IOCPC 2026 Conference

The 1st International Online Conference on Photochemistry

8–9 April 2026 | Online

Program and Abstract Book

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The 1st International Online Conference on Photochemistry

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MDPI

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Email: iocpc2026@mdpi.com

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Welcome from the Chair

Dear Colleagues,

We are excited to announce the **1st International Online Conference on Photochemistry (IOCPC 2026)**, taking place from **8–9 April 2026**. Co-organized by Dirk M. Guldi (FAU Erlangen) and MDPI, this distinguished event will bring together leading experts from the world of photochemistry and related fields for an inspiring and informative gathering.

The conference will provide an excellent opportunity to explore the latest advancements, future research directions, and key developments in the dynamic field of photochemistry. This conference will serve as an engaging platform for discussions on photochemical, photophysical, and photobiological sciences, offering an ideal environment for lively exchanges, new ideas, and potential collaborations. It's a fantastic chance to stay up-to-date with the latest trends, share exciting research, and connect with prominent scientists and top industry leaders from around the globe.

This event will be held entirely online, making it accessible to participants from around the globe—no travel hassles, no expenses, just seamless involvement from anywhere. As a fully digital conference, **IOCPC 2026** offers a dynamic platform for instant and direct exchange of the latest research breakthroughs and innovative ideas. Best of all, participation is completely free, giving you the opportunity to engage, learn, and connect with the global community without any barriers.

IOCPC 2026, proudly sponsored by MDPI and the esteemed journal *Photochem*, invites scholars and experts to join in a dynamic exchange of ideas. Conference proceedings, together with papers and presentations, will be accessible on the conference website and in **MDPI's** *Chemistry Proceedings* journal, where vibrant discussions will take place from 8 to 9 April 2026. Don't miss the opportunity to be part of this cutting-edge scientific dialogue.

After the conference, authors are invited to submit extended and enhanced versions of their proceedings papers to a prestigious Special Issue in *Photochem*. As a token of our appreciation, a generous 20% discount on article processing charges will be offered, providing an excellent opportunity to further showcase your research in a high-impact journal.

Best regards,

Prof. Dr. Dirk M. Guldi
Conference Chair
Department of Chemistry and Pharmacy, Interdisciplinary Center for Molecular Materials, Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

photochem
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Photochem (ISSN 2673-7256) is an international, peer-reviewed, open access journal (free for readers). The aim of the journal is to provide a platform for research into all aspects of photochemistry. The subject stands as the principal artery into the heart of interactions of UV, visible, and IR radiation with molecules and materials. Photochemistry has important associations across a wide spectrum of science, including physics, organic and inorganic chemistry, materials science, biology and medicine.

Photochem publishes regular research articles, reviews and short notes. Our aim is to encourage scientists to publish their experimental and theoretical results in as much detail as possible. Therefore, there is no restriction on the maximum length of the papers. For theory papers, full details of proofs must be provided so that results can be checked. For experimental papers, full experimental details must be provided so that the results can be reproduced. Additionally, electronic files or software regarding the full details of the calculations, experimental procedure, etc, can be deposited along with the publication as 'Supplementary Material'.

Impact Factor: 2.3 (2024); 5-Year Impact Factor: 2.7 (2024)

Session Chairs

Dr. Vincenzo Vaiano
Department of Industrial Engineering, University Salerno, Fisciano, Italy

Dr. Olga Sacco
Department of Chemistry and Biology "A.Zambelli", University of Salerno, Fisciano, Italy

Prof. Dr. Rui Fausto
Department of Chemistry, Coimbra Chemistry Center (CQC-IMS), University of Coimbra, Coimbra, Portugal; Spectroscopy@IKU ERA-Chair, Istanbul Kultur University, Department of of Physics, Faculty of Sciences and Letters, Istanbul, Turkey

Prof. Dr. Dirk Poelman
Lumilab, Department of Solid State Sciences, Ghent University, Gent, Belgium

Prof. Dr. Detlef W. Bahnemann
Institute for Technical Chemistry, Leibniz University Hannover, Hannover, Germany; International Joint Center for Nature Inspired Carbon Neutrality Solutions, Saint-Petersburg State University, Saint-Petersburg, Russia

Keynote Speakers

Prof. Dr. Luís G. Arnaut

Department of Chemistry, University of Coimbra, Coimbra, Portugal

Dr. Janusz Dąbrowski

Department of Chemistry, Jagiellonian University, Krakow, Poland

Professor María Ángeles Lillo-Ródenas

Inorganic Chemistry Department, University Materials Institute of Alicante (IUMA), University of Alicante, Alicante, Spain

Professor Liudmil Antonov

Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria

Professor Stefan Haacke

University of Strasbourg - CNRS Télécom Physique Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg, Strasbourg, France

Asst. Prof. Cláudia Gomes Silva

Laboratory of Separation and Reaction Engineering-Laboratory of Catalysis and Materials (Associate Laboratory LSRE-LCM), Department of Chemical Engineering, Faculdade de Engenharia da Universidade do Porto (FEUP), Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

Dr. Vicenzo Vaiano
Department of Industrial Engineering, University Salerno, Fisciano, Italy

Program at a Glance

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***CEST**—Central European Summer Time; **EDT**—Eastern Daylight Time; **CST**—China Standard Time

IOCPC 2026 Program

8th April 2026 (Wednesday)

S2. Photochemistry for Environmental Remediation

Time: 09:00 (CEST, Basel) | 03:00 (EDT, New York)| 16:00 (CST Asia, Beijing)

CEST	Speaker	Title
09:00–09:10	**Prof. Dr. Dirk M. Guldi** Event Chair	*Welcome and Opening Remarks*
09:10–09:20	**Dr. Olga Sacco** Session Chair	*Welcome by Session Chair*
09:20–09:50	**Prof. María Ángeles Lillo-Ródenas** Keynote Speaker	From Pollutant Removal to Green Fuels: Photocatalysts for Environmental Applications
09:50–10:20	**Assistant Prof. Cláudia Gomes Silva** Keynote Speaker	From Engineered Nanomaterials to Advanced Reactors: Toward Sustainable Photocatalysis
	Contributed Oral Presentations	***Session 2. Photochemistry for Environmental Remediation***
10:20–10:35	**Badis Kahouadji** Selected Speaker	Investigation of the Photocatalytic Degradation Efficiency of Methylene Blue Using TiO₂:Sm³⁺ Luminescent Nanoparticles
10:35–10:50	**Pawel Gluchowski** Selected Speaker	Low-Dimensional Structures and Composite Materials for Environmental Remediation
10:50–11:05	**Zul Adlan Mohd Hir** Selected Speaker	Sustainable Bio-derived Microcrystalline Cellulose from Bamboo Fibers Supported with TiO_2 for Enhanced Photocatalytic Degradation
11:05–11:20	**Dóra Hessz** Selected Speaker	Detection of Microplastics Using Fluorescent Probes
11:20–11:35	**Raul Losantos** Selected Speaker	Advances in Excited-State Dynamics: Bridging Small Molecules and Large Systems
11:35–14:00	**Break**	**Break**

8th April 2026 (Wednesday)

S5. Photoluminescent Materials

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

CEST	Speaker	Title
14:00–14:10	**Prof. Dr. Dirk Poelman** Session Chair	*Welcome by Session Chair*
14:10–14:40	**Prof. Liudmil Antonov** Keynote Speaker	Tautomerism and Photoswitching: Experimental vs Theoretical Spectrometer in the Design of Proton Cranes
	Contributed Oral Presentations	***S5. Photoluminescent Materials***
14:40–14:55	**Thomas J.J. Müller** Selected Speaker	One-Pot Amination-Arylation Synthesis and Structure-Property Relationships of Luminescent and Redox-Active Aryl-Triarylamines and -Phenothiazines
14:55–15:10	**Kai Li** Selected Speaker	Dy3+, Mn4+ Co-Doped Sr4GaNbO8 Materials Towards Dual-Mode Thermometry, Anti-Counterfeiting and Information Encryption Applications
15:10–15:25	**Michaila Akathi Pantelaiou** Selected Speaker	Aggregation-Induced Emission (AIE) Dye–Polymer Nanoformulations via Electrostatic Complexation
15:25–15:40	**Jiaren Du** Selected Speaker	Facilitating Tunable Near-Infrared Persistent Luminescence through Chemical Unit Co-Substitution
15:40–15:55	**Shafiga Alakbarova** Selected Speaker	Photoluminescence Tuning in Sonochemically Synthesized CdS Nanostructures via Controlled Cd:S Stoichiometry
15:55–16:10	**Xiao Huang** Selected Speaker	Theoretical Study on the Design and Optical Properties of Carbon Nanoring System
16:10–16:25	**Debosreeta Bose** Selected Speaker	Deciphering Bio-Interfacial Interactions of photoactive Imidazo-Pyrimidine Derivatives: Linking Photophysics, SAR, and Molecular Dynamics Simulations

9th April 2026 (Thursday)

S1. Photocatalysis and S3. Photocatalytic Energy Conversion

Time: 09:30 (CEST, Basel) | 03:30 (EDT, New York) | 16:30 (CST Asia, Beijing)

CEST	Speaker	Title
Session 1. Photocatalysis		
09:30–09:35	**Dr. Vincenzo Vaiano** Session Chair	*Welcome by Session Chair*
09:35–10:00	**Dr. Vincenzo Vaiano** Keynote Speaker	Innovative Photocatalytic Materials for Sustainable Selective Oxidation
	Contributed Oral Presentations	***Session 1. Photocatalysis***
10:00–10:15	**Fedor Uskov** Selected Speaker	Oxidation of Phenyl-Derived Ethers to Esters via Photocatalytic C-H Activation
10:15–10:30	**Kei Ohkubo** Selected Speaker	Photocatalytic C-H Oxygenation of Hydrocarbons with Chlorine Dioxide
10:30–10:45	**Jorge Herrera Luna** Selected Speaker	Aerobic & Anaerobic Borylation of (Hetero)arenes Triggered by Visible-Light
10:45–11:00	**Linghua Wang** Selected Speaker	Decarboxylative Borylation of Aliphatic Esters via Visible-Light Photoredox Catalysis
11:00–11:15	**Isabella Goveia** Selected Speaker	Assessment of Structure-Property-Catalytic Activity Relationships in Photocatalyst-Bound Cotton for Driving Organic Reactions Under Light
S3. Photocatalytic Energy Conversion		
11:15–11:20	**Prof. Dr. Detlef W. Bahnemann** Session Chair	*Welcome by Session Chair*
11:20–11:45	**Prof. Stefan Haacke** Keynote Speaker	Ultrafast Spectroscopy of Molecules Designed for Light-Energy Conversion
	Contributed Oral Presentations	***S3. Photocatalytic Energy Conversion***
11:45–12:00	**Patrycja Kolbusz** Selected Speaker	Light-Assisted CO2 Conversion on Electrodeposited Cu2O-Based Composite Layers
12:00–12:15	**Svetlana Boshnakova** Selected Speaker	Investigation of a New Additive Manufacturing DED Application for Waste-to-Hydrogen Conversion
12:15–14:00	**Break**	**Break**

9th April 2026 (Thursday)

