



# INTERNATIONAL SUMMIT ON CATALYSIS & CHEMICAL ENGINEERING

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# ABOUT SCITECHSERIES CONFERENCES

## **Spreading Science and Technology Research Outcome to Remote Corners of the Globe.**

**Scitechseries** offers a platform that is more inclusive and diverse, with researchers from the global North and the emerging South. A vast fraternity of budding researchers, experienced scholars, academicians, and seasonal professionals, join our conferences each year to deliberate on pure and applied Medical, Engineering, Technology, and Life Sciences research. We never deterred from adding emerging fields of research and our conferences spread across the destinations in Europe, Asia, the Middle East, the United States, and Canada.

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Our conferences extend exceptional benefits to emerging, experienced, and emeritus scholars in many ways. Join us for Networking, new project funding options, exploring new fields of scientific research, and unveiling successful formulas and solutions to promote your ideas.


## **Scope of the International Summit on Catalysis and Chemical Engineering:**

Scitechseries extends a warm invitation to the esteemed “International Summit on Catalysis and Chemical Engineering” (ISCC 2024) scheduled during June 19-20, 2024 as Virtual Event. This conference is evolving with the theme “From Lab Bench to Marketplace: Bridging the Gap in Catalysis Innovation”. ISCC 2024 serves as a dynamic platform for the exchange of cutting-edge research discoveries and innovative methodologies. Catalysis and chemical engineering, integral to advanced technology, encompass both present and future industry requirements. Yearly, this conference unites leaders from industry, academia, and regulatory spheres to curate an all-encompassing program covering traditional and avant-garde subjects, technologies, and applications. ISCC 2024 provides a meeting point for established professionals and emerging industry visionaries to deliberate, contribute, and glean insights into the sectors promising trajectory.

# KEYNOTE PRESENTATIONS



DAY 01



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**JIANXIN ZOU**

Shanghai Jiao Tong University  
China

## Hydrogen storage in Mg based nano composite materials

### Abstract:

Magnesium hydride ( $MgH_2$ ) has been regarded as one of the most promising solid-state hydrogen storage materials, due to highly reversible capacity, high abundance, and low cost. However, the practical application of  $MgH_2$  has been hampered by its high thermodynamic stability and sluggish kinetics, both usually requiring high operation temperatures and slow ab/de-sorption rate. In recent years, a large amount of researches have focused on the modification of Mg-based hydrogen storage materials. Among the numerous modifications, nanotechnology is considered to be an efficient strategy to improve their thermodynamic and kinetic properties, simultaneously. In this work, we summarize the preparation and characterization of nano-sized Mg-based composites. Herein, the fundamental theories, recent advances, and practical applications of the nanostructured Mg-based hydrogen storage materials are discussed. The synthetic strategies of Mg-based nano composites include mechanical milling methods, construction of core-shell nano-structured Mg-based composites by chemical reduction approaches, and multi-dimensional nano-sized Mg-based heterostructure by nanoconfinement strategy. The synthetic strategies of different scaffolds, the fabrication methods of Mg-based nano composites, and the characterization of their performances and morphologies are highlighted. The thermodynamic and kinetic properties, microstructure, phase changes, and hydrogen ab/de-sorption mechanisms of Mg-based hydrogen storage materials are investigated using advanced characterization techniques such as synchrotron radiation, neutron diffraction, HRTEM, XPS etc. Finally, we look forward to the future development and applications of Mg-based hydrogen storage materials.

### Biography

**Jianxin Zou**, born in 1978, is currently a tenured professor in Materials Science at Shanghai Jiao Tong University in China, the Fellow of the Royal Society of Chemistry and the International Association of Advanced Materials. He obtained his PhD degrees from the University of Lorraine in France and Dalian University of Technology in 2007. He then served as a postdoctor at the University of British Columbia. He has published over 170 academic papers in journals such as *Science*, *Adv Mater.*, *Adv Energy Mater.*, etc. He is now mainly engaged in the design, preparation, characterization and application of advanced magnesium-based energy materials. He holds 26 national and international patents and research funds from Shanghai Municipal Government, the Ministry of Education, National Science and Technology committee and NSFC.



## TADAYUKI IMANAKA

Ritsumeikan University

Japan

### **An efficient way of producing fuel hydrocarbon from atmospheric CO<sub>2</sub> and activated water**

#### **Abstract:**

Here we show that petroleum can be formed efficiently at normal temperatures and pressures from atmospheric carbon dioxide and activated water. The CO<sub>2</sub> nano-bubble containing water was treated with photocatalyst in the presence of oxygen under UV irradiation to form radical water. The activated radical water was mixed vigorously with kerosene or light oil. The mixture gradually separated into a two-phase solution. After phase separation, the volume of kerosene or light oil, depending on which oil was utilized, increased by 5 to 10 %. When n-tetradecane was used, n-tetradecane was only produced. These results suggest template-dependent synthesis. It is also shown that commercial light was purified by removing organic and inorganic impurities, resulting in premium oil. It has also been shown that atmospheric CO<sub>2</sub> was directly converted to hydrocarbon by measuring <sup>14</sup>C (radioisotope) in the newly synthesized hydrocarbon. The industrial machine for continuous production of oil was constructed.

#### **Biography**

**Tadayuki Imanaka** has received PhD from Osaka University in 1973. Postdoctoral research associate at Massachusetts Institute of Technology (USA). He was a Professor at Osaka University, Kyoto University and Ritsumeikan University. He was awarded many prizes, including Fellow in American Academy of Microbiology. He received the Purple Ribbon Medal in 2010, and The Order of the Sacred Treasure, Gold Rays with Neck Ribbon from Japanese Emperor in 2018.



## PANGKUAN CHE

Beijing Institute of Technology  
China

### $\pi$ -Conjugated Main-Group chiral macrocycles with circularly polarized luminescence and Open-Shell character

#### Abstract:

Organic luminescent materials with low-energy absorption and emission properties, especially those in the red-to-near-infrared (NIR) region are used as photodetectors and laser filters in optoelectronics and medical applications. However, synthesis of such materials with unique  $\pi$ -conjugation effect has rarely been reported. Incorporation of main group elements into aromatic systems has been established for decades to tune the electronic structures of organic materials. Those B/N-doped main-group compounds have particularly attracted considerable research interests due to notable contribution to the optoelectronic properties. New chiroptical materials with circularly polarized luminescence (CPL) have recently found numerous applications in photonics, smarting sensing and (bio) imaging as well as information technology. In pursuit of new main-group chemistry, this work will focus on the design, synthetic approach and characterization of B/N-doped macrocycles and CPL-active materials with emission in the red-to-NIR region and with the open-shell characters.

#### Biography

**Pangkuan Chen** has completed his PhD from Rutgers University with Prof. Frieder J kle, and postdoctoral studies from MIT with Prof. Niels Holten-Andersen. He is the full professor of Beijing Institute of Technology School of Chemistry, and he also serves as the director of Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials. He has published more than 60 papers in reputed journals. His current research builds on organoborane chemistry,  $\pi$ -conjugated macrocycles, Near Infrared (NIR) circularly polarized luminescence, chiral radical chemistry and dynamic B/N Lewis pairs.





