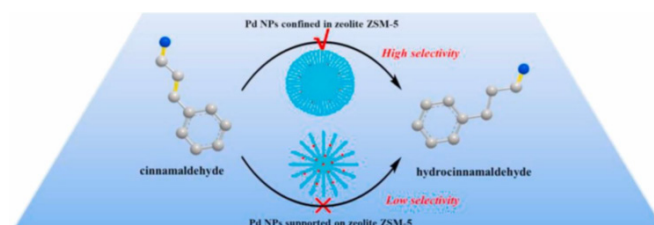
Saudi Aramco, KSA

**Biography**

Lujain R. Alfifil is a Chemist who graduated in 2009 from King Faisal University, Saudi Arabia, with a Bachelor Degree of Science in Chemistry. Received her Master Degree in 2013 from the University of New Brunswick, Canada. The research was about VUV double-photoionization and ionic fragmentation of allene and 1,3-butadiene using synchrotron radiation at the Canadian Light Source facility, located at the University of Saskatchewan in Saskatoon. Joined Saudi Aramco Research and Development Center, Fuels and Chemicals Division in 2014. Successfully defended her Ph.D. dissertation in January 2022, titled encapsulation of metal particles in zeolite crystals for various catalytic reactions from King Abdullah University of Science and Technology, Saudi Arabia.

**Highly dispersed Pd nanoparticles confined in ZSM-5 zeolite crystals for selective hydrogenation of cinnamaldehyde**

Selective hydrogenation of  $\alpha,\beta$ -unsaturated aldehyde catalyzed by supported Pd nanoparticles (NPs) is challenging, especially under harsh reaction conditions. Here, we report a facile method to prepare a catalyst composed of highly dispersed Pd NPs (~2.6 nm) confined in zeolite ZSM-5 crystals. When used in the hydrogenation of cinnamaldehyde, the prepared catalyst (Pd@SG-ZSM-5) exhibited excellent performance for the selective production of hydrocinnamaldehyde (HCAL) due to the confinement effect. Compared with the traditional supported Pd catalyst prepared by impregnation, Pd@SG-ZSM-5 showed a 2.5-fold enhancement in the HCAL selectivity (73% vs. 30%). Liquid adsorption combined with infrared spectroscopy characterization revealed that compared with the traditional catalyst, Pd@SG-ZSM-5 adsorbed much less reactant as well as product molecules and desorbed the generated HCAL quickly, thereby suppressing the formation of by-products and leading to high selectivity of HCAL.



**Maddalena D'Amore**

University of Turin, Italy

**Biography**

Maddalena D'Amore is a Post-doc at University of Turin, research activity stands in the field of theoretical and computational chemistry and aims at the investigation of large dimensions systems by means of both periodic and cluster approaches. Grown up, at first, in a group of Gaussian developers she adopted quantum mechanical approaches mostly based on Density Functional Theory (DFT) to simulate structures, spectroscopic parameters, electric response and magnetic behaviour. Then, in the CRYSTAL group, her activity focused on simulation methods for solids, mainly on surface science topics: efficient and selective catalysts, materials for a wide range of energy, environmental and industrial applications.

**Revisiting the identity of  $\delta$ -MgCl<sub>2</sub>: Structure and properties of nano-clusters by DFT, spectroscopy and machine learning. How modelling uncovers the origin of industrial catalysis**

MgCl<sub>2</sub>-supported Ziegler-Natta (ZN) catalysts for olefin polymerization are intrinsically complex multi-component systems. Nano-size and disorder are key features of ZN catalysts; DFT modelling seems to be the most powerful weapon to get insights into these systems. A detailed investigation of the atomic dynamics in disordered and nanosized  $\Delta$ -MgCl<sub>2</sub>-supported ZN catalysts was performed by DFT spectroscopic simulations on both ordered and disordered models and related surfaces, coupled to Far-IR spectroscopy and inelastic neutron scattering (INS) on a series of activated samples. We concluded: the mechanical ball-milling of naked MgCl<sub>2</sub> not only promotes an increase in the total surface area, but also changes the relative extension of the surfaces and fosters the formation of the lateral surfaces exposing strongly acidic Mg<sup>2+</sup> sites (i.e., the (1 1 0), (0 1 2) and (0 1 5) ones) at the expenses of the basal (0 0 1) one. Theoretical calculation predicted the existence of several possible edges involving the (1 1 0) surface, they are remarkably relevant because they are supposed to be the privileged places for stereo-selective active sites. We also determined vibrational spectroscopic fingerprints of 50MgCl<sub>2</sub> and 50MgCl<sub>2</sub>/3TiCl<sub>4</sub> clusters obtained by non-empirical structure determination based on an evolutionary algorithm and DFT





**Pavan Kumar Reddy**

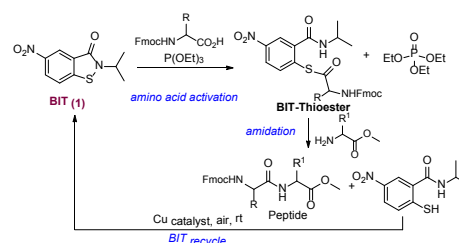
NSJ Prayog Life Sciences Pvt. Ltd., India

**Biography**

PavanKumar Gangireddy born in a village Simhadri-  
puram, Andhra Pradesh state, India, in the year 1978.  
He graduated from the Sri Venkateawara University,  
Thirupathi (2000) and completed Ph.D. under the su-  
pervision of Dr. Srivari Chandrasekhar from the Uni-  
versity of Pune, India (2010). After, he moved to pur-  
sue postdoctoral research at University of Rennes  
1, France (2011-2013) and subsequently to Emory  
University, USA (2013-2017) where he contributed  
for the significant inventions in the field of catalysis  
(a novel peptide catalyst) and novel therapeutics for  
neurodegenerative disorders (positive allosteric mod-  
ulators of NMDA receptor). Thereafter, he served as  
an assistant professor in the medicinal chemistry de-  
partment at NIPER-Hyderabad for 1.5 year where he  
developed BIT as an efficient and recyclable reagent for  
solid phase peptide synthesis. After scientific and  
professional enrichment, he was co-founded contract  
research and manufacturing service company NSJ  
Prayog Life Sciences Pvt. Ltd., for translating innova-  
tive academic research into industrial applications.

**Benzoisothiazolone (BIT): A Fast, Efficient, and Re-  
cyclable Redox Reagent for Solid Phase Peptide  
Synthesis**

In recent years, peptide therapeutics are drawing  
greater attention due to their high therapeutic effect  
and safety profile. In contrast to biochemical meth-  
ods, amidation via chemical synthesis can offer flexi-  
bility to access customized peptide sequences. Solid  
phase peptide synthesis (SSPS), a preferred synthe-  
tic tool to synthesize longer and complex peptide se-  
quences. In recent past significant technical advance-  
ment has been made in peptide coupling reagents,  
most of them successfully applied to SPPS. Howev-  
er, these reagents generate multiple equivalents of  
by-products for one equivalent of the desired peptide.  
The minimization of waste production and improve-  
ment of safety profile is key objective in large-scale  
production peptides that demands the development  
of a new coupling reagent with a catalytic turnover  
capacity or a stoichiometric recyclable ability. Previ-  
ously Liebeskind et al., demonstrated a catalytic pro-  
tocol for peptide synthesis using benzoisothiazolones  
(BITs) as a catalytic oxidant. As provided mechanistic  
investigations revealed that benzoisothiazolone (BIT)  
derived thioesters were excellent electrophiles readily  
reacts with amine to generate amide and o-mercap-  
tobenzamide. The o-mercaptobenzamide was easily  
oxidized to BIT under Cu catalyzed aerobic conditions  
(Scheme 1). We have demonstrated a fast and effi-  
cient coupling protocol for SSPS using BIT as acid ac-  
timator, which can be fully recycled. Full details of this  
protocol and its application will be discussed in the  
presentation.



Scheme1: BIT mediated peptide synthesis and recclle

**Cheng Tang**

The University of Adelaide, Australia

**Electrocatalytic Refinery for Sustainable Production of Chemicals**

Access to green, flexible and reliable energy and chemicals is the key to global sustainable development and increasing prosperity, especially in the post-COVID-19 and carbon-neutral economy. Aiming at creating changes in energy technologies and chemicals manufacturing, we proposed the electrocatalytic refinery (e-refinery) to defossilize, decarbonize and decentralize present chemical industry. We for the first time established the concept, principles, and methodologies of e-refinery. Based on it, we aim to develop new technologies that can creatively produce some key chemicals (e.g.,  $H_2$ , hydrogen peroxide, ammonia, formate, urea) directly from abundant sources (e.g., water, air,  $CO_2$ ) and powered by renewable electricity.