S4. Photodynamic and Photothermal Therapy and Flash Poster Session

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

CEST	Speaker	Title
14:00–14:10	**Prof. Dr. Rui Fausto** Session Chair	*Welcome by Session Chair*
14:10–14:40	**Prof. Luís G. Arnaut** Keynote Speaker	Flash Photodynamic Therapy: New Opportunities for More Selective and Efficient Treatments
14:40–15:10	**Dr. Janusz Dąbrowski** Keynote Speaker	From Molecular Design to Hypoxic Tumor Models: The Critical Role of Triplet Lifetime in Photodynamic Efficacy
	Contributed Oral Presentations	***S4. Photodynamic and Photothermal Therapy***
15:10–15:25	**Kave Moloudi** Selected Speaker	Evaluation of Nano-Formulation of Pheophorbide-A Mediated Photodynamic Therapy Against 3D Lung Cancer Cells
15:25–15:40	**Aleksandra Pawska** Selected Speaker	Amphiphilic Phthalocyanines as Dual-Mode Photo- and Sonosensitizers for Antimicrobial Applications
15:40–15:55	**Vladimir Sorokin** Selected Speaker	A Photocontrollable Conjugate of a Natural Chlorin and a Chemotherapeutic Agent for Combined Photodynamic Therapy
Flash Poster Session		
	Poster Presentation	***Flash Poster Session***
15:55–16:00	**Alicja Makarec** Poster Presenter	Photodynamic Activity of Hypericin-Loaded Liposomes in Breast Cancer Cells
16:00–16:05	**Dušan Milojkov** Poster Presenter	White-Emitting Dy^{3+}/Eu^{3+} Co-Doped Fluorapatite Nanoparticles for Multispectral Biomedical Applications
16:05–16:10	**Anca Vasile** Poster Presenter	Investigation of Bimetallic Pt-Co and Pt-Ni Catalysts in the Photoreduction of Nitrate
16:10–16:15	**Nelda Martínez-Galero** Poster Presenter	Treatment of Effluents Contaminated by Synthetic Dyes Using Heterogeneous Photocatalysis

16:15–16:20	**Fivos Florides** Poster Presenter	Titanate Nanotubes for the Selective Cleavage of Lignin-Inspired β-O-4 Linkages Towards Value-Added Aromatics Under Visible Light
16:20–16:25	**Beatriz Valadares** Poster Presenter	Solar-Driven Photocatalytic Degradation of Amoxicillin Using TiO2/Carbon Quantum Dots Nanocomposites Immobilized in Electrospun Polycaprolactone Fibers
16:25–16:30	**Katarina Hainz** Poster Presenter	The Impact of Intial pH Value and H2O2 on the Efficiency of Glyphosate Photocatalytic Degradation in Aqueous Suspension Using Simulated Solar Irradiation
16:30–16:35	**Valentina Silva** Poster Presenter	Matrix Influence on Antibiotics Photocatalytic Removal from Water by Magnetic TiO2–Carbon Quantum Dots Composites
16:35–16:40	**Dušica Jovanović** Poster Presenter	Sustainable Photolytic and Photocatalytic Removal of Antibiotic and Antipsychotic from the Aquatic Medium in the Presence of H2O2, KBrO3, and (NH4)2S2O8
16:40–16:45	**Nina Finčur** Poster Presenter	Shining Light on Ciprofloxacin Removal: How Reaction Conditions Shape Photodegradation Efficiency
16:45–16:50	**Ashwani Chikara** Poster Presenter	Optimising Titanium Oxo Cluster-Based Materials for Photocatalysis
16:50–16:55	**Daria Polivanovskaia** Poster Presenter	Photooxidation of Organic Sulfides in the Presence of New metal(IV)porphyrinate-Monocapped Fe(II)-, Ni(II) and Co(III)-Centered Pseudoclathrochelates
16:55–17:05	**Prof. Dr. Dirk M. Guldi** Event Chair	*Closing Remarks*

Session 1. Photocatalysis

sciforum-166903: Development and optimisation of a novel magnetic TiO_2 and Carbon Quantum Dots photocatalyst for water remediation

Valentina Guimarães Silva [1,*], João Costa [2], Nuno J. O. Silva [3], Goreti Pereira [1], Marta Cabero Otero [4], Vânia Calisto [1] and Diana L. D. Lima [5,6]

[1] CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[2] Department of Chemistry & CICECO, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portuga
[3] Department of Physics, Department of Chemistry & CICECO, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portuga
[4] Department of Chemistry and Applied Physics, University of León, León, 24071, Spain
[5] Polytechnic University of Coimbra, Coimbra, 3045-093, Portugal
[6] H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, Coimbra, 3046-854, Portugal

The revised EU Urban Wastewater Treatment Directive came into force in 2025 and mandates the implementation of quaternary treatments until 2045 for treatment plants with a load equivalent to a population of 150,000 or more. These quaternary treatments involve removing micropollutants, such as antibiotics. The application of solar-driven photocatalysis is a possible strategy to address this challenge. However, many photocatalysts in the literature lack efficiency and/or are difficult to implement, recover, and reuse. First, in this work, different synthesis methodologies (oxidative hydrolysis, hydrothermal treatment, co-precipitation, sonication and calcination, and functionalization and coupling via carbodiimide chemistry) were evaluated to produce a novel photocatalyst based on TiO_2, Carbon Quantum Dots (CQD) and magnetic nanoparticles were proposed for the removal of three antibiotics: amoxicillin (AMX), sulfamethoxazole (SMX), and trimethoprim (TMP). Then, experimental conditions for the selected synthesis methodology (co-precipitation) were optimised using two experimental designs: a central composite design and a full factorial design to maximise antibiotic removal, photocatalyst magnetisation saturation, and synthesis yield. The optimal conditions were tested in triplicate, and the results were compared with the predicted values from the applied experimental designs. Among the synthesis methodologies, the co-precipitation provided photocatalysts with consistent properties and high efficiency in antibiotic removal. The optimal synthesis conditions were a molar ratio of 1.2:1 for Fe:Ti and a mass ratio of 4.0% for CQD:TiO_2. Only 100 mg/L of the so-synthesised magnetic TiO_2/CQD composite removed 34±2% of AMX and 64±5% of TMP in 1 h of irradiation and 46±5% of SMX in 1.5 h of irradiation, presenting a *Ms* of 38.8±0.6 emu/g and a synthesis yield of 70.5±0.4%. The obtained results provide an excellent starting point for developing a sustainable solution for removing antibiotics from water using magnetic TiO_2/CQD photocatalysts and further application as a quaternary treatment in urban wastewater treatment plants.

sciforum-162446: Assessment of the Effect of Shade on the Performance of Photocatalyst-Dyed Cotton

Theneza Metra * and Rohit Bhide

Department of Chemistry and Biochemistry, California State Polytechnic University, Pomona, CA, 91768, United States

This project focuses on immobilizing the photocatalyst Eosin Y onto cotton fabric and evaluating its potential as a reusable, solid-supported catalyst for photoredox reactions. In the first phase, Eosin Y was successfully dyed and immobilized onto pre-treated cotton, as indicated by the bright pink coloration of the fabric. This was performed by first converting Eosin Y from a carboxylic acid form to a reactive acid chloride form using N,N′-Dicyclohexylcarbodiimide (DCC) as the coupling agent. Thin Layer Chromatography (TLC) was performed to monitor the formation of the acid chloride derivative; however, no significant difference in Rf values was observed with or without the use of DCC. The acid chloride form was then reacted with cotton samples to covalently attach Eosin Y to the surface of the fabric. Repeatability of the process was tested, and samples showed slight shade variations, reflecting natural differences in dye uptake during the immobilization process. Tests to further confirm the covalent attachment of the photocatalyst to cotton are in progress.

In the second phase, the Eosin Y treated cotton was tested for its photocatalytic activity in the oxidation of benzyl sulfide. The reaction mixture containing benzyl sulfide and the photocatalyst-attached cotton was illuminated with blue light (450 nm) over 72 hours. TLC was used to track the reaction progress, and it showed the formation of benzyl sulfoxide, demonstrating that the photocatalytic system is active.

The next steps of the project will focus on standardizing the immobilization procedure by increasing replicates, improving fabric submersion, and adjusting both reaction steps to achieve more uniform dye loading. After optimization, the project will advance to monitor sulfide oxidation kinetics and evaluate catalyst reuse cycles to assess durability and long-term activity. Together, these studies aim to determine the viability of cotton-supported Eosin Y as a sustainable solid-phase photocatalyst.

sciforum-162467: Perylene-Attached Glass Beads as Metal-Free Photocatalysts for Synthesizing Complex Organic Compounds

Ryan Jolin * and Rohit Bhide

Department of Chemistry and Biochemistry, Cal Poly Pomona, California Polytechnic State University Pomona, Pomona, 91768, United States

With the rising cost of pharmaceutical drug synthesis, new ways of creating base molecules like sulfoxide are high in demand. The state-of-the-art methods for these oxidation reactions involve toxic heavy metals like chromium and vanadium as catalysts, which have long reaction times and require many purification steps. However, perylene-based compounds like perylenetetracarboxylicdianhydride (PTCDA) and perylene diimide (PDI) have shown very promising results when replacing these metals. These organic compounds are non-toxic and have the potential to be reusable when attached to different substrates, for instance, glass beads. When varying the amount of photocatalyst that is loaded onto the surface, the catalytic performance would, theoretically, be affected. Also, with varying concentrations, the color shade should also get darker with more concentrated solutions. Due to this correlation with the color shade and concentration, we seek to relate the color shade to its photocatalytic performance, which has not been done before. Glass beads have been etched utilizing a base bath followed by an acid bath. Then, the beads were refluxed in a toluene-PDI mixture for 48 hours to covalently attach the PDI photocatalyst. After washing, the beads were shown to retain a light pink color, proving that the attachment was successful. In the future, the beads will be characterized using colorimetry shade analysis and Fourier-Transform Infrared Spectroscopy done on the beads in order to characterize them. The photocatalytic performance of the photocatalyst-attached beads will be assessed by monitoring the rate of sulfide oxidation using Thin Layer-Chromatography and Nuclear Magnetic Resonance.

sciforum-162689: Assessment of structure-property-catalytic activity relationships in photocatalyst-bound cotton for driving organic reactions under light

Isabella Goveia *, Verona Peterman, Genevieve Huynh and Rohit Bhide

Department of Chemistry and Biochemistry, California State Polytechnic University Pomona, Pomona, 91768, United States

Traditionally, pharmaceutical syntheses have relied on the use of toxic and precious metals, which poses concerns with safety and sustainability. Homogeneous photocatalysts, which use light to drive organic reactions, are offered as a solution; however, their recoverability and reuse is poor. This work reports on the development of photocatalyst-bound cotton to achieve higher reaction yields and selectivities, along with effective photocatalyst recyclability. These photocatalysts are synthesized following a two-step process: (i) a silanization reaction to covalently attach the (3-aminopropyl)triethoxysilane (APTES) linker to cotton, and (ii) a nucleophilic acyl substitution reaction between APTES-functionalized cotton and perylene-3,4,9,10-tetracarboxylic dianhydride to yield the photocatalyst-bound cotton. The lack of rigorous characterization techniques has limited the large-scale use of such heterogeneous photocatalysts. The major goal of this work is to develop a new technique to characterize the synthesized textile-bound heterogeneous photocatalysts using color shade-catalytic performance relationships. Specifically, a calibration curve relating the sample shade to the rate of photocatalytic reaction will be experimentally derived. Using spectrocolorimetry, the color of photocatalyst-bound cotton with varying photocatalyst loading was quantified. Procedures to dye cotton with photocatalysts were optimized to get evenly dyed samples, as determined by the lower standard deviation of L* values – the color intensity of the samples. Moreover, the applicability of these photocatalysts was tested in the oxidation of sulfide to sulfoxide, a functional group present in many pharmaceuticals. The progress of the reaction was monitored using thin layer chromatography (TLC) and nuclear magnetic resonance (NMR). Preliminary data accounting for several controls suggested that sulfoxide was formed only with the photocatalysts and illumination with blue light. Additionally, the recovery and reuse of these photocatalysts is under investigation. Overall, this work will serve as a foundation in the development of low-cost textile-bound photocatalysts in sustainable and efficient synthesis which can be applied to pharmaceutical drug syntheses.