**THOMAS J. WEBSTER**

Hebei University of Technology  
China

## **Using cells as the environmentally catalyst for nanoparticle Synthesis: Killing Bacteria, Inhibiting Inflammation, and Growing Tissues**

### **Abstract:**

While conventional nanoparticles have revolutionized medicine including to improve the prevention, diagnosis, and treatment of numerous diseases from cancer to infection, traditional nanoparticles are made with toxic catalysts. As a way to both improve human health and do less harm to the environment, this presentation will cover how nanoparticles can be made via cells. Bacteria, mammalian cells, and cancer cells can be programmed to make nanoparticles out of a wide range of chemistries and sizes without using toxic catalysts. This presentation will highlight such synthesis techniques as well as in vitro and in vivo assays using such nanoparticles to selectively kill cancer cells, inhibit bacteria function, and grow tissues. It will also present a clinical study where over 30,000 patients have been helped through nanotextured spinal implants in which no implant failures have been reported to date (over the past 5 years where the conventional failure rate is 5 – 10%). This presentation will also provide future directions for how environmentally-friendly nanoparticles can continue to revolutionize medicine.

### **Biography**

**Thomas J.** Webster's (H index: 125; Google Scholar) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). He has served as a professor at Purdue (2000-2005), Brown (2005-2012), and Northeastern (2012-2021; serving as Chemical Engineering Department Chair from 2012 - 2019) Universities and has formed over a dozen companies who have numerous FDA approved medical products currently improving human health in over 20,000 patients. His technology is also being used in commercial products to improve sustainability and renewable energy. He is currently helping those companies and serves as a professor at Brown University, Saveetha University, Vellore Institute of Technology, UFPI, and others. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology); 2022, Best Materials Science Scientist by Citations (Research.com); and is a fellow of over 8 societies. Prof. Webster is a former President of the U.S. Society For Biomaterials and has over 1,350 publications to his credit with over 55,000 citations. He was recently nominated for the Nobel Prize in Chemistry. Prof. Webster also recently formed a fund to support Nigerian student research opportunities in the U.S.

# ORAL PRESENTATIONS

DAY 01

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**JUAN DANG**

Shandong University  
China

## **New insight into the removal process of benzotriazoles in advanced oxidation processes: Integrating quantum chemical calculation with CFD simulation**

### **Abstract:**

Benzotriazole UV stabilizers (BT-UVs) are important UV absorbers. As high-production chemicals and potential hazards, their ubiquitous presence in aquatic environments is of greatly pressing concern. Herein, the removal of six typical BT-UVs by UV/H<sub>2</sub>O<sub>2</sub> was comprehensively investigated by quantum chemistry calculation integrated with CFD simulation. Utilizing such a micro and macro incorporated model in treating contaminants is the first report. From the micro-view, the degradation mechanisms of BT-UVs by •OH oxidation were determined, and corresponding rate constants were obtained with values of 10<sup>9</sup>~10<sup>10</sup> M<sup>-1</sup>s<sup>-1</sup>. In a macroscopic aspect, combining the established kinetic model and CFD simulation, the effects of UV lamp power (P), volumetric flow rate (Q<sub>v</sub>), and H<sub>2</sub>O<sub>2</sub> dosage ([H<sub>2</sub>O<sub>2</sub>]<sub>0</sub>) on removal yields of BT-UVs were expounded, increasing P or [H<sub>2</sub>O<sub>2</sub>]<sub>0</sub> or decreasing Q<sub>v</sub> are effective in improving removal yields of BT-UVs, but the enhancement was abated when P or [H<sub>2</sub>O<sub>2</sub>]<sub>0</sub> increased to a certain level. In addition, rapidly predicting energy consumption for target removal rates of organic pollutants is crucial for the industrial application of UV/H<sub>2</sub>O<sub>2</sub>. Thus, we explored the UV/H<sub>2</sub>O<sub>2</sub> treatment process for potential organic contaminants by extending the degradation rate constants to a wide range of 10<sup>9</sup> ~ 10<sup>11</sup> M<sup>-1</sup> s<sup>-1</sup>. Based on massive simulation data, we innovatively developed a model to meet the demands. This work proposed a new operable solution for rapidly predicting operation performance and energy consumption for organic contaminant removal in industrial applications of AOP, offering valuable information for practical applications and saving experimental expenses as well as improving efficiency.

### **Biography**

**Juan Dang**, Associate professor at Environment Research Institute of Shandong University, she is the recipient of Hong Kong Scholars Program and the Young Scholars Future Program of Shandong University, and mainly engaged in related research on pollutants migration and transformation, atmospheric chemistry and advanced oxidation process. She has published more than thirty papers in the international academic journals in the field of environment.



## YINGHUAI ZHU

Sunshine Lake Pharma Co. Ltd  
China

### **In Silico assessments of small molecular boron agents for boron neutron capture therapy**

#### **Abstract:**

Boron neutron capture therapy (BNCT) is a highly targeted, selective and effective technique to cure various types of cancers, with less harm to the healthy cells. In BNCT, it is crucial to have high quality boron agents with acceptable bio-selectivity, homogeneous distribution and deliver in required quantity, similar to chemotherapy and other radiotherapy for tumor treatment. Nevertheless, boron drugs currently used in clinical trials yet to meet the full requirements. On the other hand, BNCT processing has opened up the era of renaissance due to the advanced development of the high-quality neutron source and the global construction of new BNCT centers. Consequently, there is an urgent need to use boron agents that have increased biocapacity. In silico molecular docking and molecular dynamic simulation technologies have been used to accelerate screening, particularly for small molecules of boron agents. The boron agent and interacting protein's binding energy (BE), geometric shape complementary score (GSCS) and dynamic simulation results will certainly be helpful to researchers in optimizing druggable boron agents for the BNCT application. This work reports the in silico docking and molecular simulation results of the optimized small boron agents, such as 4-borono-L-phenylalanine (BPA) with optimized proteins like the L-type amino acid transporter 1 (LTA1, also known as SLC7A5), epidermal growth factor receptor (EGFR) and cellular myelocytomatosis (MYC), will be examined. The clinical status of these proteins (SLC7A5, EGFR, and MYC), which are highly relevant to cancers that may be treated with BNCT, has been assessed using bioinformatics technology and discussed accordingly.

#### **Biography**

**Yinghuai Zhu** has completed his PhD at the age of 28 years from Nankai University and postdoctoral studies from Northern Illinois University. He is the expert in new drug R&D, Sunshine Lake Pharma Co., Ltd. He has published more than 90 papers in reputed journals and has been cited more than 3600 times.



## MIRZA MUHAMMAD FARAN ASHRAF BAIG

The Hong Kong University of Science and Technology  
China

### **Recent Advances of Magnetic Gold Hybrids and Nanocomposites, and Their Potential Biological Applications**

#### **Abstract:**

Magnetic gold nanoparticles (mGNP) have become a great interest of research for nanomaterial scientists because of their significant magnetic and plasmonic properties applicable in biomedical applications. Various synthetic approaches and surface modification techniques have been used for mGNP including the most common being the coprecipitation, thermal decomposition, and microemulsion methods in addition to the Brust Schiffrin technique, which involves the reduction of metal precursors in a two-phase system (water and toluene) in the presence of alkanethiol. The hybrid magnetic–plasmonic nanoparticles based on iron core and gold shell are being considered as potential theragnostic agents. Herein, in addition to future works, we will discuss recent developments for synthesis and surface modification of mGNP with their applications in modern biomedical science such as drug and gene delivery, bioimaging, biosensing, and neuro-regenerative disorders. I shall also discuss the techniques based on my research related to the biological applications of mGNP.

#### **Biography**

My research work mainly focuses on the construction and function of DNA nanomachines, which are cutting-edge and challenging topics. I designed and constructed unique DNA motifs using a short circular DNA nanotechnology technique and functionalized these probes with fluorophores, gold nanoparticles, small molecular drugs, and peptide ligands. To achieve plasmon resonance effects, I achieved nano-specific precision in organizing plasmonic nanoparticles on the nano DNA frameworks. My work on the DNA nanomachines provided an efficient fluorescence resonance energy transfer mechanism that realizes the bio-imaging, detection of biological events, and functions of the biomolecules. I have also been working on multilayered hybrid magnetic nanoparticles for applications in nanomedicine for the last three years.