Specifically, we developed an efficient e-refinery strategy for producing  $H_2O_2$  directly from water and oxygen via two-electron oxygen reduction, which is of high flexibility to be operated in small scales and on demand. Our work innovatively engineers the structure of electrocatalysts at the molecular level, and has achieved present best activity and selectivity (> 95%) for  $H_2O_2$  production in both alkaline and acidic conditions. The obtained concentration of  $H_2O_2$  (> 1%) is high enough for practical applications such as disinfection and electro-Fenton water treatment. Besides, we also innovated the ammonia production technologies by electrocatalysis directly from air ( $N_2$  and  $O_2$ ) and water. We proposed for the first time bismuth catalysts for direct electrocatalytic nitrogen fixation into ammonia at ambient conditions. To address the significant drawbacks of tough  $N_2$  activation and poor  $NH_3$  selectivity, we developed a new two-step process through integration of plasma oxidation with electrocatalytic reduction, leading to ~2500 times higher yield and ~100% Faradaic efficiency. All the research in materials design and mechanism elucidation are achieved by combining atomic-level material engineering, electrochemical evaluation, theoretical computations, and advanced in situ characterizations



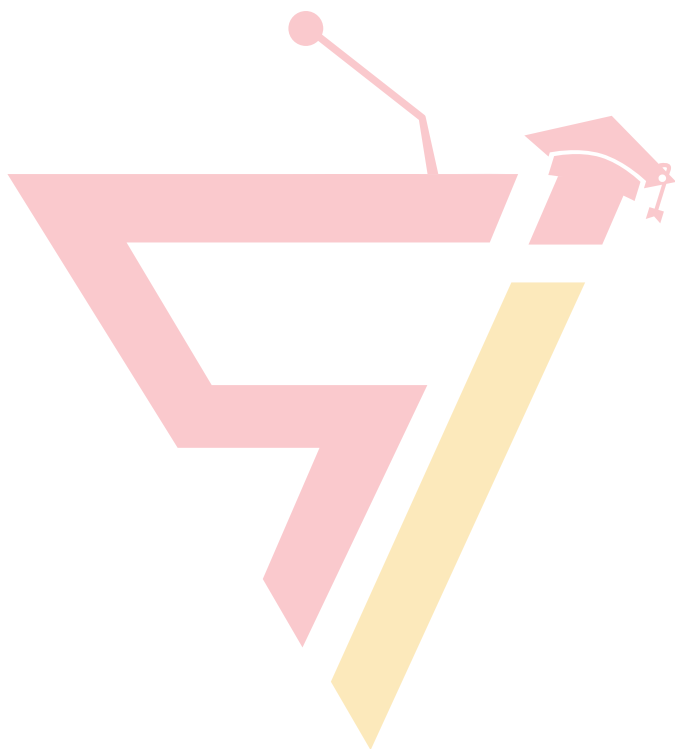
## Joint Event

Scholars International Conference on

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Posters  
Day 1



**Cheng Yee Leong**

Universiti Teknologi Malaysia, Malaysia

**Biography**

Leong Cheng Yee is a full-time Ph.D. student at the University of Technology Malaysia, after completing her undergraduate study (B.Sc. Chemistry) in 2018 from the same university. In her undergraduate research project, she carried out research on photocatalysis for dye photodegradation. Later in 2020, owing to the outbreak of the COVID-19 pandemic, she worked together with her supervisor, Assoc. Prof. Dr Lee Siew Ling, and a local textile industry, CSC Screen Process Supplies Sdn. Bhd. to invent a new photocatalytic antibacterial face mask. Since then, her research study focuses on the utilization of photocatalytic material for antibacterial application, aiming to reduce the use of antibiotics in order to combat the rapid generation of multidrug-resistant bacterial strains. During her postgraduate study, she completed a 7-months internship with Prof. Fabio Cicoira from Polytechnique Montreal, Canada, working on the fabrication of an ion-gated transistor for pH sensing.

**Novel Visible-Light-Induced Photocatalyst of Hydrophobic Copper doped Titanium Dioxide for Antibacterial Application**

The rocketing emergence of antibiotic resistance bacterial strains due to the misuse and overuse of antibiotics in this century has driven the urgent need of the invention of a novel, patent, visible light active photocatalytic antibacterial agent that could be coated on the personal protective equipment. While being able to kill the bacteria, the coated surfaces possess superhydrophobic property ( $\theta = 150^\circ$ ) to prevent the bio-film formation. In this work, a series of polydimethylsiloxane coated copper doped titanium dioxide (PDMS/Cu-TiO<sub>2</sub>) photocatalysts with different concentration of reactants were synthesized via sonochemical method. Three different commercialised TiO<sub>2</sub> precursors were used, namely TR595, P25 and Anatase TiO<sub>2</sub>. According to the particle size analysis and FESEM results, the concentration of PDMS should be below 10 wt% to prevent particles agglomeration. Meanwhile, XRD analysis depicted that the modified TR595 samples have higher crystallinity than the modified P25 and Anatase TiO<sub>2</sub> samples. DR UV-Vis analysis demonstrated that the modified TR595 appeared to have a better visible light absorption and lower band gap energy as compared to P25 and Anatase TiO<sub>2</sub>. Photoluminescence analysis proved the addition of copper dopants would suppress the electron-hole pair recombination, while PDMS has insignificant effect on the optical properties of TiO<sub>2</sub>. FTIR analysis manifested successful synthesis of PDMS/Cu-TiO<sub>2</sub> with proper incorporation of copper dopants into the TiO<sub>2</sub> lattice and integration of PDMS. The photocatalytic antibacterial activities of Cu-TR595\_2:98 and PDMS/Cu-TR595\_2:98 with varied PDMS concentrations were tested under visible light for 1 h. The antibacterial results showed that Cu-TR595\_2:98 exerted inhibitory effect against the Gram-positive while displayed bactericidal effect against Gram-negative bacteria. With PDMS loading, Cu-TR595\_98:2 not only inhibited the growth of Gram-positive bacteria but killed them. Among the PDMS/Cu-TR595\_2:98 photocatalytic antibacterial agents, 8wt% PDMS/Cu-TR595\_2:98 illustrated the best photocatalytic antibacterial efficiency, with 91.67% and 98.29% against the *Staphylococcus aureus* and *Escherichia coli*, respectively.

**Hari Krishna Namballa**

City University of New York, USA

**Biography**

Sebastian Dudek is a PhD student at the International Doctoral Studies in Chemistry at Maria Curie-Skłodowska University (Lublin, Poland). Since October 2018 he has worked on a doctoral thesis under the supervision of Prof. Dorota Kołodyńska. The topic of his doctoral dissertation concerns the removal of arsenate ions on the ion exchangers modified with lanthanide ions. Since 2019 he has been also employed as a lecturer at the Faculty of Chemistry at MCSU.

**Synthesis and Evaluation of C3/C9 Alkoxy Analogues of (-)-Stepholidine as Dopamine Receptor Ligands**

Background and Aim: Dopamine receptor ligands are sought after as biological tools and as potential therapeutics for a range of neuropsychiatric disorders. Tetrahydroprotoberberine (THPB) alkaloids have been reported to possess strong affinity for dopamine receptors.

Based on previous studies with selective D1 agonist and D3 antagonist ligands, compounds with dual targeting D1 agonist/D3 antagonist activity present a promising new therapeutic strategy to treat schizophrenia and substance use disorders. The Aim of this project is to synthesize analogues of the lead molecule – the THPB (-)-stepholidine (SPD), in order to obtain novel D1 agonist/D3 antagonist compounds.

Results: a) Synthesis. The synthetic route to the required analogues (Fig. 1) features a Bischler-Napieralski reaction and subsequent Noyori reduction to generate the tetrahydroisoquinolines of general structure 5. The core THPB structure in compounds 6 was generated via a Pictet-Spengler cyclization. Compound 6 was then transformed into SPD analogues bearing various substituent groups at the C3 and C9 positions. (see analogue library, compounds 7 - 14 in Fig. 1). b) In vitro data. The analogues were evaluated for affinity at dopamine D1, D2 and D3 receptors. Most of the synthesized compounds displayed affinity at the concentrations of 5 to 20 nM at the dopamine D1 receptors. From the structure-activity relationship (SAR) viewpoint it is observed that there is a general trend in the decrease in the affinity with the increase in the alkyl group at the C9 position. However, the C3 alkyl group has no substantial effect on the affinity. c) In vivo data. The effect of SPD on the development and expression of cocaine conditioned place preference (CPP) was studied. The data indicate that SPD can block the expression of a cocaine CPP but has no effect on its development, suggesting that it inhibits the effects of cocaine cues on cocaine incentive motivated behavior. These results suggest that SPD is a potential treatment for cue-driven aspects of cocaine use disorder.

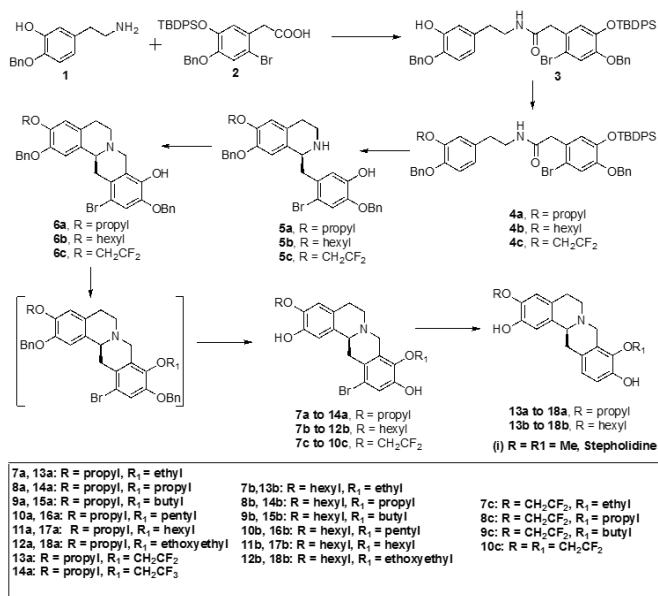



Figure 1. Synthetic route to (-)-stepholidine (SPD) analogues



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Virtual  
Keynote Speakers  
Day 2

**Takeshi Mine**

The University of Tokyo, Japan

**Biography**

Takeshi Mine is Professor in the University of Tokyo, Japan, he did Graduated from The University of Tokyo and joined Mitsui Chemicals, Inc in 1966 . He got Master's degree in Economics, The Johns Hopkins University in 197.