sciforum-162412: Assessment of Photocatalytic Performance of Silica-Bound Photocatalysts For Sulfide Oxidation

Kaitlyn Miller [1,*], Lance Paquette [2], Josh Limas [3] and Rohit Bhide [1]

[1] Department of Chemistry, Cal Poly Pomona 3801 W. Temple Ave, Pomona, CA 91768, USA
[2] Department of Chemistry, UC Irvine 260 Aldrich Hall, Irvine, CA 92697, USA
[3] Department of Chemistry, UC Berkeley, 110 Sproul Hall, Berkeley, CA 94720, USA

Studying the surface of heterogeneous photocatalysts has been a long-standing challenge in the catalysis community. This project investigates the effect of surface loading on the properties and performance of colloidal photocatalysts. Using detailed spectroscopic analyses, this research addresses challenges with catalysis and will help understand how surface engineering influences the properties of photocatalysts in different organic solvents. These studies will help improve synthesis of complex organic compounds and high recovery rates for the photocatalysts used for catalyzing reactions. To synthesize our photocatalyst particles, (3-Aminopropyl)triethoxysilane (APTES) was bound to silica particles before covalently attaching the photocatalyst perylene tetracarboxylic acid dianhydride (PTCDA). The photocatalysts were characterized using several spectroscopic and chemical analyses. To assess the performance of these catalysts, the oxidation of sulfide to sulfoxide with the PTCDA-bound modified silica was tested in a photoreactor using 450 nm blue LED light over 12 hours. This reaction has wide applications in the synthesis of commercial pharmaceutical drugs making it the best reaction to test these silica particles. The photocatalytic oxidation of sulfide was monitored by thin layer chromatography and nuclear magnetic resonance. The catalytic performance at varying photocatalyst loading on silica was tested. Analyses of these data showed a faster rate with lower photocatalyst concentration which is the opposite of expected results. A plausible reason for this observation could be attributed to the effect of photocatalyst loading on their excited state lifetimes. Excited states of photocatalysts can be more effectively quenched at higher surface concentrations, leading to poor catalytic performance. To test this hypothesis, the surface loading-photophysical property relationships will be further assessed. Moreover, careful photochemical studies were performed to confirm that both the photocatalyst and the light illumination were required to drive sulfide oxidation. With this collected data, more experiments will be conducted to test the reproducibility of observed outcomes.

sciforum-162528: Investigation of the Photocatalytic Activity of Nickel Ferrite-Iron Oxide Materials

Michail Evgenievich Fedosenko [1,*], Svetlana Vasilievna Saikova [2] and Diana Igorevna Nemkova [2]

[1] School of Non-Ferrous Metals, Faculty of Physical and Inorganic Chemistry, Siberian Federal University, Krasnoyarsk, 660012, Russian Federation
[2] School of Non-Ferrous Metals, Siberian Federal University, Institute of chemistry and chemical technologies SB RAS, Krasnoyarsk, 660078, Russian Federation

Photocatalysis is a highly promising approach to environmental pollution. However, the practical application of many photocatalysts is limited by the difficulties of efficently separating them from the reaction medium. Using magnetic materials is a viable solution to this problem. Nickel ferrite is a material that has proven to have high chemical stability and magnetic properties. Unfortunately, its application in photocatalysis is limited by the rapid process of charge recombination. The two primary mechanisms for separating charges are as follows: The first involves creating a contact between two semiconductors to form a solid-state heterojunction. The second is the addition of sacrificial agents in the liquid phase, which react irreversibly with charges from the semiconductor, thereby inhibiting rapid recombination. Therefore, the aim of this work is to synthesize and characterize nickel–ferrite-based materials and investigate their photocatalytic activity in the presence of sacrificial agents. NiFe2O4/Fe2O3 photocatalysts were prepared via co-precipitation of $Fe(NO_3)_3$ and $Ni(NO_3)_2$ using NaOH, followed by calcination at 650 °C for 3 hours. The synthesized materials were characterized by XRD, TEM, UV-Vis, and photoluminescence spectroscopy. Photocatalytic activity was evaluated via the degradation of an indigocarmine dye (20 mL, 4.0×10^{-5} mol·L^{-1}) under a13 W lamp with λmax =340 nm. Experiments to identify the most effective sacrificial agent ($NaHCO_3$, Na_2CO_3, sodium citrate, or H_2O_2) were conducted under the same conditions. The most promising photocatalyst was also tested for recyclability. The highest photocatalytic activity (73% degradation of indigocarmine under 340 nm irradiation for 45 minutes) was achieved using hydrogen peroxide (0,011 mol*L^{-1} in the reaction medium) as a sacrificial agent. An indigocarmine degradation reaction mechanism is proposed.

sciforum-165133: Novel Arenimidazolyl Porphyrins for Use in the Photocatalytic Oxidation of Organic Substrates

Timur Khomyakov [1,*], Daria A. Polivanovskaia [2], Kirill P. Birin [1,2] and Aslan Yu. Tsivadze [2]

[1] MIREA — Russian Technological University, 119454 Moscow, Russia
[2] Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, 119071 Moscow, Russia

The ability of porphyrins and their derivatives to generate reactive oxygen species (ROS) upon irradiation allows these compounds to serve as mild and highly selective agents for various photooxidation reactions. The wide range of possible modifications at the periphery of the heterocycle, as well as variation of the coordinated metal cation, enables precise tuning of the photophysical properties of the macroheterocycles and increases the rate of singlet oxygen generation under light exposure.

In this research, we present a novel synthetic route to β-arenimidazolylphenyl porphyrins. A series of target compounds was synthesized and fully characterized using standard physicochemical methods. We employed a set of tetraarylporphyrins to investigate the influence of meso-substituents on the reaction pathway, solubility, and photocatalytic efficiency.

In order to evaluate the effect of the arenimidazolyl fragment on the photocatalytic activity of porphyrins, we used the oxidation of sulfides as a model reaction. Even with a very low catalyst loading (0.5×10^{-4} mol %) and under blue-light irradiation (λ = 430-505 nm, 5 W), complete substrate conversion was achieved with >99% selectivity toward the corresponding sulfoxides. We also measured the photostability of the obtained free-base porphyrins. No significant photodegradation was observed for more than five hours of irradiation, which is comparable to the performance of existing industrial photocatalysts.

The high efficiency in model photooxidation reactions, combined with excellent photostability, allows us to consider target substances as potential photocatalysts in production of medicinal substances, bearing sulfoxide functional groups.

This work was performed with financial support from the Ministry of Science and Higher Education of the Russian Federation.

sciforum-162543: Optimising Titanium Oxo Cluster-Based Materials for Photocatalysis

Ashwani Chikara [1,*], Bin Wang [2], Frederik Tielens [2], Frank De Proft [2] and Sebastian D. Pike [1]

[1] Department of Chemistry, University of Warwick, Coventry CV4 7AL, United Kingdom
[2] Algemene Chemie (ALGC) - Chemical Theory and Materials Modelling Group, Vrije Universiteit Brussel, Brussel, 1040, Belgium

Titanium dioxide (TiO_2) is one of the most widely studied photoactive metal oxides, with applications that span self-cleaning windows, air-purifying surfaces, and a range of photocatalytic technologies aimed at improving urban environmental quality. At the nanoscale, titanium-oxo clusters provide a precise and well-defined bridge between molecular systems and bulk materials, offering precise control over both structure and electronic behaviour. Such tunability makes these clusters particularly attractive for photocatalytic applications, where their properties can be tuned more directly than those of extended solids.

In this work, we investigate the electronic structure and photochemical response of a series of Ti_6-oxo clusters and assess how these features shape their broader photocatalytic potential. Through time-dependent density functional theory (TD-DFT), we show that the energies and distributions of the frontier orbitals are strongly influenced by the ligands coordinated to the metal-oxo core. This ligand-controlled modulation closely parallels bandgap-engineering strategies commonly applied to nanoscale semiconductor materials.

Our findings reveal that adjusting the ligand environment, including the use of extended π-conjugated ligands, can optimise photocatalytic behaviour by deliberately tuning the underlying electronic landscape. These insights broaden the understanding of photoactivity in titanium-oxo clusters and highlight new routes for their use in sustainable energy conversion, environmental remediation, and chemical synthesis.

sciforum-166653: A High-Entropy Zirconate Pyrochlore for Multifunctional Photocatalysis

Anandkumar Mariappan

High-Entropy Materials Research Laboratory, South Ural State University, Chelyabinsk, 454080, Russia

The urgent need for advanced wastewater treatment drives the search for efficient photocatalysts. In this study, we have synthesized a single-phase high-entropy zirconate pyrochlore oxide (Ce0.2Pr0.2Zn0.2Nd0.2Tb0.2)2Zr2O7 via a modified Pechini technique. Several characterization techniques, such as X-ray diffraction, UV–visible spectroscopy, field emission scanning electron microscopy, and X-ray photoelectron spectroscopy, were used to explore the physicochemical features of the synthesized nanoparticles. Cationic dye (methylene blue), anionic dye (Congo red), and Cr(VI) were used to test the photocatalytic capabilities of high-entropy zirconate pyrochlore oxide $(Ce_{0.2}Pr_{0.2}Zn_{0.2}Nd_{0.2}Tb_{0.2})_2Zr_2O_7$. The photocatalytic findings show that the high-entropy $(Ce_{0.2}Pr_{0.2}Zn_{0.2}Nd_{0.2}Tb_{0.2})_2Zr_2O_7$ zirconate pyrochlore oxide that was made could break down dyes and lower Cr(VI) levels. Radical trap experiments indicate that hydroxyl radicals, superoxide radicals, and holes were responsible for the photocatalytic activity. Furthermore, the placement of the valence band and conduction band decided the photocatalytic reaction kinetics. The prepared photocatalyst also exhibited excellent structural stability and reusability, maintaining its high photocatalytic activity over three consecutive cycles without significant loss of performance. These results underscore the high-entropy pyrochlore's robust activity, stability, and versatility in treating diverse water contaminants. This study establishes high-entropy zirconate pyrochlore oxide $(Ce_{0.2}Pr_{0.2}Zn_{0.2}Nd_{0.2}Tb_{0.2})_2Zr_2O_7$ as a highly promising and effective photocatalyst for broad-spectrum environmental remediation applications.

sciforum-167716: Aerobic and Anaerobic Borylation of (Hetero)arenes Triggered by Visible-Light Irradiation

Jorge Carlos Herrera Luna [1,*], Diego Sampedro [2], David Díaz Díaz [3,4], María Consuelo Jiménez Molero [1] and Raúl Pérez Ruiz [1]