**HAJIME HIRAO**

The Chinese University of Hong Kong  
China

## Cytochrome P450 Enzymes: Computational Insights into Catalytic and Bonding Properties

### Abstract:

Cytochrome P450 enzymes (P450s) are among the most robust biological catalysts, playing indispensable roles across various organisms, including humans. However, experimental characterization of various short-lived intermediates and transition states of P450s is challenging, leaving the catalytic mechanism not yet entirely clear. Additionally, P450 inhibition is a significant public health concern due to its close relevance to adverse drug reactions arising from drug-drug interactions (DDIs). Understanding the molecular mechanisms of cytochrome P450s is therefore crucial, not only for academic interest but also for accurately predicting the DDI liabilities of drug candidates. To this end, we employ computational chemistry techniques to illuminate various facets of P450s.

### Biography

**Hajime Hirao** is a Professor at the School of Medicine at the Chinese University of Hong Kong, Shenzhen. He received his bachelor's degree and master's degree from Kyoto University in 1998 and 2000, respectively, and earned his PhD from the University of Tokyo in 2004. He has published over 175 papers in international journals.



## MOHAMMAD HASSAN HADIZADEH

Shandong University  
China

### Water droplet interfaces as novel catalytic platforms for chemical transformations

#### Abstract:

The air-water interface of water microdroplets can act as a catalyst and dramatically accelerate various chemical reactions compared to bulk water or the gas phase. This phenomenon is known as “on-water catalysis” or “interfacial catalysis”. Many chemical and photochemical reactions experience a remarkable rate acceleration when occurring at the air-water interface of microdroplets, aerosols, sprays, and extended air-water interfaces. The underlying mechanism is thought to be the ultrahigh electric fields present at the air-water interface, with smaller droplets having larger interfacial areas and producing higher yields of products like hydrogen peroxide. The air-water interface provides a unique microenvironment that can orient and align functional groups, facilitate proximity effects, and promote reactions essential for processes like peptide synthesis, mimicking prebiotic systems. Interfacial reactions are widespread in atmospheric chemistry (e.g., oxidation of SO<sub>2</sub> in cloud droplets), synthetic green chemistry (e.g., electrospray reactions), and origin of life studies (e.g., prebiotic chemistry in aerosols or ocean surfaces). Hydrophobic and hydrophilic microenvironments on catalyst surfaces can create reaction platforms, with the air-water interface playing a crucial role in biomass conversion, CO<sub>2</sub> reduction, and other catalytic processes.

#### Biography

**Hadizadeh's** research focuses on using computational chemistry techniques to study atmospheric and environmental processes. As a leader of a project related to NSFC, he has made significant contributions to this important research area.



# POSTER PRESENTATIONS

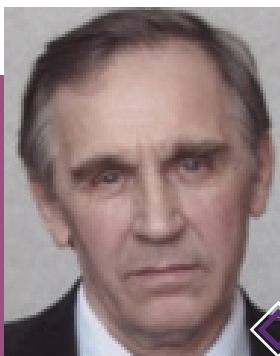
DAY 01

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## VLADIMIR VORONOV

Irkutsk National Research Technical University  
Russia

### **The nature of hyperfine coupling in paramagnetic complexes of iron group elements with 1-vinylimidazole and features of their structure according to NMR**

#### **Abstract:**

The NMR spectra of 1-vinylimidazole, transformed by the additives of paramagnetic complexes of manganese, cobalt, nickel and copper chlorides with this azole, have been studied. It is shown that the coordination atom in a solution has octahedral surrounding, four ligand molecules being located in the equatorial position. The nature of hyperfine coupling in the above complexes is evaluated by comparison of the experimental constants of hyperfine coupling with theoretically calculated spin densities of unpaired electrons on s-orbitals in the vinylpyrrole radical, which is isostructural to the molecule of 1-vinylimidazole. It is found that in the complexes of cobalt, nickel and copper, the molecules of 1-vinylimidazole are coordinated to the central ion by the pyridine N-3 atom. Therefore, paramagnetic shifts observed for the specified complexes are mainly caused by unpaired spin density delocalized in  $\sigma$ -system of the ligand molecule. Notably, in the paramagnetic complex of manganese, hyperfine coupling is transferred both through  $\sigma$ - and  $\pi$ -systems of the 1-vinylimidazole molecule. Localization of the unpaired spin density is due to the fact that molecules of this azole can also be coordinated by the pyrrole N-1 atom at a certain range of temperatures. In its turn, the specified possibility is explained by non-planar structure of a heterocycle in 1-vinylimidazole.

#### **Biography**

**Vladimir Voronov's** research interests are related to solving problems of molecular spectroscopy and physico-organic chemistry by methods of nuclear magnetic resonance and quantum chemistry. In addition, for the last twenty years or so, his research interests have included scientific and methodological issues related to cognitive barriers of university students. He is the author of more than three hundred publications in periodicals, including more than thirty books. He received a number of awards established by the Russian Academy of Natural Sciences, including the Gold Medal "For innovative work in the field of higher education". Member of the American Chemical Society.



**EIMAN SHAHROUR**

Tishreen University

Syria

## Genetic association between symptoms of mild Osteogenesis Imperfecta (OI) and postmenopausal osteoporosis according to NMR

### Abstract:

**Background:** Mild osteogenesis imperfecta OI and postmenopausal osteoporosis are both bone disorders. Mild OI may be associated with postmenopausal osteoporosis. According to NCBI, COL1A2rs72658152 (COL1A2G661S) is a pathogenic proven cause of the association between mild OI and postmenopausal osteoporosis. Aims: The challenges facing DEXA and the treatment plans of the World Health Organization WHO for osteoporosis require a search for new diagnostic solutions such as genetic methods. Methods: COL1A2rs72658152 was detected by Restriction Fragment Length Polymorphism RFLP and DNA sequencing on 150 EDTA blood samples from pre and post menopause women in Tishreen University Hospital. BMD was measured using DEXA. A clinical examination was conducted for the participants. A questionnaire was filled out with information related to the study. Related-Samples McNemar Change Test, Chi-Square Test, and binary logistic regression was used as a statistical method to estimate the correlation between mild OI and postmenopausal (osteopenia or osteoporosis) under 95% confidence level ( $\alpha \leq .050$ ) as well as the correlation between (mild OI, postmenopausal osteoporosis or osteopenia) and some morphological characteristics under 95% confidence ( $\alpha \leq .050$ ). Results & Discussion: The significant chance to the occurrence of mild OI with postmenopausal osteopenia or osteoporosis is 10.8% with confidence level of 95% or more ( $p \leq .05$ ). Strong asymptotic significance of (2-sided) correlation is found between mild OI, on one hand, and postmenopausal osteopenia or osteoporosis on the other (Chi-Square = 29.066,  $p = .000 < .05$ ). Mild OI has a significant impact on postmenopausal osteoporosis or osteopenia ( $p = .000 < .05$ ). They are in positive correlation relationship according to the nature of tendency slope ( $B = 1.758$ ). Conclusion: Mild OI is associated with postmenopausal osteopenia and osteoporosis with statistical significance with reasons other than COL1A2G661S, and no specific morphological characteristics are found. Postmenopausal osteoporosis is not a primary osteoporosis because there are causes for it to occur. This is contrary to WHO classification.

### Biography

**Eiman shahrour** has completed his PhD at the age of 35 years from tishreen University. He is the director of medical laboratory. She has published about 10 papers in reputed journals and has been serving as an editorial board member of repute.