He is Chief Representative in China on behalf of Mitsui Chemicals. Inc in 1994-1999. He got Ph.D. in Economics from The University of Tokyo in 2008

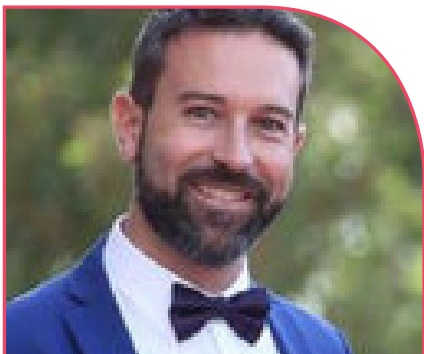
**China's small-scale production and its change through the reform and opening-up policy**

In the pre-war China 50,000t/y ammonia plant was constructed in Dalian and newly 50,000 t/y ammonia plants were constructed owing to the USSR aid in the late 1950's. Mao Zedong considered that USA and/or USSR will attack and invade into China, and aimed to construct the geographically dispersed production structure since the concentration of production will cause a serious damage on the Chinese economy in case USA and /or USSR attack China. Therefore

despite the established 50,000 t/y plants ammonia technology, China newly developed the technology of small-scale ammonia plants, namely 800 t/y or 2,000t/y. And around 1,500 small-scaled ammonia plants were constructed in the rural area of all over China. Using those ammonia as raw material China developed technology to utilize ammonium bicarbonate ( $\text{NH}_4\text{HCO}_3$ ) as nitrogen fertilizer.

Ammonium bicarbonate is not an effective fertilizer since it is easy to deteriorate during transportation and storage. But ammonium bicarbonate plant is easy to construct and operate and production cost is very low, enabling to provide poor farmers with the cheap price. China constructed the ammonium bicarbonate plants all over the rural areas. The geographically dispersed production reduced the loss during transportation and storage and redeemed the defects of ammonium bicarbonate. China is the only nation in the world which utilized ammonium bicarbonate as the fertilizer. Nowadays almost all ammonium bicarbonate plants has been converted into urea plants.

The fertilizer industry in the Mao era had changed, however, through the reform and opening-up policy. In the latter half of 1980's China succeeded to convert ammonium bicarbonate plants into urea plants. China is now the largest urea producer in the world. China's urea production from the small-scale plants, namely ammonium bicarbonate converted urea plants, is larger than the production from the large-scale plants which adopted the imported western technology. This paper concludes that the small-scale production of the fertilizer industry in the Mao era was the so-called 'intermediate technology' of Schumacher and was also the 'appropriate technology' of United Nations and other international organizations.

**Simone Carradori**

D'Annunzio University of Chieti - Pescara, Italy

**Biography**

Simone Carradori graduated with honors in 2003 in "Drug Chemistry and Technology", in 2009 with honors in Pharmacy, and then with honors in "Applied Pharmaceutical Sciences" in 2016. In 2006 he completed his PhD in "Pharmaceutical Sciences". In 2007 he received with honors the II level Master in "Natural Organic Substances". Since 2006 he has held national research grants in the Scientific Sector CHIM/08 (03/D1) (Medicinal Chemistry)

**Cobalt-based Carbon Monoxide Releasing Molecules (CORMs): Design, synthesis and anti-inflammatory activity**

Carbon monoxide (CO) is endogenously produced and it has been reported as an anti-inflammatory and cytoprotective gaseous substance at low concentrations. However, the administration of exogenous CO is complicated due to its gaseous state, and obtaining specific cell responses is challenging because of the lack of specialized targets. In this context, CO releasing molecules (CORMs) have attracted enormous interest, being reported to downregulate immune and inflammatory responses in both in vitro and in vivo models of diseases, such as Rheumatoid Arthritis (RA), Rotator Cuff Tears (RCTs) and Rotator Cuff Disease (RCD). In parallel, it has been broadly reported that Carbonic Anhydrase (CA; EC 4.2.1.1) is involved

in the pathogenesis and maintenance of many inflammation-related diseases. Levels of the isoform IX have been found in human fetal tendons as a marker of mechanical stress, and an overexpression of CA IX and XII in inflamed joints has been recently reported. In this light, the synthesis of small molecule hybrids consisting of CA inhibitors or not linked to a CORM section (CAI-CORMs) has been proposed. This strategy aims at strengthening a counteraction of the sustained oxidative stress and inflammation occurring in many diseases.

Evaluation of the CO released over time, performed by using a myoglobin carbonylation assay, revealed the organic portion linked to the CORM section to have a deep influence on the CO releasing properties. On the other hand, the DCH insertion did not highly hamper the CA inhibition. In vivo pain relief efficacy studies in the RA rat model showed that some derivatives were more efficient in terms of intensity as well as time distribution when compared to the single entities CAI and CORM administered separately, confirming the success of the hybridization strategy. These very promising results fostered our interest in studying the anti-inflammatory and anti-oxidant properties of such hybrids at a biological and molecular level on LPS-stimulated RAW 264.7 mouse macrophages and H<sub>2</sub>O<sub>2</sub>-stimulated tendon-derived human primary cells in comparison with N-acetyl cysteine (NAC) and the NSAID meloxicam, respectively.

Our results revealed that compounds counteracted the induced inflammation and some hybrids displayed a better profile in terms of enhanced viability, decreased cytotoxicity, and augmented cell proliferation in both the cell model. In the inflamed tendon cell model, compound 7, as a potent superoxide scavenger, exerted its action inhibiting the NF- $\kappa$ B translocation and downregulating iNOS, whereas compound 2 was more effective in increasing collagen I deposition.

Taken together, these data lay the grounds for further investigations in this field and pave the way for the use of CAI-CORMs in inflammatory-related diseases.



**Alina Adams**

RWTH Aachen University, Germany

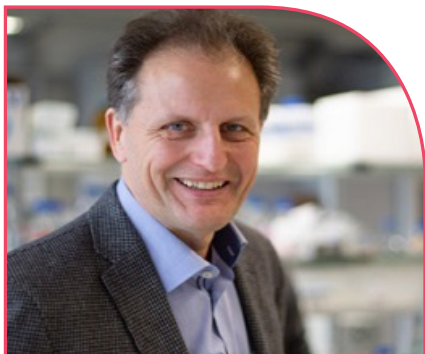
**Biography**

Alina Adams studied physics at Babes-Bolyai University in Cluj-Napoca, Romania. She received her PhD and Habilitation in the field of Nuclear Magnetic Resonance (NMR) at RWTH Aachen University, Germany, where she currently holds an interim Professor position. Her expertise is in the field of NMR methodology, solid-state NMR, low-field NMR, and material science.

**Advances in Compact NMR for Analysis of Complex Samples**

Nowadays, Nuclear Magnetic Resonance (NMR) is a primer analytical method for structural analysis of small and large molecules and as a main method for simple and quantitative analysis of complex mixtures. This information are of key importance, as for example, for the design of materials with tailored properties and the prediction of different properties of various mixtures. Most of such analyses are conducted using expensive equipment, which requires trained users and special laboratory place. Yet, many investigations are readily possible with the help of compact and low-cost NMR devices. Since some couple of years is such equipment also commercially available and raises as an interesting alternative to the standard NMR for many applications. In our contribution, we will demonstrate, with the help of selected examples, the potential of compact NMR in solving questions of current interest in various fields of activities. They will include:

- 1) Novel methodologies for quantifying the structure and content of plasticizers in solution and in polyvinyl chloride (PVC) products, with PVC being the third most produced polymer worldwide.
- 2) A new approach for fast screening of the separation power of Metal-Organic Frameworks (MOFs) for binary solvent mixtures. MOFs are regarded today as efficient alternatives to the current separation and purification procedures, which are very time and energy consuming.
- 3) The design of a novel low-cost and versatile setup for high-pressure NMR spectroscopy analysis with benchtop NMR and its application on various pressurized samples with focus on their composition quantification and the establishment of a NMR-based strategy as an alternative to Gas Chromatography (GC).

**Michael Hennig**

leadXpro AG, Switzerland

**Biography**

Michael Hennig studied Physics and Biochemistry, received the Ph.D. in structural biology at EMBL Hamburg, and the Charité, Humboldt University Berlin, Germany. It followed two years postdoc work at the Biozentrum, University of Basel, Switzerland. He is author of more than 80 scientific peer reviewed paper and, since 2011, guest professor in structural biology at the University of Basel. He worked 20 years in pharmaceutical industry at Roche, Basel, Switzerland in various positions and finally Global Head and Principle Leader of discovery technologies with responsibility for structure-based drug discovery, protein science, assay development and HTS, Roche corporate compound library, stem cell platform and analytical physical methods. In 2015, he co-founded leadXpro, a corporation dedicated to structure-based drug discovery for membrane protein targets (GPCR's, Ion-channels, Transporter) and utilizing most advanced technologies such as the X-ray free electron laser (at PSI, SwissFEL) and cryo-electron microscopy (at University of Basel, cryo-EM).