[1] Chemistry Department, Polytechnic University of València (UPV), Camí de Vera S/N, 46022, Valencia, Spain
[2] Chemistry Department, Research Chemistry Institute of University of La Rioja, Madre de Dios, 53, 26006, Logroño, Spain
[3] Organic Chemistry Departament, University of La Laguna, Avda. Astrofísico Francisco Sánchez 3, 38206, La Laguna, Spain
[4] Antonio González Bioorganic Institute, University of La Laguna, Avda. Astrofísico Francisco Sánchez 3, 38206, La Laguna, Spain

Organoboronate esters have attracted significant attention due to their broad utility in organic synthesis as versatile intermediates, as well as their relevance in medicinal chemistry and materials science. These environmentally benign building blocks can be readily transformed into a wide range of functional groups, enabling their application in the synthesis of advanced materials. In particular, heteroaryl boronates such as thiophene-derived esters are of special interest owing to their diverse applications, ranging from conjugated materials for organic electronics and LED devices to antimicrobial agents in medicinal chemistry.[1]

Accordingly, the development of innovative and efficient synthetic strategies for their preparation remains highly desirable. Over the past decade, numerous methodologies based on transition-metal catalysis or metal-free approaches have been reported for the synthesis of organoboron derivatives and their subsequent functionalization.[2] Among the available precursors, aryl halides stand out as ideal starting materials due to their low cost and widespread commercial availability. In this context, visible-light photoredox catalysis has emerged as a powerful strategy for the activation of aryl halides, enabling the generation of radical intermediates that can be efficiently trapped by boron-based nucleophiles to afford aryl boronate esters.[3]

Herein, we report our latest results on the borylation of (hetero)aryl halides under anaerobic and aerobic mild conditions using an easy-to-handle gel nanoreactor. This photocatalyst-free protocol proceeds under visible-light irradiation at room temperature and in the presence of air, highlighting its operational simplicity and sustainability. Notably, the gel network provides a stabilizing microenvironment that enables a broad substrate scope.

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sciforum-167479: Carbon Dots/TiO_2 hybrids for photocatalytic degradation of drugs in the aquatic environment

Daniela Kujawa [1,*], Marzena Fandzloch [1], Anna Grzegórska [2], Anna Zielińska-Jurek [2] and Paweł Głuchowski [1]

[1] Department of Spectroscopic Properties, Institute of Low Temperature and Structural Research, Polish Academy of Sciences, Okólna 2, Wrocław, 50-422, Poland
[2] Department of Process Engineering and Chemical Technology, Faculty of Chemistry, Gdańsk University of Technology, G. Narutowicza 11/12, Gdańsk, 80-233, Poland

The occurrence of pharmaceutical residues in water bodies represents a growing environmental and public health concern, as many of these compounds are poorly removed by conventional wastewater treatment technologies. Carbamazepine (CBZ), a widely prescribed antiepileptic drug, is among the most persistent pharmaceuticals detected in aquatic environments and is frequently used as an indicator of treatment inefficiency. This study presents an advanced photocatalytic material designed to enhance the removal of carbamazepine from water by combining mesoporous titanium dioxide (TiO_2) with luminescent and phosphorescent carbon dots (CDs and PhCDs).

Two anatase TiO_2 photocatalysts with distinct porosity and morphology were prepared via solvothermal synthesis and thermal conversion of a titanium-based metal-organic framework, respectively. The materials were modified by impregnation with carbon dots and thoroughly characterised to assess their structural, optical, and surface properties. The photocatalytic performance of the resulting hybrids was evaluated under UV-Vis irradiation using carbamazepine degradation and total organic carbon (TOC) removal as key indicators of treatment efficiency.

The incorporation of carbon dots broadened the light absorption range of TiO_2 toward the visible region, enabling more effective utilisation of solar irradiation. In particular, phosphorescent carbon dots significantly improved photocatalytic performance by prolonging the lifetime of photogenerated charge carriers and reducing electron-hole recombination. As a result, the PhCDs@TiO_2 hybrid achieved faster carbamazepine degradation and higher mineralisation efficiency compared to unmodified TiO_2, even at reduced photocatalyst loadings.

These findings demonstrate the potential of phosphorescent carbon dot-modified TiO_2 as a practical photocatalyst for water treatment applications. The use of low-cost, metal-free carbon dots combined with a well-established TiO_2 platform offers a promising and scalable approach for removing persistent pharmaceutical contaminants in advanced oxidation processes and solar-driven wastewater treatment systems.

sciforum-162032: Cobalt and iron-exchanged $LiLaTa_2O_7$ layered perovskites and their applicability in sustainable photocatalytic processes

Monica Pavel *, Irina Atkinson, Crina Anastasescu, Florica Papa and Ioan Balint

"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 Spl. Independentei, 060021, Bucharest, Romania

Solar energy catalysis remains an environmentally friendly technology that effectively addresses numerous global issues, including pollution removal, CO_2 reduction or clean hydrogen fuel generation. Dion--acobson-type layered perovskites are applicable semiconductors for sustainable photocatalytic processes, particularly for the photocatalytic H_2 production as well as for the degradation of organic pollutants. Their effectiveness arises from the capacity to adjust their electronic and structural properties through multiple modification methods, including ion exchange processes. For an efficient photocatalytic system, its activity is decided by factors such as the band gap, crystallinity, morphology, specific surface area, and defects. Therefore, the strict control of the synthesis parameters affecting these properties is decisive.

This study focuses on the synthesis, structure, and properties of perovskite-related layered transition oxyhalides of the type $(MeCl)LaTa_2O_7$ (Me = Co, Fe) along with their assessment for sustainable photocatalytic processes (e.g. H_2 generation from water splitting). The development of $(MeCl)LaTa_2O_7$ type functional materials was achieved through ion-exchange reactions, in which the starting compound, $LiLaTa_2O_7$, was combined with a two-fold molar excess of $MeCl_2$, under mild conditions (350 °C, 3 h). The XRD analysis confirms the successful incorporation of Co and Fe species within the perovskite-type $LaTa_2O_7$ layers. The intercalation of transition metal species influences the electronic band structure of materials by creating a new, higher-energy valence band and reducing their band gap values. The preliminary photocatalytic experiments for water splitting, conducted in the absence of a sacrificial reagent, have demonstrated the potential activity of these layered-perovskite-related materials. Subsequent research will aim to enhance reaction rates through the addition of various co-catalysts and understanding the reaction mechanisms, thereby making these materials suitable for practical applications.

sciforum-167179: Decarboxylative Borylation of Aliphatic Esters via Visible-Light Photoredox Catalysis

Linghua Wang

School of Life Science and Technology, Xi'an Jiaotong University (Innovation Harbor Campus), Xi'an, ShaanXi Province, 710110, China

Alkylboronates serve as pivotal intermediates in synthetic chemistry; however, their preparation through mainstream methods—such as transmetalation, hydroboration, or transition-metal-catalyzed borylation of (pseudo)halides—typically demands strictly anhydrous conditions and often exhibits limited compatibility with sensitive functional groups.

Herein, we report a mild, operationally straightforward, and versatile alternative: a decarboxylative borylation of readily available alkyl N-acyloxy-phthalimide esters under visible-light photoredox catalysis. This new protocol directly addresses the common synthetic challenges by proceeding efficiently under ambient conditions, utilizing non-anhydrous solvents, and critically, requiring no stoichiometric sacrificial additives. The reaction is catalyzed by an inexpensive iridium photosensitizer ($[Ir(ppy)_2dtbpy]PF_6$) upon irradiation with compact fluorescent light, employing tetrahy-droxydiboron as the boron source. A broad range of primary and secondary alkyl boronic acids are obtained in good-to-excellent yields. These products, which can be isolated as air-stable trifluoroborates after a simple KHF_2 workup, tolerate a diverse array of functional groups, including esters, ethers, halides, and heterocycles, highlighting the exceptional chemoselectivity of this radical-based pathway. Mechanistic investigations, including control experiments, support a catalytic cycle initiated by the single-electron reduction of the redox-active ester.

This generates an alkyl radical, which subsequently engages with an in situ formed, base-activated diboron species to forge the critical C–B bond. The method provides a general and practical strategy for converting abundant, stable aliphatic carboxylic acids—via their activated derivatives—into valuable alkylboron building blocks under remarkably mild conditions, offering a complementary and robust tool for complex molecule synthesis.

sciforum-166304: Enhanced photocatalytic degradation of oxytetracycline using $LaFeO_3$ supported on Mullite ceramic foam

Renato Pelosato * and Isabella Natali Sora

Department of Engineering and Applied Sciences, University of Bergamo, Bergamo, Italy

Photocatalysis is an accepted technique for persistent pollutant remediation. Compared to conventional photocatalytic systems based on a powdered catalyst, the immobilization of the catalyst on a solid support is essential for practical environmental applications. $LaFeO_3$ is a stable p-type oxide semiconductor with a medium bandgap of 2.48 eV. Undoped-$LaFeO_3$, like many ABO_3 perovskite-type oxides, presents an extensive recombination rate for photogenerated electron–hole pairs, but it is stable in acidic solutions (pH>3) and non-toxic.

Thus, we applied a thin active layer of catalyst on the surface of sintered mullite-based ceramic foam. The photocatalyst powder covering the outer surfaces was placed layer by layer through adding the alcohol slurry of $LaFeO_3$ powder dropwise and then thermal treatment in air at moderate temperature. With this procedure, the catalyst particles remain nanometric. Parallel tests for the photocatalytic degradation of oxytetracycline (OTC) $c_0 = 5.0 \cdot 10^{-6}$ M under visible-light irradiation in three different configurations were carried out: H_2O_2 $c_0 = 3.0 \cdot 10^{-3}$ M solution, H_2O_2 + $LaFeO_3$ supported on the mullite foam, and H_2O_2 + mullite foam without catalyst. In this study, the OTC solution was buffered at pH = 5.0, so OTC had a zwitterionic form. The OTC solutions were stirred in the dark for 20 minutes, and then two fluorescent lamps (daylight, 8 W each) emitting in the 380-780 nm region were turned on for 240 min.

H_2O_2 + mullite foam and H_2O_2 + $LaFeO_3$ supported on the mullite foam degraded 34% and 50% of OTC, respectively, after 240 min of irradiation. The small addition of H_2O_2 increases the photodegradation rate of organic pollutants by removing the surface-trapped electrons, thereby lowering the electron–hole recombination rate. The final results show that mullite foam with a thin layer of $LaFeO_3$ has a promising and stable photocatalytic activity for oxytetracycline degradation under visible light.

sciforum-161580: From DPZ to DTQ: Organic Catalysts for Homo- and Heterogeneous Photoredox Processes

Eva Prokopová *, Zuzana Burešová and Filip Bureš

Institute of Organic Chemistry and Technology, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice 2, Czech Republic

Photoredox catalysis has emerged as a powerful strategy for driving redox reactions under exceptionally mild conditions by using light as a clean and controllable energy source. A suitable photocatalyst capable of harvesting light energy and promoting electron-transfer processes is essential for this methodology.[1] Common classes of purely organic photocatalysts include xanthene, acridinium dyes, perylenediimides, and cyanoarenes.[2]

In 2014, dicyanopyrazine **DPZ** was introduced as organic photocatalyst, which has been employed in numerous photoredox transformations so far.[3] Its mechanism of action and catalytic activity were investigated,[4] while a recent study revealed that, under blue-light irradiation, **DPZ** undergoes a Mallory-type photocyclization to dithienoquinoxaline (**DTQ**).[5] Its double excited **DTQ**$^{-\cdot}$ proved to be an exceptionally strong organic reductant capable of chemodivergently reducing nitroaromatics. Hence, utilizing ^{3}**DTQ** or ***DTQ**$^{-\cdot}$ and a single blue light source, diethienoquinoxaline can be employed either as a one-electron oxidant or reductant via PET and conPET processes.