**S.KUDIYARASAN**

BHAVINI

India

## **Paroxysmal nocturnal hemoglobinuria and eculizumab (monoclonal antibody) as membrane attack complex inhibitor**

### **Abstract:**

PNH is a Complement mediated intravascular blood cell lysis which is caused by the mutation of Phosphatidylinositol glycan A (PIG-A) gene. A membrane anchor lipid called Glycophosphatidylinositol (GPI) is coded by PIG-A gene, which is responsible to bind with several other proteins like decay accelerating factor (DAF), CD59 etc. These kinds of anchoring, inhibit the action of cell lysis by complement system and keep the necessary body cells safe from the immune and complement system attack. Now if there is any problem in the synthesis of GPI due to PIG-A mutation/ inactivation then those anchoring activities will be interrupted and complement system will accelerate the lysis (called membrane attack complex-MAC) and the blood cells will be destructed. Even though the name suggest that the disease is acute in nature, it will occur at night and there will be hemolysis but it is chronic in nature, it can occur any time and it is not related to hemolysis, PIG-A mutation also can cause leucopenia and thrombocytopenia. This paper will elaborate the detailed pathology of the diseases and how the MAC could be inhibited using a monoclonal antibody.


### **Biography**

**S.S.Biswas** obtained his Bachelor of Engineering degree in Electronics and Telecommunication Engineering from Indian Institute of Engineering Science and Technology (formerly Bengal Engineering College), PG Diploma in Radiology and Imaging Technology, MBA in System and M.Tech in Power Electronics and Drives. He joined a reputed multinational software company just after completion of degree, later quit from there and now he is a nuclear scientist. He is also a Faculty to handle “Process Analysis & Control”, “Maintenance Engineering”, “Process Design & Control” and “Reliability Engineering” courses for Trainee Nuclear Engineers/Scientists. He is qualified in Level-II Ultrasonic NDT technique, trained in “Design for Additive Manufacturing” and Life member of Institute of Engineers (India), Instrument Society Of India & International Association of Engineers. During his industrial carrier, few of the important activities are design of large electrical machine and power converters, analysis in Finite Element Modelling, CFD etc. His main area of interests are Induction motor control, Micro-controller Applications, Power Electronics & Control and Medical Instrumentation.

# ORAL PRESENTATIONS



DAY 01



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## DELIA TERESA SPONZA

Dokuz Eylül University  
Turkey

### Removal of some endocrine disruptors like polibrominated diphenyl ether (PBDE) and etinilestradiol (17 alfa-etinilestradiol, EE2) with ZnO/Graphene nanocomposite

#### Abstract:

The aim of this study was the photodegradation of two endocrine disruptors namely polybrominated diphenyl ether (PBDE) and etinilestradiol (17 alfa-etinilestradiol, EE2) using ZnO/Graphene nanocomposite. The effects of endocrine disruptors concentration, nanocomposite concentration, photodegradation time, temperature and pH, and sun light powers on the yields of polibrominated diphenyl ether (PBDE) and etinilestradiol (17 alfa-etinilestradiol, EE2) were investigated. For maximal photodegradation of polibrominated diphenyl ether (PBDE) and etinilestradiol (17 alfa-etinilestradiol, EE2) (99%) the optimal operational conditions should be as follows: nanocomposite ,polibrominated diphenyl ether (PBDE) and etinilestradiol (17 alfa-etinilestradiol, EE2) concentrations were 1,4 mg/L, 300 mg/L, respectively. The photodegradation time, temperature , pH, and sun light should be 20 min, 25 °C temperature, pH=7 pH and 30 watt/m<sup>2</sup>dir. The photodegradation kinetic was zero for 300 mg/L polibromlu difenil eter (PBDE) and etinilestradiol (ya da 17 alfa-etinilestradiol, EE2) konsantrasyonunda with  $k_0 = 0,00311 \text{ day}^{-1}$  and  $R^2 = 0,994077$ .

#### Biography

**Delia Teresa Sponza** is currently working as a professor at Dokuz Eylül University, Department of Environmental Engineering. Scientific study topics are; Environmental engineering microbiology, Environmental engineering ecology, Treatment of fluidized bed and activated sludge systems, Nutrient removal, Activated sludge microbiology, Environmental health, Industrial toxicity and toxicity studies, The effect of heavy metals on microorganisms, Treatment of toxic compounds by anaerobic / aerobic sequential processes, Anaerobic treatment of organic chemicals that cause industrial toxicity and wastewater containing them, Anaerobic treatability of wastewater containing dyes, Treatment of antibiotics with anaerobic and aerobic sequential systems, Anaerobic and aerobic treatment of domestic organic wastes with different industrial treatment sludges, Treatment of polyaromatic compounds with bio-surfactants in anaerobic and aerobic environments, Treatment of petrochemical, Textile and olive processing industry wastewater by sonication, Treatment of olive processing industry wastewater with nanoparticles and the toxicity of nanoparticles. She has many international publications with an H index of 42 and 6000 citations.



**JANA PISK**

University of Zagreb  
Croatia

## Materials incorporating molybdenum and vanadium as active catalysts

### Abstract:

Transition metal catalysts, specifically those anchored on molybdenum, vanadium, and tungsten, possess recognized activity as catalysts in facilitating oxidation reactions. The initial exploration encompassed molecular catalysts (both single and multiple coordination complexes containing Mo, V and W metal cores, along with diverse supramolecular architectures) to supported catalysts (polyoxometalates adhered to Merrifield supports). These catalysts were tested in different (ep)oxidation reactions, following the principles of green chemistry. The focal points included minimizing catalyst quantities, excluding organic solvents from the reaction media, and employing oxidants available in aqueous solutions. Additionally, recent research aimed the preparation and evaluation the derived materials for their conductivity and catalytic potential. Notably, impedance spectroscopy was introduced for the first time to track the real-time transformations of mononuclear to polynuclear molybdenum complexes, complementing findings obtained by thermal analysis. Thus far, the outcomes have revealed a compelling correlation between structural attributes and the material's conductivity and catalytic efficiency. Moreover, all investigated complexes exhibited augmented conductivity with rising temperatures, displaying semiconductor-like behavior. Our recent investigations have ventured into a new realm: preparation of the oxide glasses and glass-ceramics. Despite extensive knowledge about the electrical properties of glass-ceramics, there remains a considerable gap in exploring their catalytic applications. As a response, our focus has shifted towards exploring the potential of glass-(ceramic)-based materials as catalysts in analogous oxidation processes previously conducted. This innovative approach extends the application scope of glass-(ceramics), traditionally employed as catalyst supports, toward catalytic functionalities.

### Biography

**J. Pisk** got a Ph.D. in Chemistry in 2012. In 2010 she spent one year at LCC Toulouse and IUT P. Sabatier Toulouse III, France, where she learned the basics of catalysis. She was Marie Curie Cofund's fellow and did postdoctoral research at the LCC, Toulouse (Project "Diligent search for chemical bio-sources: Solvent-free homogeneous and heterogeneous oxidation processes catalyzed by polyoxometalates"). She was an Assistant Professor at the Faculty of Science, Zagreb, in 2018, and from 2023 she is an Associate Professor. Her major interest is the coordination chemistry of molybdenum and vanadium and the investigation of catalytic properties of the obtained materials.