**Structure-based drug discovery enabled for membrane protein targets**

Integral membrane proteins such as GPCR's, ion-channels or transporters are drug targets for more

than 60% of all approved drugs. Structure based drug discovery on soluble proteins is managed well within the project timelines and portfolio changes in pharmaceutical industry, but transmembrane proteins are still underexplored because of their challenges to be expressed, purified and made them work for high resolution structure determination and ligand characterization by biophysical methods.

The presentation includes recent advances in the technologies and their application to relevant drug targets.

Construct engineering, application of in meso in situ serial X-ray crystallography (IMISX) is exemplified with the GPCR structure of CCR2 in complex with an antagonist ligand. This study is combined with detailed binding characterization using grating-coupled interferometry (GCI, Creoptix) to facilitate drug design with binding kinetic, affinity. Furthermore, the cross-talk between allosteric and orthosteric ligand binding could be investigated.

The structure of the human TRPV4 ion-channel with bound small molecule agonist shows activation of the channel opening with a significant structural change enabling direct observation of agonist pharmacology by high resolution cryo-EM analysis. Next example is LPTDE, a clinically validated antibiotics drug target. Due to limited size of 120 kDa and the monomeric  $\beta$ -sheet transmembrane architecture, the leadXpro proprietary tool of Pro-Macrobodies was essential for the successful EM structure at 2.9 Å resolution.

The outlook at future perspectives includes further advances in cryo-EM and the application of serial X-ray crystallography using femtosecond pulsed Free Electron Lasers (FEL) for determination of room temperature structures and observation of structural dynamic of ligand binding and associated conformational changes. All new developments in structural biology will further enhance the impact to the design of candidate drug compounds.

**Anne Gaffney**

Idaho National Laboratory/University of South Carolina, USA

**Biography**

Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished National Lab Fellow (2014 – present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 256 patents. Dr. Gaffney is also a distinguished Joint Appointment Fellow at the University of South Carolina (2018 – present) where she is the Technical Direc-

tor of the National Science Foundation Center for Rational Catalyst Synthesis. Some of her recent awards include: the 2019 American Chemical Society, Energy & Fuels, Distinguished Researcher Award in Petroleum Chemistry; the 2015 Eugene J. Houdry Award of the North American Catalysis Society; the Chemical Heritage Foundation, Women in Science Inductee, 2014; and the American Chemical Society, Industrial Chemistry Award, 2013. Dr. Gaffney received her BA in chemistry and mathematics from Mount Holyoke College and her Ph.D. in physical organic chemistry from University of Delaware.

**New Perspectives and Insights into Silver Catalyzed Direct Propylene Epoxidation**

A series of Ag-based catalysts were studied for direct PO epoxidation with O<sub>2</sub> as the oxidant. Ag supported on CaCO<sub>3</sub> and α-Al<sub>2</sub>O<sub>3</sub> were prepared as base materials to study. Promoters (K<sup>+</sup>, Cs<sup>+</sup>, Mo) and feed additives (EtCl, NO, CO<sub>2</sub>) were added to the catalyst and feed stream, respectively, in order to evaluate their effects on PO selectivity and yield. Ball-milling of the catalyst during preparation was a significant factor in ensuring proper blending of promoter species in the Ag particle. Surface characterization (chemisorption, XPS, SEM-EDX), bulk composition characterization (XRD, ICP-OES), and reaction kinetic evaluation were conducted to understand the nature of PO selectivity.

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Virtual  
Speakers  
Day 2





**Sujun Guan**

Toyo University, Japan

**Biography**

Guan is an associate professor working in the Bio-Nano Electric Research Center at Toyo University from April 2021, focusing on visible-NIR-driven photocatalysis and their environmental and bio application. Prior to this, he worked at the Department of Physics at Tokyo University of Science from April 2017, researching on the visible-driven photocatalysis, p-type ZnO semiconductor films and their related devices. Before the work, he gained his PhD in Department of Mechanical Engineering at Chiba University, working on enhancement of visible-light absorption and photocatalytic activity of photocatalyst coatings.

**Creation of core-shell TiC-TiO<sub>2</sub> nanoparticles for visible-NIR-driven photocatalysis**

TiO<sub>2</sub> photocatalysis has received much research interest, but the applications of TiO<sub>2</sub> nanoparticles (NPs) as photosensitizing agents in the attention should be

paid to the last mentioned, but exceptional category containing metallic and treatment of cancer as well as in photodynamic inactivation of antibiotic-resistant bacteria. However, the large band gap of TiO<sub>2</sub> and fast recombination of photogenerated charge carriers limit its overall photocatalytic efficiency.

Presently, we had successfully enhanced the photocatalytic activity of TiO<sub>2</sub> coatings on Al<sub>2</sub>O<sub>3</sub> balls (Fig. 1) encompassing the increased surface accessible area with porous structure, narrowed band gap around 1.08 eV, and effect of charge transfer between TiC and TiO<sub>2</sub>. Based on the current achievement, we had applied the above modification strategies into create the visible-NIR-driven core-shell TiC-TiO<sub>2</sub> NPs, via changing the `TiO<sub>2</sub> balls` into the `TiC NPs`, and further try to verify their potentials application in bio field.

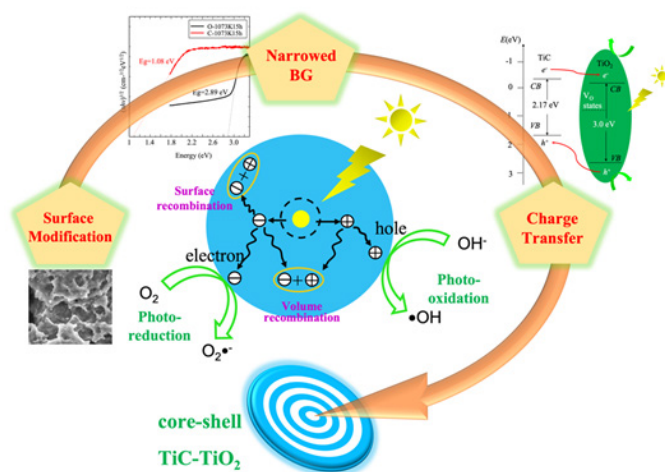
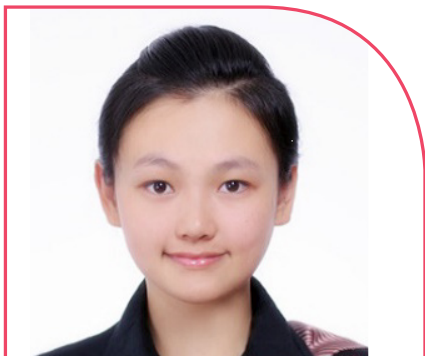


Fig. 1 Modification strategies of TiO<sub>2</sub> photocatalysis.



**Yumei WANG**

National University of Singapore (Chongqing)  
Research Institute, China

**Biography**

Yumei WANG received her Ph.D. degree at National University of Singapore (NUS) in 2018. Later, she works as a postdoctoral research fellow in NUS from 2018 to 2020. In 2021, she joins in National University of Singapore Chongqing Research Institute and works as a research fellow. Her research interests include advanced materials for rechargeable batteries and ferroelectric ceramic films for Microelectromechanical System (MEMS) transducers/sensors. She has secured research projects which are supported by Natural Science Foundation of Chongqing, China and Huaqiao University Sci-Tech Innovation Platform program, China.

**Ferroelectric Engineered Electrode-Composite Polymer Electrolyte Interfaces for All-Solid-State Sodium Metal Battery**

With continuous improvements in ionic conductivity of the solid-state electrolytes, poor electrolyte-electrode compatibility and large interfacial impedances that limit the cyclic performances of batteries have become the main challenges for solid-state batteries. To enhance the compatibility between the polymer-based electrolytes and electrodes, and promote the interfacial ion conduction, we introduce a novel approach to engineer the interfaces between all-solid-state composite polymer electrolyte and electrodes using thin layers of ferroelectrics. The well-designed and ferroelectric-engineered composite polymer electrolyte demonstrates an attractive ionic conductivity of  $7.9 \times 10^{-5} \text{ S cm}^{-1}$  at room temperature. Furthermore, the ferroelectric thin layers can effectively suppress the growth of the solid electrolyte interphase (SEI) at the interface between the polymer electrolyte and Na metal electrode, and it can also enhance the ion diffusion crossing the electrolyte-ferroelectric-cathode/anode interfaces. Notably, an extraordinarily high discharge capacity of  $160.3 \text{ mAh g}^{-1}$  with 97.4% capacity retention has been achieved after 165 cycles at room temperature. Moreover, the cell has demonstrated outstanding stability with a high discharge capacity retention of 86.0% over 180 full charge/discharge cycles after 2 months' aging. This work provides new insights in enhancing the long-cyclability and stability of the solid-state rechargeable batteries.