DTQ was further immobilized through copolymerization with styrene, generating a polymer-bound photocatalyst (**iDTQ**). Both powdered material and a flexible monolithic column based on **iDTQ** were prepared, each retaining the key photophysical and catalytic features of the homogeneous **DTQ**. **iDTQ** was successfully applied in both batch and continuous-flow heterogeneous photocatalytic processes.[6]

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sciforum-167098: FT-Based Study of Photoinduced Charge Transfer in Functional Carbon Materials

Gururaj Kudur Jayaprakash

Department of Chemistry, Nitte Meenakshi Institute of Technology, Nitte University, Bangalore, 560064, India

Photochemical reactions are significantly affected by the electronic configuration of materials when exposed to light irradiation. This study employs rapid density functional theory (DFT) calculations, as implemented in the deMon2k package, to investigate photoinduced charge transfer in functionalized carbon-based materials. An analysis of frontier molecular orbitals, HOMO–LUMO energy gaps, and charge density distributions is conducted to elucidate light-induced electron excitation and reactivity. The findings indicate that basic molecular functionalization can efficiently adjust the electronic response during photoexcitation. The deMon2k method's efficiency enables rapid calculations at a minimal computational expense, rendering this approach appropriate for the swift screening of photoactive materials. This study demonstrates that rapid simulations can provide reliable photochemical insights and facilitate the development of experimental and industrial materials. Moreover, the computational workflow is deliberately simplified by employing established exchange–correlation functionals and compact basis sets accessible in deMon2k. This facilitates the rapid completion of geometry optimization and electronic structure analysis using standard computing resources. This expedited simulation approach is especially advantageous for initial material selection, where numerous candidate systems require efficient evaluation. This methodology can be readily expanded to investigate light–matter interactions pertinent to photocatalysis, chemical sensing, and environmental remediation, thereby underscoring the practical significance of rapid theoretical photochemistry.

sciforum-162561: High-Performance Ti–Ni Nanocomposites for Wastewater Photoremediation

Ali Aqeel Salim and KaiXuan Gan *

Physics Department and Laser Centre, ISI-SIR (CsNano), Faculty of Science, Universiti Teknologi Malaysia, 81310 Skudai, Johor Bahru, Malaysia

Synthetic dyes such as methylene blue (MB) and methyl orange (MO) is widely released from textile industries pose a serious global hearth concern due to their carcinogenic and mutagenic properties, threatening public health and disrupting natural ecosystems. In this study, titanium-nickel nanocomposites (Ti-Ni NCs) were synthesized using pulse laser ablation in liquid (PLAL) method for efficient dye removal applications. The optical and chemical properties of TiO_2 NPs, NiO NPs and Ti-Ni NCs were characterized using ultraviolet-visible (UV-Vis), fluorescence (FL), and Fourier-transform infrared (FTIR) spectroscopy. The UV-Vis spectra exhibited a prominent absorption peak at ~361 nm in UV region, while Tauc plot analysis showed significant bandgap blue shift upon incorporation of NiO into TiO_2 NPs. FTIR spectra showed the presence of Ti-O, Ni-O and Ti-O-Ni vibrational bands, proving the interfacial interaction between TiO_2 and NiO upon mixing. The Ti-Ni NCs revealed enhanced photocatalytic activity, achieving up to 97.1% degradation of MB and 89.6% MO removal within 45 minutes, showing advance photocatalytic properties under UV light irradiation. This enhancement is attributed to the synergistic effect between TiO_2 and NiO, which forms a p-n heterojunction, effectively improve charge separation efficiency. These findings proposed the potential of high purity PLAL-synthesized Ti-Ni NCs as advance photocatalysts for wastewater remediation.

sciforum-162620: Light-Induced Optical and Interfacial Charge Modulation in SiC/PS Nanocomposites for Photocatalytic Applications

Sevinj Natiq Hamidova * and Vusal Usub Mammadov

Faculty of Physics, Baku State University, Baku, Azerbaijan

Silicon carbide/polystyrene (SiC/PS) nanocomposites with 1–10 wt% SiC were synthesized to investigate how structural, optical, and interfacial properties govern light-induced behavior relevant to photocatalysis and photochemical processes. SEM and XRD measurements confirmed that micron-scale, highly crystalline β-SiC is successfully incorporated into the amorphous PS matrix, with progressively intensified SiC reflections as loading increases. Williamson–Hall analysis showed that the 7 wt% composite exhibits the largest crystallite size (≈30.23 nm) and minimal microstrain, suggesting reduced lattice distortion and more efficient pathways for charge separation at polymer–ceramic interfaces. UV–Vis spectroscopy demonstrated that SiC concentrations of 1–5 wt% sharpen the absorption edge and increase the direct band gap from 3.91 to 4.22 eV and the indirect band gap from 2.91 to 3.82 eV. This band-edge modulation indicates suppression of defect-assisted transitions and improved generation of photo-excited carriers under UV illumination—properties essential for photocatalytic activity. At higher loadings (≥7 wt%), strong absorption and scattering prevent reliable gap extraction, pointing to intense photon attenuation within the composite. FTIR analysis revealed preserved PS vibrational signatures together with progressively strengthened SiC-related modes (Si–O–C at 1100–1150 cm^{-1}, Si–C/Si–C–O at 800–600 cm^{-1}, and a ~910 cm^{-1} surface phonon), confirming physical rather than covalent interactions and indicating increased exposure of optically active SiC surface sites. Dielectric spectroscopy showed a systematic rise in ε' and ε'' with increasing filler concentration due to Maxwell–Wagner–Sillars interfacial polarization, highlighting enhanced charge accumulation and migration under alternating fields. These results establish a direct correlation between SiC loading, photon absorption behavior, and interface-driven charge dynamics, identifying 3–5 wt% as optimal for UV-activated photochemical applications and 7 wt% as the most structurally stable composition.

sciforum-167569: Magnetic carbon-based photosensitizers for the removal of antibiotics from water

Beatriz Valadares [1, 2,*], Valentina Silva [3], Vânia Calisto [3], Diana L. D. Lima [3,4] and Goreti Pereira [3]

[1] Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[2] Polytechnic University of Coimbra, Coimbra Health School, Rua 5 de Outubro – S. Martinho do Bispo, Apartado 7006, 3046-854 Coimbra, Portugal
[3] CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[4] H&TRC – Health and Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3045-043, Coimbra, Portugal

Water scarcity combined with the increasing presence of pharmaceuticals, such as antibiotics, in aquatic systems, poses a significant threat to environmental integrity and to human and animal health. The increasing demand for efficient and sustainable materials for water treatment has driven research towards photocatalytic technologies. In this work, magnetic TiO_2/Carbon Quantum Dots (CQDs) nanocomposites were synthesised and evaluated to assess the influence of synthesis methodology on the final material's photocatalytic performance. CQDs were synthesised via a hydrothermal method using spent brewery grains (SBG) as a sustainable carbon precursor. The process involved hydrothermal carbonisation at 200 °C, with or without prior stirring at 70°C of the precursors, followed by filtration and purification. Magnetic TiO_2/CQDs nanocomposites were then prepared by co-precipitation of iron salts, either in-situ or ex-situ, enabling facile recovery of the materials by magnetic separation. For the ex-situ methodology, TiO_2/CQDs nanocomposites were previously prepared through ultrasonication, followed by the co-precipitation with iron oxide. In the in-situ synthesis, CQDs, TiO_2, and iron salts were added together. Four magnetic TiO_2/CQDs composites were obtained by combining stirring and the synthesis route (in-situ or ex-situ).

The prepared materials were evaluated for the photocatalytic degradation of 10 mg/L trimethoprim (TMP) and sulfamethoxazole (SMX) in phosphate buffer (0.001 mg/L, pH 8) under simulated solar irradiation. The results show that all nanocomposites enhanced the degradation of both TMP and SMX compared to photolysis. The best-performing photocatalysts removed above 70% after 1h of irradiation, against less then 20% removal in photolysis. Under tested conditions (500 mg/L), the ex-situ photocatalyst with prior stirring exhibited the highest activity, yet the results were comparable to the in-situ photocatalyst without prior stirring, which was selected as the most suitable photocatalyst due to simpler and faster synthesis.

sciforum-166911: Matrix influence on antibiotics photocatalytic removal from water by magnetic TiO_2–Carbon Quantum Dots composites

Valentina Guimarães Silva [1,*], Marta Cabero Otero [2], Vânia Calisto [1] and Diana L. D. Lima [3,4]

[1] CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[2] Department of Chemistry and Applied Physics, University of León, León, 24071, Spain
[3] Polytechnic University of Coimbra, Coimbra, 3045-093, Portugal
[4] H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, Coimbra, 3046-854, Portugal

Over the years, global consumption of antibiotics has increased, as has their presence in the environment, mainly due to the discharge of ineffectively treated wastewater. Until 2045, Urban Wastewater Treatment Plants (UWWTP) with a population equivalent load of 150,000 or more must implement quaternary treatments to promote the removal of micropollutants, such as antibiotics. For such a purpose, solar-driven photocatalysis is considered promising. In this study, a novel photocatalyst composed of TiO_2, Carbon Quantum Dots (CQD), and magnetic nanoparticles was produced using co-precipitation. The produced magnetic TiO_2/CQD composite was tested for the removal of 3 antibiotics (amoxicillin (AMX), sulfamethoxazole (SMX) and trimethoprim (TMP)) under simulated solar irradiation and different operation conditions: pH (6, 7, 8 and 9), dissolved organic matter (10, 20 and 40 mg/L), and water matrices with distinct complexity (phosphate-buffered ultrapure water at pH 8 and secondary UWWTP effluent (sUWWTPe)). Tests at different pH levels revealed no significant effect of pH for most antibiotics. Conversely, 10 mg/L of dissolved organic matter enhanced the photodegradation of the tested antibiotics, whereas higher concentrations slowed the removal of all antibiotics and decreased photocatalyst efficiency. In PBS, the magnetic TiO_2/CQD photocatalyst resulted in a 154-fold increase in the photodegradation kinetic rate compared to photolysis. Meanwhile, in sWWTPe, the photodegradation kinetic rate increased by 2 times for both TMP and SMX, whereas external factors hindered precise quantification of the kinetic rate enhancement for AMX. Furthermore, the magnetic TiO_2/CQD photocatalyst improved antibiotics mineralisation, reaching 80% after 15 h of irradiation for AMX and TMP and 30 h for SMX, compared with only 20% without the photocatalyst. Therefore, the applied photocatalyst is a promising option for solar-driven quaternary wastewater treatments in UWWTP, enabling the sustainable removal of antibiotics.

sciforum-164308: Outstanding photocatalytic activity of new metalloporphyrins

Alina D. Oparina [1,2,*], Daria A. Polivanovskaia [2], Kirill P. Birin [2] and Aslan Yu. Tsivadze [2,3]

