

11<sup>th</sup> World Conference on

# CHEMISTRY AND CHEMICAL ENGINEERING

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# ADVANCED MATERIALS, NANOSCIENCE AND NANOTECHNOLOGY







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# **ADVANCED MATERIALS, NANOSCIENCE AND NANOTECHNOLOGY**

May 21-22, 2026 | Vienna, Austria

**BOOK OF ABSTRACTS**

# Abstracts of the 11<sup>th</sup> World Conference on Chemistry and Chemical Engineering & 11<sup>th</sup> World Conference on Advanced Materials, Nanoscience and Nanotechnology

## Conference Dates:

May 21-22, 2026

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# TABLE OF CONTENTS

S.No.	Section	Page
1	<b>About Eurasia Conferences</b>	<b>6</b>
2	<b>Scientific Program</b>	<b>7-9</b>
3	<b>Keynote Session</b>	<b>10</b>
3.1	Crystallographic Transformations and Reversible Characteristics of Shape Memory Alloys	11
4	<b>Speaker Sessions</b>	<b>12</b>
4.1	Influence of Operating Conditions on Electrochemical Phenomena in Carbon Fuel Cell	13
4.2	Never-Ending Change: Atomic Models, Incommensurability, and the Tentative Nature of Science	14
4.3	Rethinking Chemical Education for Systemic Sustainability: Beyond Green Chemistry – From Molecules to Mindsets	15
4.4	Silicon/Carbon Anodes for Lithium-Ion Batteries	16
4.5	Room-Temperature Valley-Spin Photonic Devices Based on TMDC Metasurface Heterostructures: Enabling Nanophotonic Quantum Technologies for Space Application	17
4.6	Structure and Electronic Properties of Graphene-Triazine Bilayer Complexes: A Computational Investigation	18
4.7	Real-time Dynamic Analysis of Liquid Matrices with Online Measurements: Determination of Initial Headspace Concentration and Gas-Liquid Equilibrium	19
4.8	Acetaminophen Adsorption Properties Using Graphene-Triazine Bilayer Composites	20
4.9	Treatment of Crude Oil Contaminated Water Using Metal Oxide Nanocomposites	21
4.10	Hybrid Magnetic Activated Carbon–Polyaniline Nanocomposite for Superior Lead Removal from Aqueous Media	22
4.11	Advanced Oxide-Based Antireflective Coatings for Optical Applications	23
4.12	Comparative Analysis of Classical and Quantum Machine Learning Models for Nanomaterial Property Classification	24
5	<b>Participants Index</b>	<b>26</b>

# ABOUT EURASIA CONFERENCES

Established in 2022, Eurasia Conferences has rapidly gained recognition for organizing high-quality conferences across a diverse range of fields including science, technology, social sciences, humanities, business and economics, life sciences, medicine, and healthcare. Our mission is to drive progress and innovation through dialogue and collaboration among professionals worldwide.

Since our inception, we have successfully hosted over 50 conferences, providing platforms for scholars, researchers, professionals, and students to exchange knowledge and cultivate new ideas. Our events are strategically designed to foster networking, stimulate in-depth discussions, and facilitate the sharing of cutting-edge research and practical solutions to address contemporary challenges.

At Eurasia Conferences, we are dedicated to delivering an exceptional conference experience, with a focus on inclusivity and the broad dissemination of knowledge. Participants at our events become part of a community committed to making a positive impact on global society. We invite you to join us at our conferences, where we continually strive for excellence in promoting academic and professional development.



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May 21-22, 2026 | Vienna, Austria

**SCIENTIFIC PROGRAM**

08:55-09:00 @

**Introduction and Welcome Note  
(Virtual Session via Zoom) UTC/  
GMT +2 (Vienna Time)**

**MAY 21, 2026**

## keynote Sessions

**09:00-09:30**  
**Title: Crystallographic Transformations and Reversible Characteristics of Shape Memory Alloys**  
Dr. Osman Adiguzel, Department of Physics, Firat University, Elazig, Turkey.

## Speaker Sessions

**09:30-09:50**  
**Title: Influence of Operating Conditions on Electrochemical Phenomena in Carbon Fuel Cell**  
Dr.-habil. Andrei Bologa, Institute for Technical Chemistry, Karlsruhe Institute of Technology, Eggenstein -Leopoldshafen, Germany.

**09:50-10:10**  
**Title: Never-Ending Change: Atomic Models, Incommensurability, and the Tentative Nature of Science**  
V́ctor Mart́nez-Mart́nez, Department of Specific Didactics, University of Burgos, Burgos, Castilla y Le3n, Spain.

**10:10-10:30**  
**Title: Rethinking Chemical Education for Systemic Sustainability. Beyond Green Chemistry - From Molecules to Mindsets**  
Prof. Dr. Julia Krause, International Industrial Sourcing and Sales, Faculty of Business Administration, Dresden, University of applied Sciences, Dresden, Saxony, Germany.

**10:30- 10:50**  
**Title: Silicon/Carbon Anodes for Lithium-Ion Batteries**  
Georgia Moysiadou, Foundation for Research and Technology Hellas/ Institute of Chemical Engineering Sciences, FORTH/ICEHT, Greece.