# KEYNOTE PRESENTATIONS

DAY 02

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**ZLATAN DENCHEV**

University of Minho  
Portugal

## Immobilization effectiveness of various polyamide porous microparticles as carriers for enological pectinase

### Abstract:

The use of free pectinases as clarification biocatalysts constitutes a well-established practice in the large-scale production of various types of wines and juices. However, when in the form of free enzymes, the recovery and reuse of the relatively expensive pectinases is not possible. To address this limitation, we have performed noncovalent adsorption immobilization of a commercial pectinolytic preparation onto highly porous polyamide microparticulate supports (PAMS) based on PA6, PA4, PA12, and PA6-12, with and without magnetic properties, prepared via activated anionic polymerization of the respective lactams in solution. The novel PAMS/pectinase complexes resulting after immobilization underwent comparative activity and kinetic studies, contrasting them with the free enzyme preparation. The PAMS-immobilized pectinase complexes exhibited significantly higher specific activity toward the pectin substrate. The complexes displayed a higher affinity to the substrate, while acting as faster catalysts that were more resistant to inhibition. The immobilized complexes were applied in the clarification process of industrial rosé must, whereby they demonstrated accelerated performance as compared with the free enzyme. Moreover, these PAMS-immobilized pectinase biocatalysts offered the potential for three consecutive cycles of reuse, achieving complete rosé must clarification within relevant timeframes in the range of 3–36 h. All these results are in favor of the industrial application of the new PAMS/pectinase biocatalysts.

### Biography

**Z. Denchev** has completed his PhD in 1990 (Technical University of Sofia, Bulgaria) and his habilitation in 2015 (University of Minho, Portugal). Since 2000 to present he has been working as staff professor at the University of Minho, Institute for Polymers and Composites (IPC). He has published more than 100 peer-reviewed papers in reputed journals dedicated to polymer synthesis, enzyme immobilization on polymer supports, biocatalytic reactions, polymer analysis by synchrotron X-ray techniques. Author and co-author of 12 book chapters. Holds 8 patents. Currently serves as editorial board member of the MDPI journal *Micro*. ORCID data at: <https://orcid.org/0000-0002-9057-9380>



**CECILE RAILLARD**

Nantes University  
France

## Photocatalytic Oxidation for Indoor Air Treatment

### Abstract:

Photocatalytic oxidation (PCO) is a cheap and energy efficient solution for air treatment based on chemical reactions on semiconductor (mostly TiO<sub>2</sub>) catalyst surface under UV irradiation. It has been studied for several decades and can be used to remove gaseous contaminants, mainly volatile organic compounds (VOCs). It has the advantage of being a flexible solution for the degradation of a wide spectrum of gaseous pollutants in different environments such as schools, houses, hospitals. The performance of PCO systems depends on several parameters that can be categorized into two types: process parameters (e.g. air velocity, light intensity, catalyst media geometry) and environmental parameters (e.g. initial concentration, relative humidity, and presence of co-pollutants). The goal of the studies carried out in our laboratory is to define optimized process parameters to achieve the highest possible degradation rates of initial pollutants, alone or in mixture, while avoiding the formation of byproducts that could be more harmful to human health than initial compounds. Experimental works, performed in a specifically designed stainless steel close loop reactor and sometimes coupled with numerical simulations, have enabled to study the degradation of mixtures of VOCs (acetaldehyde, toluene, methylethylketone, decane, trichloroethylene, acrylonitrile, isoflurane, etc.) in operating conditions close to real ones (ppb range concentrations, high flow rates). The obtained data have been explored in order to figure out degradation pathways, to better understand interactions between the pollutants as well as the influence of process parameters and to propose solutions to improve PCO system efficiency for standalone or HVAC implanted devices.

### Biography

**Cecile Raillard** has completed her PhD at the age of 27 years from Nantes University. She is assistant-professor in the GEPEA laboratory (UMR CNRS 6144). She has published more than 20 papers in reputed journals.



## MOHAMED NAGEEB RASHED

Aswan University

Egypt

### **New Trends in Green Synthesis of Metals Nanocatalyst and its Application for Treatment of Polluted Water**

#### **Abstract:**

Green synthesis of metal nanocatalyst (MNC) is an updated green nanotechnology. There are several methods for the green synthesis of metal nanocatalyst, one of these methods used plants and microorganism extract and defined as biosynthesis of nanoparticles. Biological entities or their extracts are used for bio-reduction of metallic particles. The nanocatalyst produced by green synthesis differ from those using physical and chemical methods. Green synthesis of MNC is easy, efficient, nontoxic, eco-friendly, cost-effective, eliminates the use of toxic chemicals, and consume less energy. Several biological agents were employed for green synthesis of MNC such as plants, fungi, bacteria, and algae. Among the different agents available of MNC synthesis, the plant extract is a rather simple and easy process to produce nanoparticles at large scale relative to bacteria or fungi mediated synthesis. Additionally, various plant parts, including leaves, stems, fruits, and roots have been used for the synthesis of metal nanoparticles. Nowadays, honey bees, and human cells have been shown to be innovative resources for producing safe and nontoxic nanoparticles. This review discusses, through the recently published researches, the different methods for green synthesis of MNC, their particle sizes produced by different bio-extracts, and their environmental applications in different fields as well as their application in water, wastewater treatment.

#### **Biography**

**Mohamed Nageeb Rashed** is professor of analytical and environmental chemistry, former vice-dean for environmental affairs, Faculty of Science, Aswan University, Egypt. His research interest has been analytical and environmental chemistry with special emphasis in advanced oxidation treatment; photocatalysis, nanocatalyst, nanocomposite and adsorption techniques for water and wastewater treatment. Prof. Rashed supervised several M.Sc. and Ph.D. thesis in the field of analytical and environmental chemistry. He selected as external examiner for several Ph.D. thesis in analytical chemistry from India, Kasakhstan, Malisia and Bostuana. Prof. Rashed published about 95 scientific papers in peer reviewed international journals. He participated as invited and plenary speaker in 30 international conferences worldwide. He acts as editor-in-chief and an editorial board member in several international journals. Prof. Rashed enrolled among World's top 2% scientists by Stanford University, USA 2020-2022. He awarded the Egyptian State Award for Environmental Researches in the years 2001, and Aswan University Merit Award for Basic Science year 2020.



**OSMAN ADIGUZEL**

Firat University  
Turkey

## Shape reversibility and martensite variants in shape memory alloys

### Abstract:

Metals and alloy systems have different phases at the phase diagrams depending on the alloy compositions and exhibit different characteristics. Shape memory alloys take place at the  $\beta$ -phase region, with alloy composition. However, these alloys take place in class of smart and advanced structural materials, with the response to the variation of temperature and external conditions, by exhibiting a peculiar property called shape memory effect. This phenomenon is characterized by the recoverability of two certain shapes of material at different conditions. Shape memory effect is initiated with thermomechanical processes on cooling and deformation, and performed thermally on heating and cooling, with which shape of the materials cycle between original and deformed shapes in reversible way. Therefore, this behavior can be called Thermal Memory or Thermoelasticity. This deformation is plastic deformation, due to the soft character of the material in low temperature condition, deformation energy is stored in the material and released on heating by recovering the original shape. These alloys are used as shape memory devices in many fields such as medicine, metallurgy, building industry. This property is result of the crystallographic transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling with cooperative movements of atoms by means of lattice invariant shears in  $\langle 110 \rangle$  -type directions on the  $\{110\}$  - type planes of parent phase, along with lattice twinning and ordered parent phase structures turn into the twinned martensite structures. Twinned structures turn into the detwinned structures by means of stress induced martensitic transformation, with deformation in the martensitic condition. Atomic movements are confined to the neighbor atom distances, and martensitic transformations are diffusionless or displacive transformations. Lattice invariant shears occur as martensite variants on  $\{110\}$  -type planes of austenite matrix which is basal plane of martensite. These shears occur, in  $\langle 110 \rangle$  -type directions on the  $\{110\}$ -type planes of the parent phase. The  $\{110\}$ - plane family represent 6 certain planes,  $\langle 1 1 0 \rangle$ ,  $\langle -1 1 0 \rangle$ ,  $\langle 1 0 1 \rangle$ ,  $\langle -1 0 1 \rangle$ ,  $\langle 0 1 1 \rangle$ ,  $\langle 0 1 -1 \rangle$ , and totally 24 martensite variants occur. These alloys exhibit another property called superelasticity, which is performed with stressing and releasing material in elasticity limit at a constant temperature in parent phase region, and shape recovery is performed simultaneously upon releasing the, by recovering the original shape. Parent phase of these alloys are hard phase, stressing and releasing steps exhibit elastic material behavior. Superelasticity is performed in non-linear way; stressing and releasing paths are different in the stress-strain diagram, and hysteresis loop refers to energy dissipation. Superelasticity is also result of stress induced martensitic transformation and ordered parent phase structures turn into detwinned martensite structure with stressing. However, lattice twinning and detwinning reactions play important role in martensitic transformations. Copper-based alloys exhibit this property in metastable  $\beta$ -phase region. Lattice invariant shear and twinning is not uniform in these alloys and gives rise to the formation of complex layered structures. These structures can be described by different

unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. The unit cell and periodicity are completed through 18 layers in direction  $z$ , in case of 18R martensite, and unit cells are not periodic in short range in direction  $z$ . In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper-based CuAlMn and CuZnAl alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging duration at room temperature. This result refers to the rearrangement of atoms in diffusive manner.

## Biography

**Adiguzel** graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and studied were focused on shape memory effect in shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has been retired on November 28, 2019, due to the age limit of 67, following academic life of 45 years. He supervised 5 PhD- theses and 3 M. Sc- theses and published over 80 papers in international and national journals; He joined over 120 conferences and symposia in international and national level as participant, invited speaker or keynote speaker with contributions of oral or poster. He served the program chair or conference chair/co-chair in some of these activities. In particular, he joined in last six years (2014 - 2019) over 60 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. Also, he joined over 120 online conferences in the same way in pandemic period of 2020-2022. Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.

# ORAL PRESENTATIONS

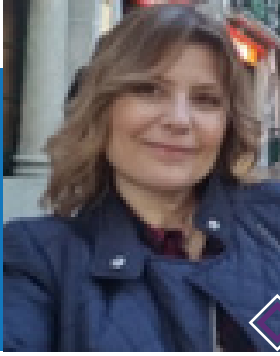
DAY 02

INTERNATIONAL SUMMIT ON  
**CATALYSIS & CHEMICAL  
ENGINEERING**

June 19-20, 2024 | Virtual Event







**NADYA VASILEVA DENCHEVA**

University of Minho  
Portugal

## **Porous Polyamide microparticles as effective carriers for cascade Bio-Catalysis**

### **Abstract:**

In the last decades, cascade biocatalysis has attracted significant interest from both academia and industry as a promising technology for green and sustainable chemical production. Unlike the step-by-step synthesis, cascade biocatalysts accomplish two or more consecutive reactions in one-pot, thus avoiding isolation and purification of intermediates. Nowadays, numerous drugs and fine chemicals, as well as some polymers are synthesized through cascade bio-catalysis. However, the industrial use of biocatalysts based on free enzymes is problematic, due to their poor stability and difficult reuse. A possible way to overcome these limitations is the application of immobilization technologies, in which two or more enzymes are co-localized close to one another on a suitable support. Major advantage of these carrier-multienzyme complexes is that the enzymes' active sites are in close proximity, minimizing the diffusion of the intermediates thereby enhancing the overall reaction efficiency. In this work various highly porous polyamide microparticles (PAM) based on Polyamide 4 (PA4), Polyamide 6 (PA6), Polyamide 12 (PA12) as well as their co-polymers with and without magnetic properties were synthesized by proper method. PAM were used as scaffolds for ordered sequential co-immobilization of Glucose oxidase (GOx) and Horse radish peroxidase (HRP). The catalytic efficiency of these hybrid bi-enzyme biocatalysts was assessed in the cascade reaction for glucose detection. The kinetic parameters, as well as the reusability and storage stability were also studied.

### **Biography**

**Nadya Vasileva Dencheva** has completed his PhD at the age of 45 years and postdoctoral studies from the University of Minho, Department of Polymer Engineering, Portugal. She is Junior Researcher at the Institute for Polymers and Composites research center at the University of Minho. She has published more than 55 papers in international peer reviewed journals, 3 book chapters and 6 patents (Index h 18; Index i10 – 32, Google scholar) <http://orcid.org/0000-0003-1698-553X>



## AMENE NASERI

Agricultural Biotechnology Research  
Institute of Iran (ABRII), , Iran

### **Nanoremediation: A sustainable approach for removal of pollutants from agricultural wastewater**

#### **Abstract:**

Population growth causes increasing in intensive food production in many developed and rapidly growing economies towards food security. To maximize crop yields and a significant increase in livestock production, high levels of agrochemicals are used, globally. The toxic agrochemicals degrade the downstream water quality and result in the eutrophication of water bodies. To remove the excess amount of agrochemicals in water, diverse approaches have been developed. Among them, nanoremediation is an emerging one that is defined as decontamination mediated by nanostructures. In the talk, recent advances of different mechanisms of nanoremediation including nanophotocatalysts, nanoadsorbents and nanobiocatalysts will be discussed.

#### **Biography**

**Amene Naseri** received her Ph.D. in Nanotechnology from the Institute for Nanoscience & Nanotechnology (INST) of Sharif University of Technology (SUT), Iran in 2018. After one year and a half of working as a postdoctoral researcher at the Physics Department of SUT on “shape-dependent electrocatalytic activity of rGO supported Pd nanoparticles”, she joined the Agricultural Biotechnology Research Institute of Iran (ABRII) (located in Karaj, Iran) in 2020 as an assistant professor of Nanotechnology Department. Her current research interests focus on the synthesis and characterization of different nanostructures for clean energy and environmental applications.





## VINAYAK ADIMULE

Angadi Institute of Technology and  
Management (AITM), India

### **Microstructure, zeta potential and enhanced photocatalytic dye degradation performances of mesoporous flower shaped Nb doped CeO<sub>2</sub> bimetallic oxide nanostructures decorated with reduced graphene oxide**

#### **Abstract:**

The unique features of reduced graphene oxide (rGO) enable their applications in the field of photocatalysis as well as unique electrical properties. In the present research work, a novel series of Nb doped CeO<sub>2</sub> decorated with rGO (2, 8 and 12 wt %) were synthesized by hydrothermal method. The structural and morphological features of nanomaterials (NMs) investigated by using different analytical techniques namely, XRD (X-ray diffraction), UV-visible, SEM (scanning electron microscopy), EDX (energy dispersive X-ray), XPS (X-ray photoelectron spectroscopy), BET (Brunauer-Emmett-Teller). The XRD analysis present polycrystalline mixed phase of tetragonal/cubic crystal structure and microstructure analysis showed flower shaped morphology having mesoporous nature. The addition of rGO results in the increased specific surface area and pore diameter. Red-shift in optical absorbance results with decrease in direct optical band gap as rGO concentration increases in NMs. The EDX/XPS studies showed the chemical composition and oxidation states of elements NB, Ce, O, C in NMs. Zeta potential studies showed increased poly disparity with increase in the mobility of the NMs. The zeta potential varies from 88.1 mV to 110.8 mV as the rGO concentration increases on bimetallic oxide NMs. Further, Photocatalytic dye degradation studies of rGO (2, 8 and 12 wt %): Nb<sub>2</sub>O<sub>3</sub>@CeO<sub>2</sub> against Methylene blue (NM), Rodhamaine B (RB) and Sudan 1 dye showed increased photocatalytic activity. The Photocatalytic performances increase with increase in rGO concentration on bimetallic oxide NMs. The findings of the present work can be better candidate for photocatalytic and an excellent material for charge transport capability.