[1] Faculty of Chemistry, Lomonosov Moscow State University, Moscow, 119991, Russia
[2] Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, 119071, Russia
[3] Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, 119071, Russia

Porphyrins are able to act as effective photosensitizers for oxidation due to the ability to generate reactive oxygen species under photoexitation. Various strategies to macrocycle functionalization, allow us to significantly impact on photocatalytic activity of porphyrins. For instance, heterocyclic annelation with additional aromatic fragments, expanding the π-system, or the introduction of the certain metal ions into porphyrin cave can contributes to an increase in the quantum yield of singlet oxygen. It is reasonable to expect that the use of both types of modification will make it possible to obtain fundamentally newand highly efficient photocatalysts based on pyrazine-annelated metalloporphyrin. In this work, a series of novel pyrazinoporphyrinato In(III), Pd(II), Zn(II) and Mg(II) were obtained. The study of the photostability of the compounds demonstrated that In(III) and Pd(II) complexes are the most resistant to photoirradiation. Furthermore, the Pd(II) and In(III) porphyrinates demonstrated superior photocatalytic activity in the oxidation of thioanisole. Under blue-light irradiation with photocatalyst loading of 1×10^{-3} mol%, Pd(II) and In(III) complexes achieved complete conversion of the substrate to sulfoxide and the turnover number (TON) up to 100000. Remarkably, the high activity of the In(III) complex allowed reduce the loading to 5×10^{-4} mol% and still achieve 100% conversion. A study of the kinetics of photooxidation of thionalizole was carried out under photocatalytic conditions. The highest oxidation rate was demonstrated by In(III) complex, which reached 52% conversion for 3 hours, with the maximum TOF value of 17333 h^{-1}. The applicability of the In(III) complex as a photocatalyst for the oxidation of a series of structurally diverse organic sulfides was further studied, and 80-100% conversion was achieved for most of the substrates, which makes it a promising material for photocatalytic applications.

The work was supported by the Russian Science Foundation grant (project No. 24-73-00168).

sciforum-164909: Oxidation of Phenyl-Derived Ethers to Esters via Photocatalytic C–H Activation

Fedor A. Uskov [1,2,*], Stepan M. Korobkov [2], Kirill P. Birin [2] and Aslan Yu. Tsivadze [2,3]

[1] Faculty of Chemistry, National Research University Higher School of Economics, Moscow, Vavilova Str., 7, 117312, Russia
[2] Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, Moscow, Leninsky pr., 31, bldg. 4, 119071, Russia
[3] Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Moscow, Leninsky pr,, 31, 119991, Russia

Functionalization of the ether fragment is a challenging task for classical organic chemistry. Meanwhile, radical C–H activation of ethers has emerged as a powerful synthetic tool. However, most transformations of this kind are described for aliphatic ethers. Thus, the search for a method of C–H activation of phenol-derived ethers may significantly expand the existing set of synthetic approaches for this class of compounds.

In this work, a method for radical C–H activation of phenol-derived ethers is proposed, affording the corresponding α-halogenated ethers. Subsequent addition of potassium tert-butoxide gives the corresponding α-halogenated ester instead of elimination. In contrast, the mixing of tBuOK with DMSO before the addition led to unsubstituted ester.

As a result, radical bromination of a series of ethers followed by the addition of a base was carried out, a mechanism of radical C–H activation was proposed, and the influence of the alkyl fragment and photocatalyst was investigated. In the second stage, the effect of the amount and nature of the base on the final product was studied. The yields and structures of the products of the first stage were confirmed by NMR spectroscopy. The second stage was monitored by GC. The work was performed with financial support from the Ministry of Science and Higher Education of the Russian Federation.

sciforum-164866: Photocatalysis of Ag Nanoparticles in Wastewater Teatment

Rebika Baruah * and Archana Moni Das

Chemical Science and Technology Division, CSIR-NEIST, Jorhat, Assam, PIN No. 785106, India

Nanomaterials are an remarkable innovation in the 21st century for humanity. Environmental pollution is a great challenge for human civilization . Water pollution is the main threat to surviving . Much wastage is drained off to the water bodies and they cause detrimental effects on the aquatic lives . Development of an innovative and novel technique to remediate water pollutants and make water safe for drinking is very necessary. Traditional methods have disadvantages of high pressure, temperature, cost, longer time, larger area, production of byproducts, etc. . Photocatalysis in the presence of nanoparticles is the most remarkable method in wastewater treatment due to its cost-effective, simple, and eco-friendly nature. Nanoparticles possess large surface to volume ratio, extra small-size NPs and these properties make them applicable in scavenging of organic pollutants within a short period to the larger extent. Ag nanoparticles (NPs) were synthesized using the plant extracts of *Phragmites australis* as reducing and capping agents. Ag NPs possessed superior photocatalytic properties in the scavenging of organic pollutants. To confirm the shape, size, optical properties, stability, and involvement of phytochemicals in the synthesis and stabilization of NPs, Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM), X-Ray Diffraction (XRD), UV-Visible, Dynamic Light Scattering (DLS), Zeta potential and Fourier Transform Infrared (FTIR) analysis were performed respectively. Photo-degradation of harmful dyes was carried out in presence of Ag NPs under sunlight. Ag NPs degraded Phenol Red (PR) and Brilliant Blue (BB) dyes up to achieving 80%. Ag NPs efficiently inhibited the growth of human pathogens like *Staphylococcus aureus* and *Escherichia coli*. ZnO NPs also showed potential antioxidant activity in the DPPH assay. Hence, *Phragmites australis* fabricated Ag NPs (PA@ZnO NPs) will be novel innovative multifunctional materials for the treatment of wastewater for safe drinking water and prevention of transmission of severe contagious diseases like COVID-19.

sciforum-160496: Photocatalysis-induced electric fields: Enhancing dichromate transport and reduction

Liping Zhang [1,*], Chen Chen [1], Siyu Zhao [1], Bingming Zhou [1], Changqing Ye [1] and Baojiang Jiang [2]

[1] Faculty of Materials Science, Shenzhen MSU-BIT University, Shenzhen, Guangdong 518172, China
[2] Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education of the People's Republic of China, Heilongjiang University, Harbin, Heilongjiang 150080, China

Photocatalysis-induced phenomena, such as active motion and superhydrophilicity, have been widely studied [1,2]. In this presentation, we introduce a previously unrecognized effect: photocatalysis-induced electric fields [3]. Using monoclinic bismuth vanadate (BiVO4) films and potassium dichromate (K2Cr2O7) as a model reduction system, we demonstrate that illumination generates long-range electric fields extending hundreds of micrometers into the surrounding solution. Spatially resolved concentration measurements and transport analysis reveal that these fields strongly bias the migration of charged reactants toward the photocatalyst surface. The same behavior is observed in an independent system based on TiO2, indicating that this phenomenon is not limited to a specific material or crystal structure.

Unlike the localized interfacial fields commonly discussed in semiconductor heterojunctions, these extended electric fields enhance dichromate transport by more than three orders of magnitude, thereby maintaining a continuous reactant supply. As a result, the overall photocatalytic reduction rate is significantly improved without additional energy input, catalyst restructuring, or complex reactor engineering. We argue that photocatalysis-induced electric fields represent a new handle for coupling light-driven redox chemistry with ion transport. This concept opens an unexplored design space for optimizing photocatalytic reactors, and may be generalized to other oxidation or reduction processes relevant to green synthesis, solar fuel production, and environmental catalysis.

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sciforum-162278: Photocatalysts based on oxidized g-C_3N_4 and their photocatalytic applications

Sofiya Kharina [1,*] and Anna Kurenkova [2]

[1] Laboratory of Processes for Alternative Energy, Boreskov Institute of Catalysis, SB RAS, Novosibirsk, 630090, Russian Federation
[2] Department of Synchrotron Research of Functional Materials, Synchrotron Radiation Facility 'SKIF', Boreskov Institute of Catalysis SB RAS, Koltsovo, 630559, Russian Federation

In the context of growing energy shortages and environmental issues, photocatalytic technologies are becoming particularly relevant. Using sunlight as the only energy source, photocatalysis enables the production of synthetic fuels, such as hydrogen and methane.

A key factor affecting photocatalytic efficiency is the choice of semiconductor material, which must combine chemical stability, visible-light activity, and favorable textural and surface properties. Graphitic carbon nitride (g-C_3N_4) with a partially oxidized surface is a promising candidate. Oxidation of g-C_3N_4 via hydrothermal treatment in H_2O_2 solution significantly increases its specific surface area, enhances photoinduced conductivity, and introduces O-containing functional groups. These modifications improve hydrophilicity, facilitate reactant adsorption, and ensure strong anchoring of cocatalyst species in the form of nanoparticles or single atoms.

The photocatalytic performance of oxidized g-C_3N_4 loaded with 0.1–1 wt.% Pt was investigated in two reactions: hydrogen evolution (HER) from aqueous organic substrates under LED irradiation (λmax = 440 nm) and simulated sunlight (AM 1.5 G), and CO_2 reduction under LED irradiation (λmax = 405 nm). In the CO_2 reduction reaction, the use of 1 wt.% Pt/g-C_3N_4 produced CH_4 as the primary product at a rate of 2.9 $\mu mol \cdot g_{cat}^{-1} \cdot h^{-1}$, with an overall electron consumption rate of 26.3 $\mu mol \cdot g_{cat}^{-1} \cdot h^{-1}$. The photocatalysts containing 0.5 and 1 wt.% Pt exhibited similar hydrogen evolution rates from glucose solutions of up to 310 $\mu mol \cdot g_{cat}^{-1}\ h^{-1}$, indicating the efficient utilization and uniform dispersion of Pt species [1].

TEM, XPS, ATR-FTIR and EXAFS analyses confirmed the structural and chemical stability of the photocatalysts before and after HER, demonstrating that the surface composition and Pt distribution remained unchanged.

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sciforum-162577: Photocatalytic C-H Oxygenation of Hydrocarbons with Chlorine Dioxide

Kei Ohkubo

Institute for Open and Transdisciplinary Research Initiatives, The University of Osaka1-6, Yamada-oka Suita Osaka 565-0871, Japan

Extensive efforts have been devoted towards the development of methods for the direct conversion of methane (CH_4), ethane (CH_3CH_3), or other abundant natural gasses into useful products, such as the corresponding alcohols, aldehydes, ketones, and carboxylic acids, liquid fuels, and precursors of chemical and pharmaceutical products. Selective aerobic oxygenation of CH_4 into liquid products without the concomitant formation of CO_2 and CO has served as an elusive target reaction. The selective oxygenation of CH_4 to CH_3OH with molecular oxygen (O_2) has been unknown because the oxidation of oxygenated products, CH_3OH and formic acid (HCOOH) is much easier than that of CH_4, leading to over-oxidation products such as CO and CO_2. Here, we report that oxygenation of methane photochemically occurred in the presence of $ClO_2^{\bullet}$. The yields of methanol and formic acid as products were 17% and 82%, respectively, with a methane conversion of 99% in a two-phase system comprising perfluorohexane and water under ambient conditions. The reaction occurred by the efficient radical chain process.[1–3]

UV light irradiation of chlorine dioxide radical results in the excited state of one-electron reduction potential to be E_{red}^{*} = +3.22 V vs. SCE. The highly oxidative power of chlorine dioxide at the excited state allowed electron-transfer oxidation of benzene and cyclohexane as hydrocarbon substrates to yield the corresponding oxygenated products. The reaction is initiated by the formation of the photoexcited state of $ClO_2^{\bullet}$. Electron transfer from benzene (Eox = 2.48 V vs SCE) to the excited state of $ClO_2^{\bullet}$ occurs to form a radical ion pair composed of a benzene radical cation and ClO_2^{-}. Phenol, as a final product, is formed from the reaction between benzene radical cation and H_2O.