**10:50- 11:10**  
**Title: Room-Temperature Valley-Spin Photonic Devices Based on TMDC Metasurface Heterostructures: Enabling Nanophotonic Quantum Technologies for Space Application**  
Rohit K Ramakrishnan, QOSMIC Satellite Systems, Bangalore, India. Indian Institute of Science, Bangalore, India.

**Tea and Refreshments Break 11:10-11:30**

**Title: Structure and Electronic Properties of Graphene-Triazine Bilayer Complexes: A Computational Investigation**

11:30- 11:50

**Dr. Keshab K. Adhikary**, Center for Green Chemistry and Environmental Biotechnology (GREAT) – Engineering of Materials via Catalysis and Characterization, Ghent University Global Campus, Incheon, South Korea.

**Title: Real-time Dynamic Analysis of Liquid Matrices with Online Measurements: Determination of Initial Headspace Concentration and Gas-liquid Equilibrium**

11:50-12:10

**Prof. Philippe M. Heynderickx**, Center for Green Chemistry and Environmental Biotechnology (GREAT), Ghent University Global Campus, Incheon 21985, Republic of Korea. Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, Belgium

**Title: Acetaminophen Adsorption Properties Using Graphene-Triazine Bilayer Composites**

12:10-12:30

**Miran Seo**, Center for Green Chemistry and Environmental Biotechnology (GREAT), Ghent University Global Campus, Incheon, Republic of Korea

**Title: Treatment of Crude Oil Contaminated Water Using Metal Oxide Nanocomposites**

12:30- 12:50

**Nawar Razzaq Salihi**, Department of Chemical Engineering, Yildiz Technical University, Istanbul, Türkiye.

**Title: Hybrid Magnetic Activated Carbon–Polyaniline Nanocomposite for Superior Lead Removal from Aqueous Media**

12:50-13:10

**Mahmoud M. Youssif, and Marek Wojnicki**, Faculty of Non-Ferrous-Metals, AGH University of Krakow, Poland.

**Title: Advanced Oxide-Based Antireflective Coatings for Optical Applications**

13:10-13:30

**Dr. Sadaf Bashir Khan**, Key Laboratory of Testing Technology for Manufacturing Process, Ministry of Education, Southwest University of Science and Technology, China.

**Title: Comparative Analysis of Classical and Quantum Machine Learning Models for Nanomaterial Property Classification**

13:30-13:50

**Chaima Gharbi**, Higher Institute of Information and Communication Technologies, University of Carthage, Tunis, Tunisia

**Closing Note 13:50-14:00**



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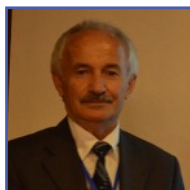
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# ADVANCED MATERIALS, NANOSCIENCE AND NANOTECHNOLOGY

May 21-22, 2026 | Vienna, Austria

KEYNOTE PRESENTATIONS | DAY 1

## Crystallographic Transformations and Reversible Characteristics of Shape Memory Alloys



**Osman Adiguzel**

Department of Physics, Firat University, Elazig, Turkey

A series of alloy systems take place in a class of advanced smart materials by giving stimulus response to external effect. Shape memory alloys take place in this group by exhibiting a peculiar property called shape memory effect with the recoverability of two shapes at different conditions. This phenomenon is initiated with thermomechanical treatments on cooling and deformation and performed thermally on heating and cooling, with which shape of the material cycles between original and deformed shapes in reversible way. Therefore, this behavior can be called Thermoelasticity. Deformation in low temperature condition is plastic deformation, with which strain energy is stored in the materials and released on heating by recovering the original shape. This phenomenon is governed by two crystallographic transformations, thermal and stress induced martensitic transformations. Thermal induced martensitic transformations occur on cooling with cooperative movement of atoms in  $\langle 110 \rangle$ -type directions on a  $\{110\}$ -type plane of austenite matrix, along with lattice twinning reaction and ordered parent phase structures turn into the twinned martensite structures. The twinned structures turn into detwinned martensite structures with deformation by means of stress induced martensitic transformations. These alloys exhibit another property called superelasticity. This behavior is performed in only mechanical manner with stressing the material and releasing in elasticity limit in the parent austenite phase region, and shape recovery occurs instantly upon releasing, by exhibiting elastic material behavior. Superelasticity is also result of stress induced martensitic transformation and ordered parent phase structures turn into the detwinned martensite structures with stressing. Lattice twinning and detwinning reactions play important role at the transformations and driven by lattice invariant shears. These alloys have dual memory characteristics, Thermoelasticity and Superelasticity, with these properties.

Copper-based alloys exhibit this property in metastable  $\beta$ -phase region. Lattice twinning and lattice invariant shear is not uniform in these alloys and cause the formation of complex layered structures, The layered 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.

In the present contribution, x-ray and electron diffraction studies were carried out on copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflection. 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.

**Keywords:** Shape memory effect, martensitic transformation, thermoelasticity, superelasticity, twinning, detwinning.

### Biography:

Dr. 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 on 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 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 230 online conferences in the same way in pandemic period of 2020-2024. He supervised 5 PhD- theses and 3 M. Sc- theses. 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.