**Koichi Nagata**

Tohoku University, Japan

**Biography**

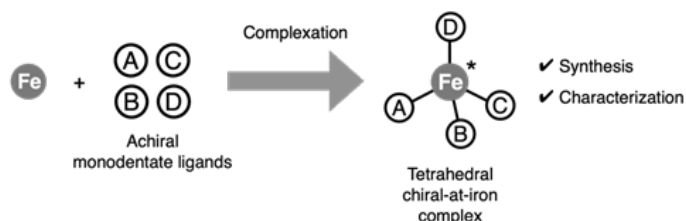
Koichi Nagata received his Ph.D. from Kyoto University (Japan) in 2016 under the guidance of supervisor Prof. Norihiro Tokitoh (Main group chemistry). During Ph.D. degree, he spent a half year as a visiting researcher at the University of Alberta, working with Prof. Eric Rivard (Main group chemistry). After obtaining his Ph.D. degree, he then undertook postdoctoral studies with Prof. Jonas C. Peters (Inorganic chemistry) at Caltech as a JSPS Overseas Research Fellow. He then joined the Shionoya group (The University of Tokyo) as a postdoctoral fellow in September of 2017. He was promoted to a project assistant professor in April of 2018, working with Prof. Mitsuhiko Shionoya (Coordination chemistry, Supramolecular chemistry). In 2020, he joined the Hashimoto group as an Assistant Professor.

**Synthesis and Properties of a Tetrahedral Fe Complex with Metal-Centered Chirality**

The synthesis and characterization of molecular chirality (ex  $sp^3$ -carbon center) is one of the most important areas in chemistry. Among various molecular groups, metal elements can also serve as chiral centers, so even if achiral ligands are used, it is possible to construct chiral metal complexes that have chirality only at the metal center. Such complexes are ex-

pected to be applied to enantioselective catalytic reactions and chiroptical materials. However, it is quite difficult to control the chirality of such metal-centers, because the dynamic and reversible nature of coordination bonds often lead to ligand scrambling or rapid racemization. So far, some excellent examples of relatively inert octahedral metal complexes with chirality at the metal-center only have been reported, but control of the metal center of tetrahedral metal complexes is still a challenge.

This study focusses on the induction of metal center chirality in tetrahedral iron complexes. We report on the synthesis of tetrahedral metal complexes composed of only achiral ligands, where only at the metal is the chiral center, and on the control of the absolute configuration of the metal center. Specifically, a chiral tetrahedral iron complex, Fe(ABCD), was synthesized as a racemic mixture using achiral monodentate ligands (A–D). The tetrahedral monomeric structure was revealed by single-crystal X-ray diffraction analysis, along with characterization based on spectroscopic measurement and theoretical calculations.



[1] E. Meggers et al. Chem. Asian J. 2017, 12, 2335. [2] M. Shionoya et al. Nat. Commun. 2020, 11, 6263.



**Wan Izhan Nawawi Bin Ismail**

UiTM Cawangan Perlis Kampus Arau, Malaysia

**Biography**

Wan Izhan Nawawi Wan Ismail have a wide knowledge in modification of  $\text{TiO}_2$  photocatalysts, electrocoagulation, germicidal,  $\text{TiO}_2/\text{PANI}$ /perovskite photovoltaic solar cell, production of activated carbon and coal desulphurization treatment process. I have a good understanding on XPS, HRTEM, Photoluminescent (PL), XRD, SEM, BET, Elemental analyzer (CHNS), TGA, HPLC, LCMS, GC-MS and UV-Vis DRS with hands on experience in handling those instruments. I also have experience in teaching chemistry subjects such as petroleum technology, energy technology, computer in chemistry, advance instrumental analysis and nuclear technology as a senior lecturer in Universiti Teknologi MARA Cawangan Perlis, Malaysia from Feb 2014 until now.

**The Role of N and Pt co-dopants in Sequential and Vice-versa Mode Preparations on  $\text{TiO}_2$  Photocatalyst for Photocatalytic Degradation of Methylene Blue Dye characteristics and dosage form designs**

Heterogenous titanium dioxide ( $\text{TiO}_2$ ) photocatalysis has frequently been studied by researchers. However, the limitation of  $\text{TiO}_2$  as photocatalyst such as larger band gap energy which only activate under UV region and give a lower photocatalytic activity. This study will report the role of the N and Pt co-dopant on modification of  $\text{TiO}_2$  photocatalyst for photocatalytic degradation of methylene blue dye under different mode

preparations ie; sequential and vice-versa mode. The sequential mode preparation of N and Pt co-dopant  $\text{TiO}_2$  photocatalyst was initially prepare the N doped  $\text{TiO}_2$  (NT) under calcination method and further doped with platinum (Pt) through photodeposition process labelled as NP- $\text{TiO}_2$  while vice-versa mode was labelled as PN- $\text{TiO}_2$ . About 0.8 wt.% N element was found in NP- $\text{TiO}_2$  photocatalyst while there is no presence of N element was detected in PN- $\text{TiO}_2$  and it was confirmed through elemental analyzer (CHNS-O) and (EDX) analysis. The optimum weight percentage of Pt for both modes was detected about 1.8 wt.% which has been confirmed by (ICP-OES). The photo-activity under methylene blue (MB) dye degradation of NP- $\text{TiO}_2$  photocatalyst is 2 and 0.5 times faster as compared to the unmodified  $\text{TiO}_2$  and PN- $\text{TiO}_2$  where the photodegradation rate was ca.  $0.04 \text{ min}^{-1}$  and  $0.8 \text{ min}^{-1}$  respectively. This is due to the N elements is being in cooperated with the  $\text{TiO}_2$  lattice which has proven by UV-Vis/DRS where the band gap energy of NP- $\text{TiO}_2$  was reduced from 3.2 eV to 2.9 eV and a lower emission peak of photoluminescence intensity indicates a lower recombination rate of electron-hole pair was identified. The XPS studies confirmed the binding energy of NP- $\text{TiO}_2$  found at 400.5 eV and 398.9 eV specifies as the interstitial and substitutional bonding of N by forming Ti-O-N, O-Ti-N and Ti-N-Ti. While the oxidation state of the Pt was formed as  $\text{Pt}^{2+}$ ,  $\text{Pt}^{4+}$  and metallic form, Pt0 where it confirms the Pt bonding has influenced on the photocatalytic activity by scavenge the electron preventing it to be recombined on NP- $\text{TiO}_2$  photocatalyst. The preparation order does not affect the Pt dopant but otherwise for N element. Therefore, different mode preparation for N and Pt co-dopant on modification of  $\text{TiO}_2$  is significant to be investigated to produce a good quality photocatalyst for photocatalytic study under photodegradation of MB dye.

**Eman Alabbad**

Imam Abdulrahman bin Faisal University, KSA

**Biography**

Eman Alabbad is assistant professor in chemistry department in Science collage. She is a graduate from Imam Abdulrahman bin Faisal University and focused on the application of water treatment and protection from pollution. She has many researches in this field. She participated in many scientific conferences and symposia. She recently won an international award for the best scientific research.

**Efficacy assessment of natural zeolite containing wastewater on the adsorption behaviour of Direct Yellow 50 from; equilibrium, kinetics and thermodynamic studies**

This study aimed to evaluate an efficient method in order to remove Direct Yellow 50 (DY50) dye from

aqueous solutions using natural zeolite in a batch system. The results indicated that the removal of DY50 was highly subjective to the pH of the aqueous solution, initial concentration of DY50, adsorbent dosage, temperature, and contact time. The research data was then tailored isothermally to the Freundlich and Langmuir isotherms, and the kinematic results were interrelated to the pseudo-first and second-order models. The removal rate of DY50 was calculated to be 58.63% for a zeolite sample of 0.05 g and 40 mg L<sup>-1</sup> as a preliminary dye concentration with 4 hrs of contact time. The description of the adsorptive behaviour of the natural zeolite was presented through a kinetic model of the pseudo-second-order. The change in enthalpy (DH), free energy (DG), and entropy (DS) were also investigated as thermodynamic parameters. The results of this study supported the theory that the initial concentration of DY50, pH of solution, adsorbent mass, contact time, and temperature, greatly affected the adsorption of DY50 on zeolite.

**Valerie Welborn**

Virginia Tech, USA

**Biography**

After completing a broad undergraduate education at ESPCI ParisTech in France, Dr. Vaissier Welborn specialized in developing computational techniques to model complex macromolecular systems.

She received her PhD in Physics from the Doctoral Training Center in Theory and Simulation of Materials at Imperial College London in 2014. Her graduate work revolved around the quantification of the kinetics of intermolecular charge transport in dye sensitized solar cells, performed under the supervision of Prof. Jenny Nelson and Prof. Piers Barnes.

Dr. Vaissier Welborn then worked as a postdoctoral fellow at MIT in Troy van Voorhis' research group where she focused on incorporating dynamical, ensemble-based, factors into electronic structure methods for a more accurate representation of solvent effects and other environmental factors. This was followed by a second postdoc at UC Berkeley in Teresa Head-Gordon's group where she gained expertise in classical molecular dynamics simulation of proteins and supramolecular catalysts with polarizable force fields.

Dr. Vaissier Welborn has since started her independent research program at Virginia Tech where she has been an assistant professor in the Department of Chemistry since 2019.

**DNA-scaffolded synthetic enzymes for tunable high performance catalysis**

A major bottleneck in synthetic enzyme design is the engineering of a stable and functional protein scaffold. Efforts to mimic natural enzyme scaffolds are only partially successful due to the complexity of reproducing such intricate folded structures that also need to be flexible and dynamic. In natural enzymes, these structurally and dynamically complex scaffolds induce strong electrostatic interactions in the active site, stabilizing the reaction transition state, which lowers the energy barrier and accelerate reaction kinetics (electrostatic preorganization theory). Thus far, the designed scaffolds of synthetic enzymes do not exhibit similar electrostatic properties, resulting in limited rate accelerations. While scaffold modifications (i.e., mutations of the protein sequence) can help to improve on the original design, the process is often tedious, expensive and rarely efficient.