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sciforum-162670: PHOTOCATALYTIC DEGRADATION OF RHODAMINE USING Bi_2WO_6/ g-C_3N_4 COMPOSITE

Ambigadevi J [1,*], Senthil Kumar P [2], Balaji Bhargav Pamula [3] and Senthilnathan Selvaraj [4]

[1] Department of Chemical Engineering, Rajalakshmi Engineering College, Chennai 602105, Tamil Nadu, India
[2] Centre for Pollution Control and Environmental Engineering, School of Engineering and Technology, Pondicherry University, Kalapet, Puducherry- 605014, India
[3] SSN Research Centre, Sri Sivabramaiya Nadar College of Engineering, Kalavakkam, Chennai 603110, Tamil Nadu, India
[4] Centre for Applied Nanomaterials, Chennai Institute of Technology, Chennai-600069, Tamil Nadu, India

Harnessing the power of photocatalysis stands out as a beacon of hope in the quest for environmental restoration. Using a coprecipitation method, highly efficient Bi_2WO_6/g-C_3N_4 heterojunction photocatalysts, activated by visible light, were successfully fabricated. The Bi_2WO_6 /g-C_3N_4 composite materials underwent characterisation utilising X-ray diffraction, UV-vis diffuse reflectance spectroscopy, scanning electron microscopy, and Fourier transform infrared spectroscopy. The seamless fusion between Bi_2WO_6 and g-C_3N_4 fosters an environment where charge carriers are efficiently separated, minimising electron-hole recombination. This harmonious synergy enhances the photocatalytic prowess of the Bi_2WO_6/g-C_3N_4 composite, promising a brighter future for environmental remediation. The optical studies showed that the band gap of the composite was 2.71 eV. The parameters, such as initial dye concentration, pH and catalyst dosage, affecting the photocatalytic activity were analysed and optimised. The study found that a pH of 2.5, a catalyst dosage of 30 mg, and a dye concentration of 5 ppm were the optimal parameters for this process. Under these conditions, the photocatalytic system achieved an impressive 95.649% degradation of Rhodamine B. The catalyst showed high stability up to five cycles. The kinetics of the photodegradation mechanism followed pseudo-first order. The rate constant of the composite showed that it folds greater than Bi_2WO_6, proving it to be an efficient photocatalyst.

sciforum-162565: Photocatalytic Performance of PLAL-Synthesized Chromium Nanoparticles Toward Methylene Blue Degradation

Ali Aqeel Salim *, KaiXuan Gan, S. K. Ghoshal, Muhammad Safwan Abd Aziz and H. Bakhtiar

Physics Department and Laser Centre, ISI-SIR (CsNano), Faculty of Science, Universiti Teknologi Malaysia, 81310 Skudai, Johor Bahru, Malaysia

Access to clean water is essential for human health, yet the persistent and poorly degradable nature of synthetic dyes continues to threaten aquatic environments. This challenge underscores the need for efficient nanoscale photocatalysts capable of enhancing pollutant degradation. In this study, an eco-friendly, simple, and cost-effective pulse laser ablation in liquid (PLAL) technique was employed to synthesize high-purity chromium nanoparticles (CrNPs) without the use of surfactants or chemical precursors. CrNPs were produced at various laser energies and evaluated for their potential in dye-degradation applications. The nanoparticles were characterized using ultraviolet–visible (UV–Vis) spectroscopy, fluorescence (FL) spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy to elucidate their optical and chemical properties. UV–Vis and FL analyses showed that laser energy significantly influences NP size distribution and optical behavior, while bandgap analysis revealed a slight shift with increasing laser energy. FTIR spectra confirmed the presence of Cr–O and O–H functional groups, which are known to contribute to photocatalytic activity. The absorption spectra of methylene blue (MB) decreased gradually with irradiation time. Photocatalytic degradation experiments under visible light demonstrated that CrNPs exhibit strong photodegradation efficiency. Overall, these findings highlight the potential of surfactant-free, PLAL-synthesized CrNPs as promising photocatalysts for the remediation of pharmaceutical pollutants and heavy-metal-contaminated wastewater.

sciforum-167690: Photocatalytic upcycling of bio-based microplastics under ambient conditions using nanostructured titania-based catalysts

Athanasia Kotsaridou [1,*], Dimitrios A. Giannakoudakis [1] and Konstantinos Triantafyllidis [2,3,4]

[1] Department of Chemistry, Aristotle University of Thessaloniki, University Campus, Thessaloniki, Greece
[2] Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia
[3] Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia
[4] Saudi Arabia Chair in Catalysis and Petrochemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

The sustainable photocatalytic upcycling of plastic waste under mild conditions represents an emerging pathway toward a circular materials economy. In this study, we present the development of innovative nanostructured titania-based photocatalysts, designed to efficiently drive polymer conversion under low-intensity UVA or visible light. The catalysts consist of mixed titanium hydroxide/titanium dioxide phases, synthesized by energy-efficient sono-chemical methods. These routes yield zero- and one-dimensional nanostructure, such as doped anatase core, shell systems embedded in amorphous carbon-rich matrices or titanate nanotubes, featuring superior light-harvesting capacity, improved charge carrier separation, and enhanced surface reactivity.

The catalytic performance of these tailored materials is demonstrated in the selective photo-depolymerization of bio-based polymers, including polylactic acid (PLA), polyethylene furanoate (PEF), and polybutylene succinate (PBS), under ambient conditions. Remarkably, the process proceeds in the absence of organic solvents, additives, or sacrificial agents, affording value-added monomers and lactic acid-derived products through a fully green transformation route. Systematic optimization of process parameters ensures both activity and selectivity, emphasizing scalability and environmental compatibility.

This work establishes heterogeneous photocatalysis as a viable and sustainable strategy for ambient-condition plastic upcycling. Using PLA as a model substrate, it provides a foundation for implementing low-energy photocatalytic technologies in real-world waste valorization applications, bridging materials design with circular economy principles.

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sciforum-165645: Photodegradation of Methylene Blue by Pla/Tio$_2$ Composite Membranes Prepared by the Phase Inversion Method

Olaolu Samuel Awobifa [1,*], Rosa Idalia Narro-Céspedes [1], Alejandro Samuel Lozano Morales [2] and Francisco José González González [2]

[1] Faculty of Chemical Science, Department of Material Science for Autonomous University of Coahuila, Blvd. V. Carranza s/n. Col. Republica Oriente Saltillo, Coahuila. C.P. 25280, Saltiilo, Mexico
[2] Department of Macromolecular Chemistry for Center for Research in Applied Chemistry, Blvd. Enrique Reyna Hermosillo No. 140 Saltillo, Coahuila, CP 25294, Mexico

Fresh drinking water in the environment is scarce due to the contamination of water bodies by pollutants such as dyes, pharmaceuticals, heavy metals, and other industrial waste. Dyes have been a major concern in industries, especially the textile, paper, and tile production industries. When these dyes are deposited in the environment, they cause various diseases, including cancer, and disrupt photosynthesis. They are resistant to the oxidizing agent and heat because they are not biodegradable. Therefore, the ability to remove them has become a serious problem. This project deals with the preparation of biodegradable PLA/TiO_2 composites prepared by the phase inversion method for the photocatalysis of methylene blue. The composite membrane produced was characterised by FTIR to determine the functional groups of the membrane. SEM was used to identify the morphology of these porous membranes. The thermal properties of the composite membrane were determined by the TGA and DSC. The adsorption of the methylene blue and the photodegradation of the dyes were carried out at room temperature for 80 mins at 10 mins interval. The adsorption by the pure PLA was higher than that of the composite membrane throughout the 180 min time. The composites containing 10 wt. % TiO_2 showed the highest dye removal.

sciforum-162507: Photooxidation of organic sulfides in the presence of new metal(IV)porphyrinate-monocapped Fe(II)-, Ni(II) and Co(III)-centered pseudoclathrochelates

Daria A. Polivanovskaia [1,2,*], Semyon V. Dudkin [2], Kirill P. Birin [1] and Aslan Yu. Tsivadze [1,3]

[1] Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, 119071 Moscow, Russia
[2] Nesmeyanov Institute of Organoelement Compounds Russian Academy of Sciences, 119334 Moscow, Russia
[3] Kurnakov Institute of General and Inorganic Chemistry Russian Academy Of Sciences, 119071, Moscow, Russia

One of the priority areas of scientific development today is the search for new approaches to efficient and selective transformations of organic substrates. This challenge can be successfully overcome using catalytic approaches to various reactions, including oxidation reactions. Due to their broadly conjugated polyaromatic system, porphyrins possess unique optical and electronic properties upon photoexcitation, namely the ability to transfer energy and electrons to molecular oxygen, forming its reactive oxygen species (ROS). In turn, the ROS allows selective oxidation reactions to be performed under mild conditions and prevents the formation byproducts and degradation products of chemical oxidants. This is fully consistent with the principles of atom economy and green chemistry. Thus, porphyrins could be considered as promising photocatalysts for effective oxidation processes. Nevertheless, the known porphyrin-based photocatalysts require significant efforts for the optimization of their photocatalytic characteristics, including activity, photostability, and conditions of photocatalytic reactions.

In this study, we developed an approach to control the physicochemical properties of the tetrapyrroles by introducing into the axial positions of Zr and Hf(IV) porphyrinates additional coordination structures—tris-pyridinoximate complexes of Fe, Ni(II) and Co(III). Thus, new metal(IV)porphyrinate-monocapped Fe, Ni(II) and Co(III)-centered pseudoclathrochelates were prepared.

It was shown that this functionalization of porphyrinates was shown to significantly increase photostability and the photocatalytic activity of the macrocycles in oxidation compared to their precursors. Irradiation with low-power light (LED lamp, 3W, 410-510 nm) in most cases resulted in complete conversion of thioanisole as model organic sulfide while maintaining >99% selectivity of the formation of the target sulfoxide. This type of photocatalyst has demonstrated high applicability for the oxidation of a series of aryl alkyl and alkyl alkyl sulfides with various substituents at extremely low catalyst loading (0.02 mol%).