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**SPEAKER PRESENTATIONS | DAY 1**

## Influence of Operating Conditions on Electrochemical Phenomena in Carbon Fuel Cell



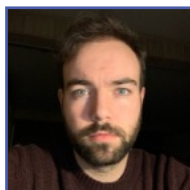
**A. Bologna, K. Aleksandrov, H.-J. Gehrman, K. Woletz, D. Stapf**  
Institute for Technical Chemistry, Karlsruhe Institute of Technology, Eggenstein  
-Leopoldshafen, Germany

The study contributes to investigation of the influence of operation conditions on electrochemical phenomena in an experimental carbon fuel cell (CFC). The cell is heated inside an electric oven. The CFCI includes ceramic crucible with a cover, anode, cathode and reference electrode. An eutectic ternary carbonate salt mixture is used as electrolyte. The atmospheric air is purged through the CFC crucible during the cell operation. The novelty of the study consists in use of Carbon Fibers (CF) as cell fuel. The research project involves the study of CFC electrodes' design, heating temperature, as well as, of the mass CF-fuel on experimental cell parameters. The test facility periphery is applied for control of temporal evolution of temperature inside and outside the CFC crucible, fuel cell voltage and current, as well as, of concentration of carbon dioxide in the output purged atmospheric air. The Light Microscopy and Laser Induced Plasma Spectroscopy are applied for analysis of the state of carbon fibers and CFC electrolyte after the short- and long-term tests. The results of the study allows better understanding of the electrochemical phenomena and their temporal evolution during the cell operation. In perspective, the research should be extended to the study of the phenomena, related to the direct conversion of Carbon Fibers Reinforced Polymers into electric power.

### Biography:

Dr.-habil. Andrei Bologna is a scientist with over 40 years of experience in the field of charged aerosols, electrohydrodynamics, gas cleaning technologies, carbon fuel cells. His experience includes design, development and investigations of electrostatic precipitators for gas cleaning from waste, as well as, small scale biomass combustion, cleaning of exhaust gases from chemical industrial processes and machinery. The research interests cover also development of electrostatically augmented condensation systems for pyrolysis processes, as well as, the design and investigation of carbon fuel cells. He is the author of over 250 publications and over 50 patents.

## Never-Ending Change: Atomic Models, Incommensurability, and the Tentative Nature of Science



**Víctor Martínez-Martínez**<sup>1</sup>

<sup>1</sup>Department of Specific Didactics, University of Burgos, Burgos, Castilla y León, Spain

The historical development of atomic models provides a compelling illustration of the tentative and continually revisable nature of scientific knowledge. From Thomson's early corpuscular conception to Rutherford's nuclear model, from Bohr's quantized structure to the probabilistic descriptions of modern quantum mechanics, each transition reflects more than a refinement of previous ideas. These shifts reveal changes in problem agendas, representational commitments, and standards of explanatory adequacy that make direct translation between models conceptually difficult. This difficulty exemplifies the partial incommensurability described in contemporary philosophy of science, showing that successive theories may construct distinct conceptual worlds rather than linear improvements of a single framework.

In chemistry education, however, atomic theory is often taught as if it followed a straightforward cumulative progression. This narrative obscures the deeper epistemological lesson: scientific models are provisional tools shaped by evolving evidence, methods, and theoretical priorities. Presenting atomic models through the lens of tentativeness and incommensurability helps students recognize that scientific knowledge is open to revision and that theoretical change often involves rethinking fundamental assumptions rather than merely adding new details.

Integrating these ideas into chemistry instruction enriches students' understanding of how science operates, encouraging them to navigate multiple models critically and to appreciate the conceptual discontinuities that accompany scientific progress. This approach strengthens scientific literacy by demonstrating that uncertainty, revision, and theoretical plurality are not weaknesses of science, but essential features of its dynamic and self-correcting character.

### Biography:

Víctor Martínez-Martínez holds a degree in Chemistry and a PhD in Science Education, with a dissertation focused on the nature of science and STEM education. He is currently completing a master's degree in Logic and Philosophy of Science, deepening his engagement with the conceptual foundations of scientific practice. His research is driven by the conviction that insights from philosophy of science and social studies of science are essential for improving scientific literacy and educational practice. He works to integrate these perspectives into curriculum design, teacher training, and the broader understanding of how science operates within contemporary societies.

## Rethinking Chemical Education for Systemic Sustainability. Beyond Green Chemistry - From Molecules to Mindsets



### Prof. Dr. Julia Krause

International Industrial Sourcing and Sales, Faculty of Business Administration, Dresden University of Applied Sciences, Dresden, Saxony, Germany.

Chemical education is at a turning point. While sustainability has become a strategic priority in industry and policy frameworks worldwide, it is often introduced into chemistry curricula as an add-on topic rather than as a structural principle.

This contribution argues that sustainability in chemistry must be embedded by speaking the language of chemists. Instead of abstract ethical appeals, sustainability can be integrated through core chemical categories: materials, reactions, energy systems, process design, resource efficiency, circularity, and risk assessment. By reframing sustainability within the epistemological logic of chemistry, students can understand it not as external regulation but as an intrinsic dimension of chemical innovation.