In this talk, I will present an alternative for improving synthetic enzymes that relies on designing a DNA scaffolding. Within electrostatic preorganization theory, enzyme catalysis is governed by both short-range (from the active site) and long-range (from the scaffold and beyond) electrostatic interactions. Here, the polar sugar-phosphate backbone of DNA induces further long-range electrostatic interactions in the active site, accelerating reaction kinetics. I will illustrate this concept by showing how DNA fragments are predicted to lower the reaction barrier by 2.0 kcal/mol in the active site of synthetic enzyme KE15.



**Lianghai Zhang**

The University of Illinois at Chicago, USA

**Biography**

Zhang received her M.D. from Medical School of Fudan University and Ph.D. in Pharmacology from University of Rochester. Dr. Zhang's research interests have been focused on exploring the mechanisms of inflammatory endothelial injury and repair using acute lung injury mouse model and developing novel mechanism-based regenerative strategies. Her scientific training began with her graduate work under the instruction of Dr. Alan Smrcka at the University of Rochester to dissect signal pathways of cardiac hypertrophy (Cell 2013). Dr. Zhang's postdoctoral training in lung vascular biology was with Dr. Jalees Rehman and Dr. Asrar Malik in the Department of Pharmacology at the University of Illinois at Chicago (Circulation 2017, Nature Communications 2019). Dr. Zhang started her own laboratory in 2021 with the funding support from NIH R01. She recently published the SARS-CoV-2 work in Nature Chemical Biology 2022.

**Engineered ACE2 Decoy Mitigates Lung Injury and Death Induced by SARS-CoV-2 Variants**

Vaccine hesitancy and the continuous emergence of SARS-CoV-2 variants of concern that partially escape vaccine-induced immune responses highlight the urgent need for the development of effective therapeutics for COVID-19 patients. Current therapeutic approaches rely on therapeutic cocktails of monoclonal antibodies or the delivery of a soluble

ACE2 decoy peptide which competes host cell ACE2, a cell-entry receptor for the SARS-CoV-2 Spike protein. Engineering modified ACE2 peptides could significantly augment the binding affinity of decoy peptides for the Spike protein and thus increase their therapeutic efficacy against multiple viral variants. Using molecular dynamics simulations, we validated the engineering of a soluble ACE2 peptide (sACE22.v2.4-IgG1) containing three amino acid substitutions with markedly increased affinity for the SARS-CoV-2 Spike (S) protein. We demonstrate its higher binding affinity to S proteins of the original SARS-CoV-2 WA-1/2020 isolate and the B.1.1.7 (Alpha), B.1.351 (Beta), P.1 (Gamma), and B.1.617.2 (Delta) SARS-CoV-2 variants of concern compared to wild-type soluble ACE2. In humanized K18-hACE2 mice, prophylactic and therapeutic injections of sACE22.v2.4-IgG1 after viral inoculation prevents SARS-CoV-2 induced acute lung vascular endothelial injury, lung edema formation and improves survival. Therapeutic benefits persisted whether animals were infected with the original SARS-CoV-2 WA-1/2020 isolate or with P.1 (Gamma) variant which showed markedly increased virulence in this model. These studies demonstrate the broad efficacy of a single engineered ACE2 decoy peptide against multiple SARS-CoV-2 variants and underscore its potential role in treating severe COVID-19 disease induced by variants of concern (Figure 1).

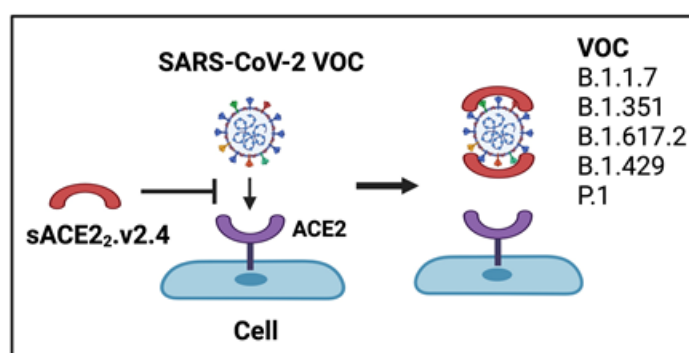


Figure 1. Graph Abstract.

**Chris G Dealwis**

Case Western Reserve University, USA

**Biography**

Chris G Dealwis major interest lies in studying the molecular basis of biological function to maintain homeostasis. I use techniques such as structural biology, including x-ray crystallography, cryo- electron microscopy and neutron diffraction, biochemical and biophysical tools to conduct my studies. One of my major interests is to alleviate human suffering by using drug design to develop new anticancer and anti-Alzheimer's therapies. In the last two decades I have been focusing on the structure – function and drug design of anticancer agents against the major cancer target ribonucleotide reductase. My lab is the first to solve the structure of the catalytic subunit of eukaryotic and human ribonucleotide reductase and demonstrated the use of structure – based drug design in developing the first reversible, small molecule inhibitor against this enzyme. Additionally, my lab has provided insights into the molecular basis of its exquisite specificity and how it achieves regulation through multimerization.

**The cancer target ribonucleotide reductase and its allosteric regulation**

Human Ribonucleotide Reductase (hRR) is an established cancer target, due to its essential role in dNTP synthesis and DNA replication. RR is involved in the rate determining step of dNTP synthesis which is essential for making DNA. RR is an exquisitely allosterically regulated enzyme and provides crucial information on allosteric regulation. RR consist of an alpha subunit that contains the catalytic site and two allosteric sites and a small beta subunit that houses a stable di-iron radical cofactor, essential for catalysis. RR demonstrates exquisite substrate specificity by catalyzing for nucleotide diphosphates selected by four nucleotide triphosphates. The antimetabolite class of chemotherapies such as gemcitabine, clofarabine and fludarabine inhibit hRR. Gemcitabine is one of the few drugs that have been approved against the treatment of pancreatic Cancer (PC). Only 10% of the PC sufferers respond to gemcitabine and gemcitabine treated patients develop resistance after a month with the average life expectancy only extended by one year. Therefore, there is a large unmet need for novel therapies for the treatment of cancer, such as PC and other nonresponsive cancers to therapies such as triple negative breast cancer and glioblastomas. Using *in silico* screening, medicinal chemistry, interspersed with synthesis, we developed a novel class of non-nucleoside, reversible, small molecule inhibitors targeting hRR. In this presentation, I will present the structure – function data generated in our lab that provided insights into the molecular basis of allosteric regulation of this enzyme. Moreover, I will present knowledge-based drug design efforts conducted in my lab to develop novel catalytic inhibitors for the treatment of cancer. The techniques presented will include but not limited to chemical biology, medicinal chemistry, x-ray crystallography, cryo- electron microscopy, biophysical and biochemical techniques. I will also briefly describe clinically approved drugs that target this cancer target.



**Raed Abu-Reziq**

The Hebrew University of Jerusalem, Israel

**Biography**

Abu-Reziq completed his doctorate at the Hebrew University under the guidance of the late Prof. Jochanan Blum and Prof. David Avnir, in catalysis and sol-gel chemistry. After receiving his Ph.D. degree in 2004, he moved to Ottawa University, Canada, to do his post-doctoral research in the labs of Prof. Howard Alper, in the field of nanocatalysis. In 2006, he joined the company Sol-Gel Technologies as Senior Researcher and spent two years in developing micro and nano-encapsulation systems based on sol-gel process as drug delivery systems. In 2008, He was appointed as Senior Lecturer at Casali Center for Applied Chemistry and Institute of Chemistry and in 2015 he was

promoted to associate Professor. His research focuses on nanocatalysis, green chemistry and developing micro and nanoencapsulation methods.

**Catalysis in Nano- and Microreactors**

Confined microenvironment in catalysis has been recently recognized as one of the elements that can affect significantly the performance of catalysts, in particular heterogeneous catalysts. It can help in stabilization of the active sites and control reactivity and selectivity. In addition, it has been demonstrated in many cases that performing chemical reactions in microdroplets can dramatically accelerate their rate.

In this talk, I will present developing new methods for preparing catalytic nanoreactors and microreactors and their application in confined catalysis. In Particular, I will describe the preparation of catalytic periodic Mesoporous Organosilica (PMO) nanoparticles from 100% bridged organo-alkoxysilane precursors,  $(OR)_1-3Si-R-Si(OR)_3$ , in the presence of a structure directing agent, which assists the creation of uniform pores and structures. These nanoparticles have uniquely a very large surface area that could reach up to 1800  $m^2/g$ . In addition, the preparation of catalytic silica microreactors containing ionic Liquids (ILs), deep Eutectic Solvents (DESs) or polyethylene Glycols (PEGs) via aqueous and non-aqueous sol-gel techniques will be described. The application of the catalytic nano- and microreactors in different organic transformations will be discussed.