#### **Biography**

Fifteen years of research experience as senior Scientist, associate research scientist in R&D organizations of TATA, Astra Zeneca India, Trans Chem Ltd. Overseas Research Fellow of Nanyang Global Research Center, Bangkok, Malaysia. Published more than 150 research articles, and 15 Books/several book chapters in Scopus, Q-rated journals with high impact factor, attended and presented papers in National and International Conferences as Key note speaker, distinguished speaker, Chaired/ Key note speaker/Organizing secretary, Editor for International and National conferences, Editorial Board Member, Life Member of many international societies. Editor of the special issues published in springer, Elsevier and Wiley. Research interest includes, Optoelectronics, Material Chemistry, Sensors and Actuators, Bio Nanomaterials, Medicinal Chemistry.



## ASHANENDU MANDAL

University of Calcutta  
India

### Phenol removal from wastewater using innovative biological and industrial wastes as adsorbents

#### Abstract:

This research aims for adsorptive removal of phenol from wastewater by solid waste materials generated from biological wastes viz. guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and industrial wastes viz. rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina. The adsorbents are characterized by SEM, XRD, FTIR and BET analyzers. The experiments of phenol removal are carried out with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum phenol removal percentage through batch absorptions has been found to be as high as 97.50%. The kinetics analysis with the experimental results shows that the pseudo-second order model is best fitted for all adsorbents except red mud. The kinetic modelings show that the adsorption mechanism is supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggests that Freundlich isotherm model is best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm are best supportive for rice husk ash and clarified sludge respectively. The thermodynamics shows the spontaneity, randomness and endothermic/exothermic nature of the adsorption processes. The ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient establishes that the experimental and predictive data are within allowable range. The scale-up designs are performed for their commercial applications. The regeneration and the safe disposal of used adsorbents are also studied for checking their wider industrial applicability. Further, the column study is also extensively carried out using the most efficient batch adsorbent neem leaves. The study concludes that these adsorbents can be used commercially for removal of toxic phenol from wastewater.

#### Biography

Fifteen years of research experience as senior Scientist, associate research scientist in R&D organizations of TATA, Astra Zeneca India, Trans Chem Ltd. Overseas Research Fellow of Nanyang Global Research Center, Bangkok, Malaysia. Published more than 150 research articles, and 15 Books/several book chapters in Scopus, Q-rated journals with high impact factor, attended and presented papers in National and International Conferences as Key note speaker, distinguished speaker, Chaired/ Key note speaker/Organizing secretary, Editor for International and National conferences, Editorial Board Member, Life Member of many international societies. Editor of the special issues published in Springer, Elsevier and Wiley. Research interest includes, Optoelectronics, Material Chemistry, Sensors and Actuators, Bio Nanomaterials, Medicinal Chemistry.



**DEBANJAN MITRA**

Raiganj University  
India

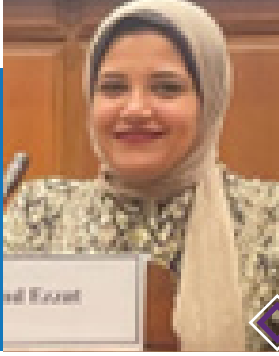
## **Insight into the mesophilic bacterial chromate reductase: an insilico study towards remediation of chromium pollution through microbes**

### **Abstract:**

Industrial use of chromium leads to the contamination of natural environment with chromium pollution and the hexavalent form is very harmful to the living system compared to the trivalent and other forms. The most sophisticated way of chromium reduction is the use of an enzyme chromate reductase exclusively produced by the bacteria. An insilico sequence and structure analysis of chromate reductase enzyme from three mesophilic bacteria *Acetobacter aceti*, *Escherichia coli*, and *Pseudomonas putida* has been studied. Amino acid variation study indicates a highest number of charged and uncharged residues in *P. putida* and *A. aceti* compared to *E. coli*. Secondary structure analysis indicates that protein from *E. coli* contains additional beta-hairpin and beta bugle. Higher number of salt bridges, aromatic-aromatic interactions, cation-pi interactions in *P. putida* chromate reductase provides its more stability than the other two. Molecular dynamics simulation studies through RMSD and RMSF indicates less fluctuation in case of *P. putida* chromate reductase while lowest Rg indicates tightly packed nature and lower SASA indicates better folding of the said protein. This is the first reporting on structural and sequence analysis of chromate reductase of the three mesophilic bacteria and among them *P. putida* proved to be the most stable one to be used in the industrial level for better chromate alleviation.

### **Biography**

**Debanjan Mitra** has completed his PhD at the age of 29 years from Raiganj University, India. He is working on bioinformatics specially in the field of proteomics, drug discovery, cheminformatics, quantum mechanics, immunoinformatics and programming. He has published more than 43 papers in reputed journals and has been serving as a reviewer and editorial board member of repute. 1st time he revealed the presence of cyclic salt bridge in protein in the field of structural biology. Till now, he got 6 international and 2 national awards in his scientific life journey.



## HEND A. EZZAT

National Research Institute of Astronomy and  
Geophysics (NRIAG), Egypt

### **Improving Li-ion battery performance for aerospace applications via efficient nanocomposites of carbon derivatives based on polyethylene oxides**

#### **Abstract:**

Industrial use of chromium leads to the contamination of natural environment with chromium pollution and the hexavalent form is very harmful to the living system compared to the trivalent and other forms. The most sophisticated way of chromium reduction is the use of an enzyme chromate reductase exclusively produced by the bacteria. An insilico sequence and structure analysis of chromate reductase enzyme from three mesophilic bacteria *Acetobacter aceti*, *Escherichia coli*, and *Pseudomonas putida* has been studied. Amino acid variation study indicates a highest number of charged and uncharged residues in *P. putida* and *A. aceti* compared to *E. coli*. Secondary structure analysis indicates that protein from *E. coli* contains additional beta-hairpin and beta bugle. Higher number of salt bridges, aromatic-aromatic interactions, cation-pi interactions in *P. putida* chromate reductase provides its more stability than the other two. Molecular dynamics simulation studies through RMSD and RMSF indicates less fluctuation in case of *P. putida* chromate reductase while lowest  $R_g$  indicates tightly packed nature and lower SASA indicates better folding of the said protein. This is the first reporting on structural and sequence analysis of chromate reductase of the three mesophilic bacteria and among them *P. putida* proved to be the most stable one to be used in the industrial level for better chromate alleviation.

#### **Biography**

**Hend Ezzat** completed his PhD at the age of 32 years from Ain Shams University. She is the director of spectroscopy and material science, a researcher in Nano Unit, Space Lab, Solar and Space Research Department, National Research Institute of Astronomy and Geophysics (NRIAG). She has published more than 25 papers in reputable journals and has been serving as a reviewer of repute.



## M. ABDELHAMID SHAHAT

National Research Institute of Astronomy and  
Geophysics (NRIAG), Egypt

### **A novel strategy for refunctionalizing Carbon-based nanosheets for utilization in photo-voltaic cells via plasma surface modification**

#### **Abstract:**

The basic concept for the future development of human society has become to reduce emissions of greenhouse gases such as carbon dioxide that cause climate change. As a result, one of the best sustainable and environmentally acceptable solutions to this challenge is to use perovskite solar cells (PSCs), which may be used as an efficient alternative for fossil fuels.

The main objective of this work is to design and improve the performance of carbon quantum dot-based PSCs. We presented a simple method for modifying the physicochemical properties of hole transport layer (HTL) and electron transport layer (ETL) as the most efficient components in solar cells, using in-situ plasma surface treatment. Following that, the effects of the treatment on the microstructure, active sites, surface area, optical, and electrical characteristics of these nanolayers were examined. Whereas, these treatments resulted in a considerable improvement in the chemical functionalization of the nanolayers, as well as a rapid increase in surface roughness, which reduced photons reflection and therefore increased the generation of charge carriers.