The presentation introduces a holistic curriculum framework based on a 7P sustainability model adapted for chemical education (Product, Process, Planet, People, Partnerships, Premises, Purpose). This model is aligned with the ORANGE Framework for systemic transformation in higher education, which integrates orientation, research-based learning, alliances, governance, and education culture into a Whole-Institution approach.

Grounded in the ORANGE Framework for institutional transformation and the 7P model for holistic business sustainability, this contribution translates systemic sustainability into the language of chemistry, creating a structured approach for curriculum development in chemical education.

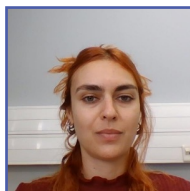
The goal is not merely to “teach about sustainability,” but to educate chemists who think systemically, innovate responsibly, and translate chemical expertise into societal value.

This contribution proposes curriculum strategies that transform sustainability from a compliance topic into a core driver of chemical education and innovation.

### Biography:

Julia Krause holds the interdisciplinary Chair of International Industrial Sourcing & Sales at HTW Dresden, bridging procurement and sales to foster holistic perspectives on global value creation. Her research focuses on the systemic implementation of sustainability in business processes and international supply chains, particularly in the chemical and plant engineering industries. With extensive industry experience in international consulting and chemical plant engineering, she combines academic rigor with practical insight. As Chair of the Scientific Advisory Board of the JARO Institute for Sustainability and Digitalization in Procurement, she advocates for integrating sustainability into education as a strategic, structural principle rather than a purely regulatory requirement.

## Silicon/Carbon Anodes for Lithium-Ion Batteries



**Georgia Moysiadou<sup>1,2</sup> and Maria K. Daletou<sup>1</sup>**

<sup>1</sup>Foundation for Research and Technology Hellas/Institute of Chemical Engineering Sciences FORTH/ICEHT, 26500 Patras, Greece.

<sup>2</sup>Department of Chemistry, University of Patras, 26504 Patras, Greece.

Lithium ion batteries are one of the most promising energy storage options for devices such as electrical vehicles etc. Silicon (Si) is a premier candidate for next-generation lithium-ion battery anodes due to its exceptional theoretical capacity of ~4200 mAh/g. However, its practical application is hindered by a ~300% volume expansion during lithiation/delithiation, which causes particle pulverization and unstable solid-electrolyte interphase (SEI) formation, leading to rapid capacity decay.

This work presents the controlled synthesis of Si/C yolk-shell nanostructures designed to accommodate this expansion within a protective conductive framework. The methodology involved the surface modification of Si nanoparticles via thermal oxidation to create a SiO<sub>2</sub> sacrificial layer, followed by the polymerization of dopamine at varying intervals. Subsequent carbonization and selective etching of the SiO<sub>2</sub> layer created the required internal void space.

Characterization through Transmission Electron Microscopy (TEM) and X-ray Diffraction (XRD) confirmed the successful formation of the yolk-shell architecture and the retention of silicon's crystallinity. Thermogravimetric Analysis (TGA) demonstrated that polymerization time is critical for controlling carbon content. Preliminary electrochemical testing showed that these yolk-shell materials exhibit enhanced structural stability compared to bare silicon, effectively mitigating pulverization and stabilizing capacity during cycling.

### Biography:

Georgia Moysiadou (Chemist) is a Ph.D. candidate in Chemistry at the University of Patras under the foundation of a national scholarship of H.F.R.I and a researcher at the Institute of Chemical Engineering Sciences (FORTH/ICEHT). Also, she has finished a Master at AUTH titled <<Science and Technology of Electrochemical Systems>>. Her research interests are centered on the synthesis, physicochemical, morphological, and electrochemical characterization of anode electrodes for Lithium-Ion batteries. Her work has been communicated through national and international conferences. Additionally, she has participated in national research projects focused on advanced electrochemical systems and material development.

## Room-Temperature Valley-Spin Photonic Devices Based on TMDC Metasurface Heterostructures: Enabling Nanophotonic Quantum Technologies for Space Applications



**Rohit K Ramakrishnan**

QOSMIC Satellite Systems, Bangalore, India

Indian Institute of Science, Bangalore, India

Space-based quantum technologies — spanning satellite quantum key distribution (QKD), inter-satellite optical links, quantum sensing, and distributed network nodes — demand photonic hardware that operates without cryogenic cooling, external magnetic fields, or thermally sensitive components. Transition metal dichalcogenides (TMDCs), atomically thin 2D semiconductors, present a platform inherently compatible with these constraints. Large exciton binding energies (100–500 meV) sustain excitonic resonances at room temperature, while the intrinsic valley pseudospin enables direct spin-photon coupling via helicity-dependent optical selection rules at the  $K^+$  and  $K^-$  valleys.

Pan et al. (Nature Communications, 2025) demonstrated room-temperature valley-selective emission in  $\text{MoSe}_2$  monolayers on silicon chiral metasurfaces, achieving a record circular polarization degree of 0.5 at 294 K, independent of excitation polarization — overcoming the valley dephasing bottleneck at ambient conditions. Parallel work on strain-engineered  $\text{WSe}_2$  has produced deterministic single-photon emitters with  $g^2(0) < 0.03$  and 92% circular polarization, with ferromagnetic proximity coupling removing the need for external magnetic fields.