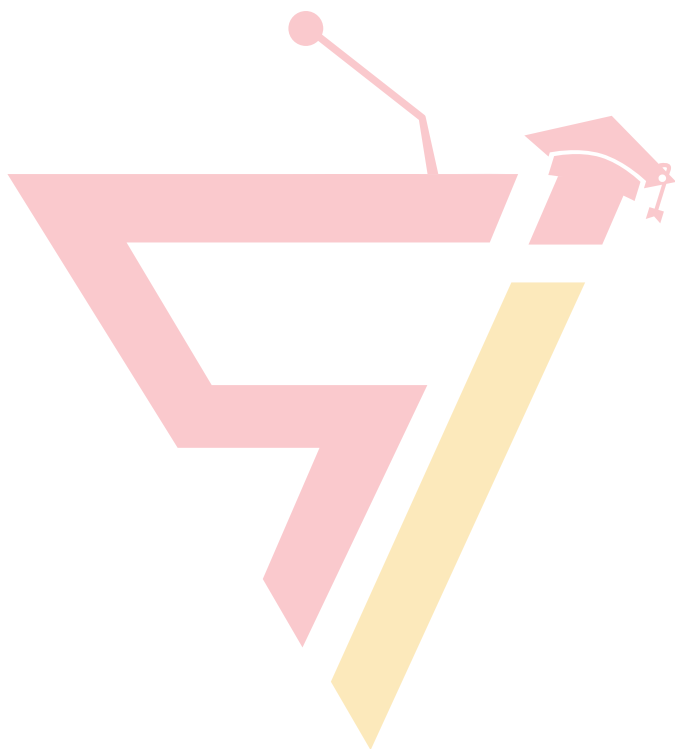
## Joint Event

Scholars International Conference on

# **CATALYSIS AND CHEMICAL ENGINEERING & SCHOLARS FRONTIERS IN CHEMISTRY FORUM**

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Posters  
Day 2



**Jimena Magdalena Jacob**

Ensenada Center for Scientific Research and Higher Education, Mexico

**Transition-Metal (Pt, Pd, Rh, Ru) Single-Atom Catalysts based on the ZnO(0001  $\bar{1}$ )-2x2 vacancy reconstructed surface: An ab-initio study**

Here we present a theoretical investigation on the transition-metal (Pd, Pt, Rh, Ru) single Atom Catalyst (SAC) based on the ZnO (000-1-) reconstructed surfaces. The model system used to incorporate the transition metals into the ZnO (000-1)-2x2 oxygen vacancy reconstructed surface. Through the first-principles thermodynamic formalism we determine the most stable site for the transition-metal atoms. The electrostatic potential isosurface calculations allows us to discuss on the potential improvement on the catalytic activity due to the single atom incorporation. Consequently, our results are compared to the SAC Cu/ZnO (000- $\bar{1}$ ) surface, previously reported in the literature. Surface engineering mediated by single-atom incorporation is a way to improve the catalytic activity of the existent materials, opening a way to achieve catalysts cheaper than the conventional based on Pt or Pd.

**Leah Kim**

Regis University, USA

**Biography**

Leah Kim is a volunteer researcher for the Chemistry department of Regis University. Leah intends to do more research and pursue her passions in chemistry. Leah worked under the supervision of Dr. Kimberly Waldron for this project.

**Examining the Degrading Effects of Acid Rain on Solar Panels and Its Reflectors**

Solar energy and panels are often used in this world

to efficiently use what is radiated by the Sun. Solar panels, also known as PV panels, convert light from the sun to a reusable energy source that can be used in real life in many ways. Since there also have been many incorporations of reflectors to increase the efficiency of the solar panels, four types of reflectors were selected to test the erosion in response to acidity of rain. This research is focused on the effect of acidic rain on the surface of the solar panels' reflectors which are exposed to rain. The objective is to show how reflectors can be incorporated into solar cells to increase the efficiency of solar energy collection. Using mirror, mylar, aluminum, and paper as the reflectors, they were first tested in three different angles – 45, 60, and 90 degrees in mA. After exposing the rectangularly cut reflector samples to HCl solution of different pHs, the energy output was measured again at 90 degrees, which resulted in the most optimal increase in the solar panel output under the sun. All reflectors showed degradation in the surfaces meaning the acidity of rain has a detrimental effect. pH 1 solution resulted in the most degradation and lessened output of the measured sunlight, which divulged the negative effect of the acid rain on solar panels' reflectors and possibly on the panels itself.

**Sebastian Dudek**

University of Maria Curie-Skłodowska, Poland

**Biography**

Sebastian Dudek is a PhD student at the International Doctoral Studies in Chemistry at Maria Curie-Skłodowska University (Lublin, Poland). Since October 2018 he has worked on a doctoral thesis under the supervision of Prof. Dorota Kołodyńska. The topic of his doctoral dissertation concerns the removal of arsenate ions on the ion exchangers modified with lanthanide ions. Since 2019 he has been also employed as a lecturer at the Faculty of Chemistry at MCSU.

**Enhanced arsenic(V) removal by commercially available ion exchanger modified with La(III) ions**

Arsenic has long been recognized as a toxin and carcinogen. Chronic exposure to arsenic may occur through natural sources such as weathering reactions, volcanic emissions as well as human activities like mining. Of the various risks, exposure to arsenic through contaminated drinking water is probably the greatest threat to human health. Therefore, it requires to look into the problem of arsenic(V) adsorption more intensely to find out an appropriate adsorbent with affinity to arsenate(V) ions. The commercially available adsorbent containing inbuilt iron nanooxide molecules of the goethite structure, Purolite Arsen Xnp (Xnp in short), was chosen to this study. Modification of this sorbent with lanthanum(III) ions lead to obtaining the new material Xnp-La(III). The modification process itself was tested for optimal pH, kinetics, and equilibrium adsorption isotherm study. The sorbent characteristics were made using, among others, SEM, FTIR, and nitrogen adsorption/desorption isotherms. Then, several tests were conducted to compare the adsorption properties of the modified and unmodified material. It was found that Xnp-La(III) was able to completely remove arsenate(V) from water with an initial concentration of up to 50 mg/dm<sup>3</sup>. Without modification, it was not possible to reach the WHO recommended 10 µg/dm<sup>3</sup> arsenic limit even at an initial concentration of 25 mg/dm<sup>3</sup>. Moreover, the maximum sorption capacity increased threefold after modification. Such La(III)-based adsorbent can be successfully applied in wastewater purification and used many times after proper regeneration what leads to cost reduction.

**Huda Alghamdi**

Imam Abdulrahman bin Faisal University, KSA

**Biography**

H. Alghamdi is a Master degree holder in physical chemistry, my interest is in the field of green chemistry for sustainability. I am passionate to learn all-new. Looking forward to gaining a Ph.D.

**Using of Chemically Modified Chitosan for the Sorption of some Toxic Metal Ions in Aqueous Systems**

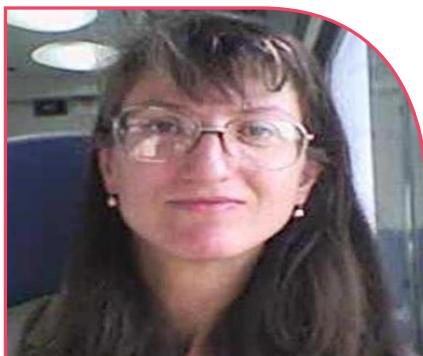
In this study, a successful grafting of three different kinds of benzaldehyde derivatives namely, (3-hydroxybenzaldehyde, 2,3-Di-hydroxybenzaldehyde, and 3,5-Di-tert-butyl-2-hydroxy benzaldehyde) onto chitosan powder to obtain polymer I, II, and III, respectively. The modification allows enhancing the sorption of Co (II) and Ni (II) ions from aqueous solutions. FTIR analysis, BET isotherm, TGA data, SEM, and XRD analysis have been utilized to specify the structure of the

prepared Schiff base bio-sorbents after the chemical modification and to emphasize binding between the sorbent and the two metallic ions. pH at zero charge has been also estimated for approaching the interaction mechanism with the two metallic ions. The environmental factors were evaluated using batch experiments. The sorption equilibrium data was modeled effectively and obeyed the Langmuir equation with  $q_{max}$  higher than  $125 \text{ mg g}^{-1}$  for the polymers. The uptake behavior follows  $\text{Co (II)} > \text{Ni (II)}$ . Further, two kinetic models have been overwhelmingly applied pseudo-first and second-order kinetic models, the best model that fitted the data was the pseudo-second-order rate equation suggested chemisorption might be the rate-determining step. The adsorption process was endothermic, feasible, and the positive value of  $\Delta S$  indicated the high randomness at the solid/solution interface.

Table 11. Sorption of cobalt ion on polymer I, II, and III at different temperatures

Table 11. Sorption of cobalt ion on polymer I, II, and III at different temperatures

T (°C)	T (K)	C <sub>0</sub> (ppm)	Polymer I		Polymer II		Polymer III	
			q <sub>e</sub> (mg g <sup>-1</sup> )	R%	q <sub>e</sub> (mg g <sup>-1</sup> )	R%	q <sub>e</sub> (mg g <sup>-1</sup> )	R%
30	303.15	20	48.689	48.689	52.378	52.378	53.615	53.615
40	313.15	20	52.747	52.747	52.902	52.902	54.214	54.214
50	323.15	20	54.891	54.891	55.379	55.379	54.729	54.729
70	343.15	20	55.922	55.922	57.12	57.12	56.168	56.168



**Ioana Stanciu**

University of Bucharest, Romania

**Biography**

Ioana Stanciu working at the University of Bucharest, Faculty of Chemistry has a 20 years experience in teaching and conducting research on the study of polymers used as additives for lubricating oils, the rheological behavior of vegetable oils and mineral oils added to polymers. Ioana Stanciu is the author of 9 books and has the recognition of publishing 90 works in the field of physical chemistry, is the editor of several international magazines. He has presented over 41 national research papers of which 9 research papers at international conferences. He has earned over 250 diplomas awarded nationally and internationally.