#### **Biography**

**Mohamed Abdelhamid Mohamed Shahat** is a Researcher at NRIAG, Egypt. He was born in April 1990. He holds a PhD in Physics of Material Science and Solar Energy, Feb. 2021. His expertise includes plasma applications in water treatment as well as photovoltaics (Perovskite, Dye-sensitized, and Organic cells). Recently,

- Efficient CO<sub>2</sub> capture and storage utilizing plasma modification of Carbon-based nanocomposite materials.
- Improved Thermophysical Properties of Nanocarbon-based Composite Clay Bricks for Sustainable Building and Construction Applications via Plasma Modification.
- A novel design for Energy, Hydrogen, and Water production utilizing Solar Energy for climate change mitigation.

**ACCEPTED  
ABSTRACTS**



**INTERNATIONAL SUMMIT ON  
CATALYSIS & CHEMICAL  
ENGINEERING**

**June 19-20, 2024 | Virtual Event**

**VICTORIA EZINNE OTTAH**

University of Nigeria

Nigeria

## **Adapting chemistry with innovations to achieve future objectives**

### **Abstract:**

According to the report given by the International Union of Pure and Applied Chemistry (IUPAC), current innovation trends of 2023 focused on the production of wearable sensors, artificial muscles, low sugar vaccines, phage therapy, synthetic electrochemistry, photo catalytic therapy, biological recycling of plastics, depolymerization, chlorine-mediated removal of carbon IV oxide and GPT language models. Innovation seeks to improve existing methods and generate new/improved ideas that better addresses current challenges and seeks to provide better solutions for future objectives. This relies heavily on the study of various materials to understand their specific characteristics such as structure and properties which influences how they behave in various systems. These characteristics must be fully comprehended, and potential ideas extensively tested, if new, and improved solutions will be realized. The scientific data generated from this is the bedrock for new innovations that can achieve future objectives. For example, a historic resolution aimed at totally overhauling the generation of plastic waste was passed in March 2022 at Nairobi by the United Nations Environment Assembly. To actualize this, chemical analysis addressing certain key questions pertaining to the structures of these plastics, their degradation into non-toxic components, and their replacement with other environmentally friendly biodegradable materials must be carried out. So, it is not out of place to say that chemistry drives innovations. It is our responsibility to look critically into these problems and conduct chemical research that can serve as a knowledge base for future innovations.

### **Biography**

**Victoria Ezinne Ottah** completed her Ph.D. in Biochemistry by age 30 from the University of Nigeria, Nsukka. She has published several papers in reputable journals that have been cited by various authors. She has served as a reviewer for reputable journals. She is interested in multidisciplinary research that focuses on the potential of catalytic biodegradation of biomaterials in biotechnology.



**XIONG WANG**

Petrochemical Research Institute

China

## **Porous organic Polymers-Based metallocene catalysts for ethylene polymerization**

### **Abstract:**

Porous organic polymers (POPs) have received increasing attentions in a wide range of areas including adsorption, separation and catalysis. In this presentation, POPs and POP/inorganic hybrid supports were designed, synthesized and used as metallocene catalyst support for ethylene polymerization. The prepared POPs and POP/NPs (POP/MMT and POP/TiO<sub>2</sub>) hybrid supports obtained excellent particle flowability with tunnable bulk density ( $\geq 0.20$  cm<sup>3</sup>/g) and specific surface area suitable for polyolefin catalysts. N<sub>2</sub> sorption porosity, TGA, IR, XRD, SEM characterization were conducted to evaluate the POP/MMT and POP/TiO<sub>2</sub> hybrid supports, and the results showed that the MMT sheets and TiO<sub>2</sub> nanoparticles could be well-dispersed in the POP matrix, and excellent particle flowability and narrow particle size distribution could also be gained. Ethylene polymerization results exhibited that the POP/NP supported metallocene catalysts could obtain better polymerization performance than the inorganic materials or the silica gel supported catalysts. The prepared POP/NPs catalysts show no obvious Zr<sup>+</sup> active sites decay during the ethylene polymerization, and gain stable polymerization kinetics in 80 °C. Furthermore, the pore structure played a significant effect on the molecular weight and molecular weight distribution by nano-confined polymerization, and larger molecular chains could be produced on the POP/NPs supported catalysts with smaller nanopore size.

### **Biography**

**Xiong Wang** was born in Hubei (China) in 1980. He received B. S. degree in chemistry (2002) and M. S. degree (2005) from Hubei University. Then he joined in Lanzhou petrochemical research center, PetroChina, focused on polyolefin catalysts and novel products. He completed his Ph. D with prof. Yanfeng Li in Polymer Chemistry and Physics (2016) from Lanzhou University. He gained the Young Scientific and Technological Talents Award of China National Petroleum Company (CNPC) in 2018, and now he serves as a senior expert in Petrochina Petrochemical Research Institute. His research interests include Olefin Polymerization Catalysis and Porous catalytic materials.



**DEHUA HE**

Tsinghua University

China

## **Photothermal catalytic process for conversion of CO<sub>2</sub> and Biomass-Based glycerol to glycerol carbonate**

### **Abstract:**

Photothermal catalytic processes are of great significance for efficiently utilizing solar energy to catalyze the reactions of transforming cheap raw materials to high value-added chemicals. Transforming CO<sub>2</sub> and biomass-based glycerol, which is by-product from the biodiesel manufacturing, into high value-added glycerol carbonate is a green and promising approach for simultaneously utilizing CO<sub>2</sub> and glycerol. However, the reaction of CO<sub>2</sub> and glycerol to produce glycerol carbonate is thermodynamically unfavorable for thermal catalysis. Breaking the thermodynamic limitation is the key to effectively utilizing this process. Introducing abundant solar energy into a thermal-driven reaction system can effectively activate reactants, break through the thermodynamic limitation, increase catalytic rate, and enhance the selectivity of target products. In this work, we have developed Co<sub>3</sub>O<sub>4</sub>-ZnO and Au/Co<sub>3</sub>O<sub>4</sub>-ZnO catalytic materials with photothermal synergistic function, and introduced solar energy into the reaction system for the synthesis of glycerol carbonate from CO<sub>2</sub> and glycerol. A series of Co<sub>3</sub>O<sub>4</sub>-ZnO and Au/Co<sub>3</sub>O<sub>4</sub>-ZnO catalysts were prepared by hydrothermal and impregnation methods. The photo-thermal catalytic reactions were carried out in a 100 mL stainless-steel autoclave. The results of characterizations and reactions showed that the cooperation between Co<sub>3</sub>O<sub>4</sub> and ZnO exerted significant functions on the catalytic activities for transforming CO<sub>2</sub> and glycerol to glycerol carbonate, light irradiation further improved their catalytic performance because of the photo-thermal synergistic effect. Meanwhile, the heterojunction structure of p-n type semiconductor Co<sub>3</sub>O<sub>4</sub>-ZnO and the localized surface plasmon resonance of Au nano-particles improved visible light absorption capacity and electron-hole separation efficiency. The separated electrons and holes activated CO<sub>2</sub> and glycerol, respectively, which played dominant roles for catalytic performance improvement under visible light irradiation.

### **Biography**

**Dehua HE** graduated from East China University of Science and Technology (Jan. 1982). He received Master degree from Okayama University of Japan (March 1987) and obtained his Ph.D. degree from Tokyo Institute of Technology of Japan (March 1990), followed by the research works at Sagami Chemical Research Center of Japan (1991-1994). He has joined Tsinghua University since 1995. He is interested in heterogeneous catalysis.

# Supporting Journal

## Journal of Chemistry and Analytical Biochemistry

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