Together, these advances define a nanophotonic platform — planar, silicon-foundry-compatible, and thermally passive — well suited to space deployment. This presentation reviews the physics of room-temperature valleytronics in TMDCs, surveys the state of the art across key device metrics, and identifies remaining integration challenges — spectral inhomogeneity, radiation tolerance, photon extraction efficiency, and free-space coupling — in the context of space qualification and next-generation quantum space systems.

### Biography:

Rohit K. Ramakrishnan is Co-Founder and CTO of QOSMIC, building optical and quantum communication infrastructure for space. He holds a PhD in quantum technologies and was a C.V. Raman Postdoctoral Fellow at the Indian Institute of Science. His research spans quantum communications, quantum AI, and optical satellite networks. He was part of quantum satellite research team at the NUS and the Australian Defence Force Academy. A keynote and invited speaker at major global conferences, he has contributed to *The Quantum Internet: The Second Quantum Revolution* (Cambridge University Press) and serves as a reviewer for Springer Nature and SPIE peer-reviewed journals.

## Structure and electronic properties of Graphene-Triazine bilayered complexes: A computational investigation



**Keshab K. Adhikary**\*<sup>1</sup> **Philippe M. Heynderickx**\*<sup>2</sup>

<sup>1,2</sup>Center for Environmental and Energy Research (CEER) – Engineering of Materials via Catalysis and Characterization, Ghent University Global Campus, 119-5 Songdomunhwa-Ro, Yeonsu-Gu, Incheon, 406-840 South Korea, Academic faculty

<sup>2</sup>Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, 653 Coupure Links, Ghent, B-9000, Belgium.

In the recent decades graphene immersed into the technology and industry with its various derivatives including with its immense functionality by making a complex, combination with other organic molecules, atoms and the combination of the both. Noncovalent functionalization creates scope of wide range of application of graphene complexes. Our intention is to characterize the stacking-like two-layered graphene nanoparticles. We selected the triazin and its substituted derivatives having donor-acceptor properties to layer on the graphene surface. We conducted the cluster and crystal model of the graphene surface to sketch the electronic and structural properties. We verified the stability of the complex using Density Functional Theory (DFT) by measure the interaction energy and charge transfer. On the other hand the macrostructural character was contemplated by the meta-dynamics simulation in material studio platform.

### Biography:

Dr. Adhikary has completed his PhD from Inha University, Incheon, South Korea, in 2003 and 3 years postdoctoral studies from the department of chemistry of the same university. He was an Associate Professor of the department of chemistry, Inha University upto the end of 2019. After Ph.D., he serves his academic role in the university of development alternative, Dhaka, Bangladesh for two years and currently academic faculty of the center for Green Chemistry and Environmental Biotechnology (GREAT) at Ghent University Global Campus (GUGC), Incheon, Korea. He has published several papers in the various reputed journals and has been serving as a guest editor of multiple journals.

## Real-time dynamic analysis of liquid matrices with online measurements: Determination of initial headspace concentration and gas-liquid equilibrium



**Philippe M. Heynderickx**<sup>1,2,\*</sup>

<sup>1</sup> Center for Green Chemistry and Environmental Biotechnology (GREAT), Ghent University Global Campus, Incheon 21985, Republic of Korea,

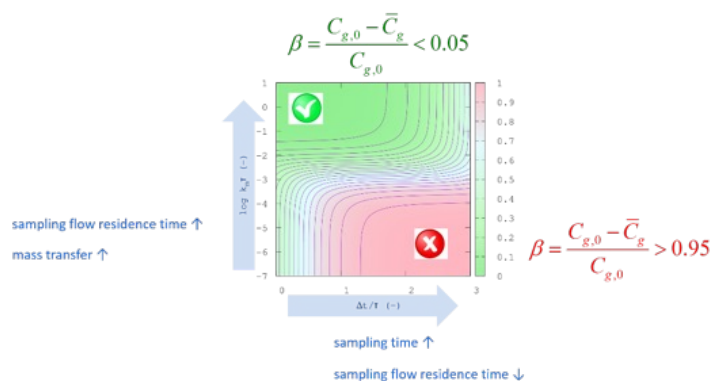
<sup>2</sup> Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, 653 Coupure Links, Ghent B-9000, Belgium

Dynamic headspace sampling is a crucial technique for analyzing consumer products, studying biological samples, and conducting environmental water tests. Specifically, initial headspace concentrations are vital in forensic investigations and in calculating Henry coefficients. In the latter context, 'initial' refers to equilibrium with the liquid phase, where deviations are undesirable. However, during dynamic measurements, achieving true equilibrium is often challenging, leading to potential inaccuracies if only the initial concentration is considered.

This work examines how experimental parameters – such as sampling time, flow rate, headspace volume, liquid volume, and Henry coefficient – affect the measured average concentrations. A corresponding analytical expression, as a function of these variables, is introduced to quantify the deviation of the initial headspace concentration. A measurement accuracy criterion (error below 5%) is also provided. The model is a bi-exponential function that consolidates various existing models for recovery in dynamic sampling into a unified expression (Heynderickx, 2019).

Additionally, the developed model can be applied to determine Henry coefficients for gas compounds in non-ideal solutions through parameter estimation, allowing the effects of real liquid phase conditions to be inferred from gas phase measurements.