**Studies spectroscopy FTIR of copolymers used as viscosity improvers for SAE 10W mineral oil**

The copolymer INFINEUM SV 206 is used as viscosity improvers for multi-grade oil. The properties chemical and physical of copolymer INFINEUM SV 260 are: physical state – solid, form – white solid blocks, colour – compressed crumbs, odourless, flashpoint > 1500C, insoluble in water, is not material hygroscopic, stable, density (15°C) – 0. 272 g.cm<sup>-3</sup> and none hazardous decomposition.

The intensity of the absorption band at 2922.45 cm<sup>-1</sup> associated with the CH<sub>2</sub> asymmetric stretch [7] had decreased significantly after aging. A similar decrease was also observed for the CH<sub>2</sub> absorption band at 2853.31 cm<sup>-1</sup>, which is associated with the CH<sub>2</sub> symmetric stretch.

The significant observation about the aged IR spectra is decomposition of the C-CH<sub>3</sub> bond with an asymmetric bend at 1459.99 cm<sup>-1</sup>. The third major observation is in the intensity of the C-CH<sub>3</sub> bond with a symmetric bend around wave number 1376.35 cm<sup>-1</sup>. A similar reduction was also observed for the out-of-plane CH bend absorption at wavenumber 699.61 cm<sup>-1</sup>.

The spectres FTIR of one copolymer presents bend characteristic groups: CH<sub>3</sub>, CH<sub>2</sub> and CH aliphatic.



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**Accepted  
Abstracts**

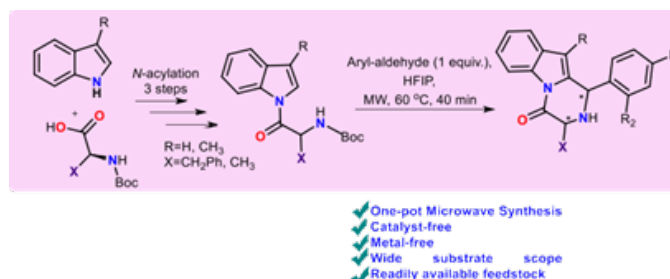
**Aarushi Singh**

University of Delhi, India

**Stereospecific N-acylation of Indoles and corresponding Microwave mediated synthesis of Pyrazinoindoles using Hexafluoroisopropanol**

We envisioned a facile construction of diversified pyrazinoindoles by using 1,1,1,3,3,3- Hexafluoroisopropanol (HFIP) as the solvent and catalyst, hence eliminating metal catalyzed routes for its development. The process is facilitated by HFIP that has emerged as a powerful tool for development of novel fused heterocycles. This cascade approach blends the asymmetric N-acylation with consecutive intramolecular cyclisation via Pictet-Spengler reaction as an efficient tool forming overall two stereogenic centers. Our approach deals with incorporation of L-amino acid on

substituted indoles to provide the chiral N-acylated indole precursor followed by cyclisation to access Pyrazinoindole derivatives in high enantiomeric excess upto >99% in good to excellent yields, which have great potential as molecular scaffolds in drug discovery. We have also described the mechanistic course of the reaction based on density functional theory.



**Qian Liu**

Second Institute of Oceanography, China

**Dissolved free amino acids and polyamines are two major dissolved organic nitrogen sources for marine bacterioplankton**

The regenerated nitrogen from dissolved organic nitrogen (DON) has been suggested to play a pivotal role in sustaining primary productivity in marine environments; however, DON cycling has not been clarified there. Dissolved free amino acids (DFAAs) and polyamines (DFPAs) are two major groups of labile DON that are used rapidly by heterotrophic bacteria, and important in nitrogen cycling. In this study, we applied radio-isotope labelled compounds for measuring turnover rates and HPLC for quantifying concentrations

of representative DFAAs (arginine and glutamic acid) and DFPAs (putrescine) in riverine, estuary and coastal shelf waters, to estimate uptake rates and evaluate their potentials to fulfill carbon and nitrogen demands of bacterial production. Furthermore, homologs of genes encoding transporter systems for arginine (*aotJ*) and putrescine (*potD/potF*) were quantified in metagenomes from sampling stations. The taxa encoding these genes were identified to gain insight into the composition of microbial communities potentially utilizing DFAAs and DFPAs. Spatial variation in uptake rates indicated that biogeochemical cycling of DFAAs was distinct from that of DFPAs. Redundancy analysis and metagenomes demonstrated that environmental variables and distinction in bacterial assemblages using DFAAs and DFPAs could both affect their dynamics in marine environments.

**Shaymaa E. Kassab**

Damanhur University, Egypt

**Structure-based design and synthesis of conformationally constrained derivatives of methyl-piperidinopyrazole (MPP) with estrogen receptor (ER) antagonist activity**

Nuclear Estrogen receptors (ER) are cytoplasmic proteins; translocated to the nucleus to induce transcriptional signals after getting bound to the estrogen hormone. ER activation implicated in cancer cell proliferation of female reproductive organs. Thus, the discovery of ER antagonists is a reliable strategy to combat estrogen-dependent breast cancer. Endometrial carcinoma is one of the complications encountered upon long-term therapy by selective estrogen receptor modulators (SERMs) like Tamoxifen (TMX) and methyl piperidinopyrazole (MPP). Thus, the ER-full antagonist is a solution to improve the safety of this class of therapeutics during the treatment of breast cancer. We selected MPP as a lead structure to design conformationally constrained analogs. Structural rigidification is a proven strategy to transform the SERMs into full antagonists. Accordingly, we

synthesized 7-methoxy-3-(4-methoxyphenyl)-4,5-dihydro-2H-benzo[g]indazoles (4), (6a-c), (8–12) along with the biphenolic counterparts (13–19) that are the anticipated active metabolites. The 4-nitrophenyl derivative (4) is with the most balanced profile regarding the *in vivo* anti-uterotrophic potential ( $EC_{50} = 4.160 \mu\text{M}$ ); and the cytotoxicity assay of the corresponding active metabolite (13) against ER+ breast cancer cell lines (MCF7  $IC_{50} = 7.200 \mu\text{M}$ , T-47D  $IC_{50} = 11.710 \mu\text{M}$ ). The inconsiderable uterotrophic activities of the elaborated ERantagonists and weak antiproliferative activity of the compound (13) against ovarian cancer (SKOV-3  $IC_{50} = 29.800 \mu\text{M}$ ) highlighted it as a good start point to elaborate potential ER-full antagonists devoid of endometrial carcinoma. Extending the pendant chain that protrudes from the 2-(4-(substituted)-phenyl) ring of the new benzo-indazoles is recommended for enhancing the potency based on the binding mode of compound (13) in the ligand-binding domain (LBD) of ER.

**Tingting Dai**

Stanford University, USA

**Biography**

Sebastian Dudek is a PhD student at the International Doctoral Studies in Chemistry at Maria Curie-Skłodowska University (Lublin, Poland). Since October 2018 he has worked on a doctoral thesis under the supervision of Prof. Dorota Kołodyńska. The topic of his doctoral dissertation concerns the removal of arsenate ions on the ion exchangers modified with lanthanide ions. Since 2019 he has been also employed as a lecturer at the Faculty of Chemistry at MCSU.

**The design and synthesis of a dual-targeting fluorogenic probe for phagocytosed *Mycobacterium tuberculosis***

With an estimated 1.7 billion latent infections, 10 million illnesses, and 1.3 million deaths in 2017, tuberculosis (TB) remains the deadliest disease caused by a single infectious agent, ranking above HIV/AIDS. TB is caused by the slow-growing airborne pathogen *Mycobacterium tuberculosis* (Mtb), which colonizes resident macrophages as their natural habitat. Fluorescence-containing trehalose probes have been tested for

labeling phagocytosed Mtb inside macrophages, but the extremely high working concentration ( $\geq 200 \mu\text{M}$ ) brought nonspecific background and potential toxicity. In this talk, I will discuss the dual-targeting design strategy in developing specific and sensitive probes for the diagnosis and imaging of Mtb. More recently, we applied this strategy to the development of a cephalosporin caged Tokyo Green-trehalose probe, CDG-Tre that is specifically activated and incorporated into the cell envelope of growing bacilli. The mechanism of CDG-Tre involves BlaC, a unique enzyme expressed by TB, and the essential trehalose mycolyltransferase enzymes, AG85s. This new dual-targeting fluorogenic strategy was validated in different bacteria species and fungi and revealed selective labeling of poles and wall structure of growing Mtb within infected macrophages at as low as  $2 \mu\text{M}$  concentration. In comparison, dead bacilli could not be labeled under similar conditions. These findings suggest that cephalosporin may act as a unique function moiety to increase Mtb uptake of unnatural trehalose and potentially many other small molecules within phagosomes. A specific and sensitive detection of growing Mtb either extracellularly or inside macrophages may find many potential applications in pathogenesis studies, drug screening, and most importantly, for detection of TB.

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[heartcongress@scmeetings.org](mailto:heartcongress@scmeetings.org)

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