### Graphical Abstract



### Reference

Heynderickx, P. M. (2019) Dynamic headspace analysis using online measurements: modeling of average and initial concentration. *Talanta*, 198, 573-584. <https://doi.org/10.1016/j.talanta.2019.02.038>

### Biography:

Philippe M. Heynderickx is professor at Ghent University Global Campus (GUGC), South Korea, where he works on catalyst characterization for indoor air cleaning purposes (gas phase pollution mitigation) and in-depth modeling of photocatalysis as pollution remediation technique for air and aqueous phase systems. He is also active in the field of hydrothermal carbonization for upgrading waste (from marine origin, but also food waste and waste plastic) into hydrochar (adsorbent material) and activated carbon (adsorbent, catalyst carrier material...). Recently, he is involved in waste plastic upgrading via hydrothermal carbonization. In addition, he works on fundamental understanding of process phenomena by combining aspects from chemistry, engineering and mathematics. He is (co-)author of +100 publications in high-impact journals (average IF = 8.0). He received the Young Scientist Award on the 14th International Congress on Catalysis (ICC) in Seoul, Korea (2008).

## Acetaminophen Adsorption Properties Using Graphene-Triazine Bilayer Composites



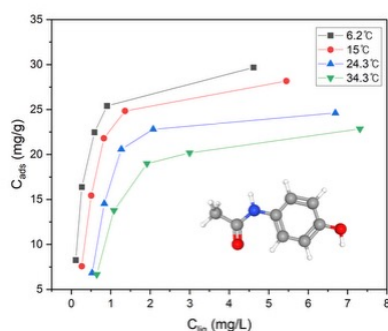
Miran Seo<sup>1</sup>, Keshab Kumar Adhikary<sup>1</sup>, Philippe M. Heynderickx<sup>1,2,\*</sup>

<sup>1</sup> Center for Green Chemistry and Environmental Biotechnology (GREAT), Ghent University Global Campus, Incheon 21985, Republic of Korea

<sup>2</sup> Department of Green Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, 653 Coupure Links, Ghent B-9000, Belgium

Acetaminophen (AMP), known as paracetamol, is widely used as an antipyretic, analgesic, and anti-inflammatory, being one of the most common pharmaceuticals found in different surface water environments (Gatrouni et al., 2024). It is frequently detected in aquatic environments and poses potential risks to human health, aquatic ecosystem and natural environment. Among removal technologies for AMP, adsorption is most promising method widely utilized to remove different organic and inorganic contaminants from aqueous solutions due to its simplicity, efficiency, and low cost (Arabkhani et al., 2025). In this work, the adsorption capacity of newly synthesized graphene-triazine bilayer nanocomposites was investigated for the removal of acetaminophen. The composites were synthesized via ultrasonication, chemical and hydrothermal methods: 1,3,5-triazine (TZN), trichloro triazine (TCT), and 2,4,6-tris (trifluoromethyl)-1,3,5-triazine (TTF) were embedded in graphene to form a noncovalently functionalized two-layered complex. Among the synthesized graphene-triazine nanocomposites, the TTF-functionalized composites with the hydrothermal method exhibited the highest AMP adsorption performance (28.3 mg/g) due to the strong electron-withdrawing and hydrophobic effects of the trifluoromethyl groups, which enhance  $\pi$ - $\pi$  stacking and electrostatic interactions induced by the conjugated- $\pi$  and sigma inductive effects, which results in the strong AMP adsorption onto the composite surface.

### Graphical Abstract



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Arabkhani, P., Asfaram, A., & Sadegh, F. (2025). Efficient treatment of acetaminophen-contaminated wastewater by a phenylboronic acid-functionalized magnetic expanded graphite nanocomposite. *Scientific Reports*, 15(1), 40574. <https://doi.org/10.1038/s41598025-24309-9>

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### Biography:

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## Treatment of Crude Oil Contaminated Water Using Metal Oxide Nanocomposites

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The contamination of rivers and oceans with crude oil pollutants and their waste poses a serious threat to human health and various animal species. With the continued expansion of global industrial activities, the demand for crude oil has increased significantly, leading to its widespread consumption. The presence of numerous offshore and onshore oil fields, along with the extensive transportation of crude oil and its derivatives, increases the likelihood of oil spills or seepages through groundwater, especially those located close to water sources. The effects of these major oil spills are not limited to the depletion of valuable energy resources but also cause severe environmental degradation in the aquatic environment, disrupting ecosystems and raising widespread concerns. In addition to these large-scale incidents, smaller oil spills occur frequently on land, in marine environments, and across inland freshwater systems. This study sought to determine the optimal laboratory conditions for the treatment of real petroleum wastewater in water resources utilizing photocatalysts for the degradation of petroleum-derived contaminants.

An experimental strategy was developed to synthesize a oxide photocatalyst composite using a combination of precipitation/Co- precipitation and sol-gel methods.

The resulting catalysts were subjected to a series of characterization techniques to evaluate their structural, morphological, and surface properties. The degradation efficiency, chemical oxygen demand (COD), total organic carbon (TOC) and Gas chromatography-mass spectrometry (GC-MS) analysis of oil refinery wastewater (DOR) were systematically analyzed and validated following treatment. The highest treatment efficiency was achieved through the nanophotocatalytic composite process.

The photocatalytic degradation efficiency of crude oil effluent was strongly impacted by catalyst type, UV irradiation, sunlight exposure, and crude oil concentrations. The TiO<sub>2</sub>-based composite catalyst improved degrading performance by effective charge separation and increased production of reactive oxygen species. UV radiation has higher photocatalytic activity than sunlight due to its greater excitation capacity for electron-hole pair production. The adjusted circumstances resulted in a high removal efficiency, showing that the proposed photocatalyst is suitable for treating crude oil pollutants.

**Keywords:** Photocatalysis, Nanocomposite, Crude oil pollutants, water resources, magnetic nanoparticles

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## Hybrid Magnetic Activated Carbon–Polyaniline Nanocomposite for Superior Lead Removal from Aqueous Media

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Lead (Pb) contamination in water poses a significant threat to both human health and the environment, as it is toxic even at very minimal concentrations. In the scope of this study, a novel magnetic composite material as AC/Fe<sub>3</sub>O<sub>4</sub>/PANI-SDS, was synthesized to efficiently eliminate Pb<sup>2+</sup> ions from polluted water. Each component in the composite has a significant impact: the activated carbon provides a large surface area for adsorption, the magnetic iron oxide (Fe<sub>3</sub>O<sub>4</sub>) allows the material to be easily magnetic recovery from water systems using a magnet, and the polyaniline (PANI) and sodium dodecyl sulfate (SDS) improve the capability of the material to attract and hold onto Pb<sup>2+</sup> ions. To assess the surface, magnetic, and structural properties of the prepared material, several characterization techniques were applied, such as FTIR, XRD, SEM-EDS, BET analysis, VSM, and zeta potential measurements. These tests confirmed that the composite has the right structure, and functional groups to work as a capable and efficient adsorbent. Batch adsorption studies were used to evaluate the effect of pH, interaction time, initial Pb<sup>2+</sup> ions concentration, and temperature on removal efficiency. The findings highlight the composite's remarkable adsorption efficiency after 220 minutes at optimal conditions, specifically at pH 6. Adsorption kinetic studies demonstrated strong agreement with the pseudo-second-order model, while isotherm analysis showed that the Langmuir model provided the highest correlation coefficient within the investigated concentration range. This fitting suggests apparent Langmuir-type adsorption behavior with a maximum adsorption capacity of 348.39 mg/g. Thermodynamic assessment demonstrates that the elimination of Pb<sup>2+</sup> ions is an endothermic and spontaneous process. In addition, the composite can be reused and recycled repeatedly without significantly reducing its effectiveness, offering an economical and ecologically sustainable approach. The findings of this research highlight the potential of AC/Fe<sub>3</sub>O<sub>4</sub>/PANI-SDS composite as new, efficient, and eco-friendly adsorbents for the elimination of Pb<sup>2+</sup> ions from solutions. In real-world applications, its high capacity for adsorption, ease in separation, and reusability make it a promising treatment for heavy metal contamination.

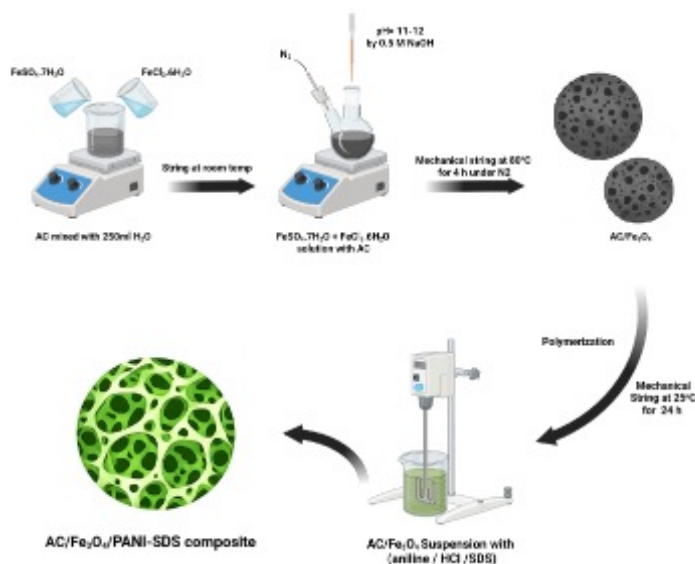


Fig 1. Synthesis process for AC/Fe<sub>3</sub>O<sub>4</sub>/PANI-SDS composite.

## Advanced Oxide-Based Antireflective Coatings for Optical Applications



### Dr. Sadaf Bashir Khan

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Herein, we present the design, fabrication, and performance analysis of multifunctional antireflective (AR) thin-film coatings using high- and low-refractive-index oxide materials, including hafnia ( $\text{HfO}_2$ ), silica ( $\text{SiO}_2$ ), and titania ( $\text{TiO}_2$ ). The multilayer coatings were deposited on different substrates to investigate their optical performance, environmental durability, and multifunctional characteristics. By optimizing the refractive-index contrast and layer configuration, the developed coatings exhibited significantly reduced surface reflectance over a broad spectral range.

In addition to excellent optical transmission, the coatings demonstrated hydrophobic behavior, omnidirectional antireflective performance, and high thermal stability under elevated-temperature conditions. The incorporation of  $\text{HfO}_2$  and  $\text{TiO}_2$  as high-index materials together with  $\text{SiO}_2$  as a low-index material enabled enhanced durability and stable optical properties. The coatings maintained their structural integrity and antireflective characteristics after thermal treatment, highlighting their suitability for demanding optical and photonic applications.

The results suggest that these multifunctional AR coatings are promising candidates for applications in solar cells, optical windows, displays, sensors, and high-temperature optical systems where low reflection, durability, and environmental stability are required.

### Key Words

Oxide thin films, Optical materials, Surface engineering, Nanostructured coatings, Broadband antireflection, Durable optical coatings

### Biography:

Dr. Sadaf Bashir Khan is a Professor at the School of Manufacturing Science and Engineering, Southwest University of Science and Technology (SWUST), P.R. China. She earned her PhD in Materials Science and Engineering from Tsinghua University in July 2018. During her doctoral studies at Tsinghua University, Dr. Khan received multiple prestigious academic honors, including the Comprehensive Scholarship, the 2017 Guorui Scholarship (awarded by the 14th Research Institute of China Electronics Technology Group Corporation), and the 2018 Best Dissertation Award. She also received the Outstanding Excellent Postdoctoral Inbound Award from Shenzhen University.

### Research Focus & Academic Achievements

Dr. Khan's long-term research centers on optoelectronics, additive manufacturing, functional materials, and advanced manufacturing processes. Her core research objective is to integrate materials science with innovative manufacturing technologies to tackle global sustainability challenges. To date, she has published more than 75 peer-reviewed academic papers (including 30 first-author papers) with a total cumulative impact factor exceeding 300, in addition to authored book chapters and authorized patents. She has been recognized with high-level talent awards at the Sichuan Provincial and municipal levels, as well as the Dongguan Special Talent Award. Dr. Khan actively contributes to the academic community as a Guest Editor for multiple renowned journals, including *Discover Applied Sciences* and *Molecules*. She has also received professional recognition for her peer-review expertise, including the 2021 Outstanding Reviewer Award (Springer Nature) and the Trusted Reviewer Award.

## Comparative Analysis of Classical and Quantum Machine Learning Models for Nanomaterial Property Classification



**Chaima Gharbi<sup>12</sup>, Wejden Gazehi<sup>12</sup>, Rania Loukil<sup>12</sup>, Mongi Besbes<sup>12</sup>**

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The accurate prediction and classification of nanomaterial properties constitute essential prerequisites for the rational design and systematic optimization of nanocomposites in chemical engineering contexts. The present study investigates the application of classical and hybrid quantum--classical machine learning frameworks to establish quantitative structure--property relationships between nanoparticle descriptors and their corresponding physicochemical attributes. Four computational approaches are systematically examined: K-Nearest Neighbors (K-NN), Decision Tree (DT), Random Forest (RF), and a novel Quantum Feature Random Forest (QFRF) architecture for nanoparticle property classification.

Model performance is rigorously assessed using standard statistical metrics, including classification accuracy, Mean Squared Error (MSE), Root Mean Squared Error (RMSE), F1-score, and precision. Comparative analysis reveals that the hybrid QFRF framework exhibits markedly superior predictive capability relative to conventional machine learning methods, achieving a classification accuracy of 91.78% with substantially reduced prediction errors (MSE = 0.2556, RMSE = 0.5055). The concomitant improvements in F1-score and precision further demonstrate enhanced model robustness and reliability.

These results establish that the incorporation of quantum-derived feature representations into ensemble learning architectures leads to significant improvements in nanomaterial property prediction. From a chemical engineering standpoint, this data-driven computational framework provides a robust and efficient methodology for nanomaterial characterization, optimization, and inverse design, thereby facilitating the accelerated development of advanced nanocomposites and streamlining materials discovery pipelines.

### Biography:

Chaima Gharbi received her Baccalaureate degree in 2020. She obtained her Bachelor's degree in Telecommunications in 2023 from the Higher Institute of Information and Communication Technologies, University of Carthage, Tunisia. She then completed a Research Master's degree in Data Science and Intelligent Services in November 2025 at ISTIC. Currently, she is a first-year PhD student at the École Polytechnique de La Marsa. Her research is at the intersection of quantum physics and artificial intelligence, with a strong focus on machine learning and deep learning techniques. Her research interests encompass nanotechnology and artificial intelligence, particularly nanoparticle classification using advanced AI-based models.



# Participants Index

A. Bologna	13
Chaima Gharbi	24
Georgia Moysiadou	16
Keshab K. Adhikary	18
Mahmoud M. Youssif	22
Miran Seo	20
Nawar Razzaq Salihi	21
Osman Adiguzel	11
Philippe M. Heynderickx	19
Prof. Dr. Julia Krause	15
Rohit K Ramakrishnan	17
Sadaf Bashir Khan	23
Víctor Martínez-Martínez	14

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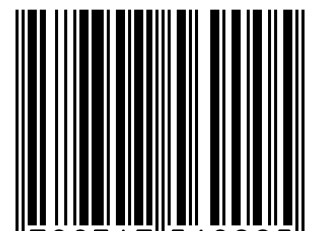
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