This work was supported by the Russian Science Foundation grant (project No. 24-23-00323).

sciforum-162348: Polystyrene with Controlled Molecular Weight via Photoinduced Reversible-Deactivation Radical Polymerizations

Daniil Varabyou [1,2,*], Aliaksei Vaitusionak [3,4] and Sergei Kostjuk [5]

[1] Research Institute for Physical Chemical Problems of the Belarusian State University, 14 Leningradskaya St., 220006, Minsk, Belarus
[2] Department of Chemistry, Belarusian State University, 14 Leningradskaya St., 220006, Minsk, Belarus
[3] Research Institute for Physical Chemical Problems of the Belarusian State University, 14 Leningradskaya St., 220006 Minsk, Belarus
[4] Institute for Regenerative Medicine, Sechenov First Moscow State Medical University, 8-2 Trubetskaya St., Moscow 119991, Russia
[5] Parisian Institute of Molecular Chemistry, Sorbonne University, Paris, 75252, France

The application of light as an external stimulus to induce polymerization processes can have significant implications in a range of scientific, medical and technological domains. Photoinduced electron/energy transfer (PET) RAFT polymerization, which employs photoredox catalysis in conjunction with the RAFT process, offers a range of advantages over conventional RAFT polymerization. In addition to the inherent benefits of the RAFT technique, this method also provides enhanced control over the polymerization process by varying light wavelength and intensity, while also being environmentally friendly. The PET-RAFT process has been thoroughly investigated with regard to the polymerization of acrylates, methacrylates and acrylamides, while comparatively less attention has been devoted to the polymerization of styrene.

In this study, in order to conduct effective PET-RAFT polymerization of styrene, we have examined a number of organic dyes and sulfur-containing compounds as potential photocatalysts and RAFT agents, respectively. It has been demonstrated that 2-(dodecylthiocarbonothioylthio)-2-methylpropionic acid is the most effective RAFT agent, while eosin Y and perylene are the most effective photocatalysts. PET-RAFT polymerization with 2-(dodecylthiocarbonothioylthio)-2-methylpropionic acid and eosin Y yielded polystyrene with a molecular weight of up to 9000 g/mol and low polydispersity ($Đ \leq 1.4$). Trithiocarbonate functionality was observed on ^{1}H NMR spectra, which is important from the perspective of further modification and synthesis of block copolymers. Moreover, this photoinitiating system allowed us to polymerize styrene under both blue and green light irradiation; to achieve temporal control of the polymerization process (by switching off/on the light); and to conduct polymerization in air without negative influence from oxygen on the rate and molecular weight characteristics of the obtained polymers.

sciforum-162775: Preparation and Characterization of PLAL-Derived Cobalt Nanoparticles for Methylene Blue Photodegradation

Dr. Ali Aqeel Salim and Aminu said Abdullahi *

Physics Department and Laser Centre, ISI-SIR (CsNano), Faculty of Science, Universiti Teknologi Malaysia, 81310 Skudai, Johor Bahru, Malaysia

This study reports a clean, surfactant-free synthesis of cobalt-based nanomaterials via pulsed laser ablation in liquid (PLAL) using deionized water as the ablation medium for advanced photocatalytic applications. A high-purity cobalt metal target was irradiated with a pulsed laser under controlled conditions to generate cobalt and cobalt-oxide nanoparticles directly in aqueous media, eliminating the need for chemical reducing agents, stabilizers, or post-treatment purification. The crystalline structure, phase composition, and crystallite size of the as-synthesized nanomaterials were systematically investigated using X-ray diffraction (XRD), confirming the formation of mixed metallic cobalt and cobalt oxide phases. Transmission electron microscopy (TEM) analysis revealed the successful formation of well-dispersed, predominantly nanospherical particles with a narrow size distribution in the nanometer range. The optical absorption characteristics were examined using UV–visible spectroscopy, demonstrating strong absorption in the visible region, which is highly favorable for photocatalytic activity under light irradiation. The photocatalytic performance of the synthesized cobalt-based nanomaterials was evaluated through the light-driven degradation of a model organic pollutant in aqueous solution. The nanomaterials exhibited a remarkable degradation efficiency under visible-light irradiation, which can be attributed to their enhanced light-harvesting capability, high surface-to-volume ratio, and efficient charge carrier generation. The superior photocatalytic response confirms the effective role of PLAL in tailoring the structural and optical properties of cobalt-based nanomaterials. Overall, this work highlights PLAL in deionized water as a green, scalable, and environmentally benign synthesis route for producing high-purity cobalt-based photocatalysts with promising potential for wastewater remediation and environmental purification technologies.

sciforum-162580: Pyrazinoporphyrins for the photooxidation of organic sulfides: the role of the metal center and functional groups

Ekaterina Sergeevna Shremzer *, Daria A. Polivanovskaia, Kirill P. Birin and Aslan Yu. Tsivadze

[1] Frumkin Institute of Physical Chemistry and Electrochemistry Russian Academy of Sciences, 119071 Moscow, Russia
[2] Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, 119071, Moscow, Russia

Porphyrins constitute a versatile platform for designing photocatalysts, and the growing interest in photocatalysis for organic synthesis and sustainable technologies underscores the need for strategies that improve their efficiency. The synthesis of the target pyrazinoporphyrins was carried out following previously developed methodologies, which involve the reduction of 2-nitro-3-aminoporphyrin to the corresponding 2,3-diamino derivative followed by condensation with aromatic carbonyl compounds. A synthetic approach enabling the introduction of phosphoryl groups on the periphery of diaryl-substituted and phenanthrene-appended pyrazinoporphyrins was established *via* phosphorylation of brominated precursors. This strategy afforded a series of photoactive compounds, including the free bases and the Zn(II) and In(III) complexes bearing various *meso*-substituents.

To assess the effect of these structural modifications on the stability of pyrazinoporphyrins, the kinetics of photodegradation were analyzed. The introduction of diethylphosphoryl groups was found to markedly enhance photostability. Indium(III) complexation further decreased the photodegradation rate by nearly 20-fold, whereas zinc(II) coordination had the opposite effect.

The introduction of phosphoryl substituents and indium(III) ions into the macrocycle also resulted in a systematic enhancement in photocatalytic activity in the photooxidation of thioanisole. At 0.0005 mol% loading, functionalized free bases and In(III) complexes achieved 78–100% conversion, whereas non-functionalized pyrazinoporphyrins produced only 66–72% even at higher loadings (0.001 mol%).

Kinetics studies of thioanisole photooxidation in acetic acid revealed that in both series of pyrazinoporphyrins, the In(III) complexes outperform the corresponding free bases. At the lowest tested loading (0.00001 mol%), an exceptional TON of 9900000 and a TOF of 309000 h^{-1} were obtained, highlighting the outstanding catalytic performance of these systems. The high efficiency of the catalysts was further demonstrated in the selective oxidation of a wide range of sulfides. Overall, the new photosensitizers outperformed previously reported porphyrin systems.

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sciforum-165630: Solar-driven photocatalytic degradation of amoxicillin using TiO_2/Carbon Quantum Dots nanocomposites immobilized in electrospun polycaprolactone fibers

Beatriz Valadares [1,*], Valentina Silva [2], Rosa Baptista [3], Bernardo Almeida [3], Diana L. D. Lima [4,5], Vânia Calisto [2] and Goreti Pereira [2]

[1] Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[2] CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
[3] Centre of Physics of Minho and Porto Universities (CF-UM-UP), Laboratory for materials and Emergent Technologies (LAPMET), University of Minho, 4710-057 Braga, Portugal
[4] Polytechnic University of Coimbra, 3045-093 Coimbra, Portugal
[5] H&TRC – Health and Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3045-043, Coimbra, Portugal

The presence of antibiotics in aquatic environments has become a growing concern due to their incomplete removal in conventional wastewater treatment plants, leading to the dissemination of antimicrobial resistance. Solar-driven advanced oxidation processes have emerged as sustainable strategies for degrading persistent pharmaceuticals. In this context, immobilizing photocatalysts onto polymeric supports may facilitate their recovery and reuse, thereby enhancing the practicality of water treatment applications. Carbon Quantum Dots (CQDs) were synthesized hydrothermally and incorporated onto commercial TiO_2 (P25) to form TiO_2/CQDs nanocomposites. These photocatalysts were embedded into electrospun polycaprolactone (PCL) nanofibers at a 1:2 photocatalyst-to-polymer ratio, and the resulting fibers were characterized by scanning electron microscopy. Photolysis and photocatalysis experiments were carried out under simulated solar irradiation using amoxicillin (AMX, 10 mg L^{-1}) in phosphate buffer (0.001 mol L^{-1}, pH 8), with a photocatalyst concentration of 1.5 g L^{-1}. AMX degradation was monitored by HPLC-UV. The kinetic parameters were determined by assuming pseudo-first-order behavior. AMX removal under irradiation was significantly enhanced in the presence of the photocatalyst, resulting in an approximately 18-fold increase in degradation efficiency compared with photolysis. The pseudo-first-order rate constant increased from 0.0112 h^{-1} to 0.201 h^{-1} with TiO_2/CQDs@PLC, reducing the AMX half-life time from 62 to 3.45 h. These results highlight the potential of this sustainable method for treating water contaminated with antibiotics.

sciforum-162390: Synthesis and Photocatalytic Activity of the Oxysulfide Perovskite $KTaO_{3-x}S_x$

Darya Sergeevna Kalugina [1,*], Andrei Trofimovich Matveev [1], Alexander Denisovich Kovalev [2], Magzhan Kaiyrzhanovich Kutjanov [1] and Dmitry Vladimirovich Shtansky [1]

[1] Research Center "Inorganic Nanomaterials", National University of Science and Technology MISIS, Moscow, 119049, Russia
[2] Department of Physical Materials Science, National University of Science and Technology MISIS, Moscow, 119049, Russia

Introduction. Perovskite $KTaO_3$ is regarded as a promising photocatalyst owing to its high stability and structural adaptability to substitution. The possibility of substituting oxygen with nitrogen or sulfur in its lattice allows the band gap to be reduced and the material response in the visible region of the spectrum to be enhanced. In this work, the oxysulfide perovskite $KTaO_{3-x}S_x$ is presented, and the effect of sulfur content on its structure and photocatalytic properties under solar-light irradiation is investigated.

Materials and Methods. $KTaO_{3-x}S_x$ powders were obtained in two steps: $KTaO_3$ was first synthesised by a solid-state reaction between K_2CO_3 and Ta_2O_5 at 800 °C for 8 h, and then $KTaO_3$ was treated at 600 °C in an H_2S atmosphere. The sulfur content was determined by EDS, and changes in the crystal structure were monitored by XRD. The photocatalytic activity of $KTaO_{3-x}S_x$ particles was evaluated from the degradation of rhodamine B (RhB), and the contribution of different catalytically active species to the photocatalytic process was assessed by scavenger experiments.

Results. Oxysulfide perovskites $KTaO_{3-x}S_x$ with sulfur contents of 1.8, 4.2 and 7.4 at.% were obtained. The samples are single-phase, and the $KTaO_3$ structure is preserved over the entire sulfur-doping range studied. The $KTaO_{2,79}S_{0,21}$ sample (4.2 at.% S) exhibits the highest photocatalytic activity under solar-light irradiation: in RhB degradation its activity is 2.25 times higher than that of pristine $KTaO_3$, with superoxide anion $O_2\bullet^-$ being the main active species.

Conclusions. It is shown that sulfurization of $KTaO_3$ in H_2S vapour enables controlled formation of the oxysulfide perovskite $KTaO_{3-x}S_x$. Sulfur doping increases the photocatalytic activity by more than a factor of two: the composition containing 4.2 at.% S exhibits an activity of 12.5 $mg \cdot g^{-1} \cdot h^{-1}$ in RhB degradation under solar-light irradiation.

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sciforum-162386: The impact of intial pH value and H_2O_2 on the efficiency of glyphosate photocatalytic degradation in aqueous suspension using simulated solar irradiation

Katarina Hainz *, Szabolcs Bognár and Daniela Šojić Merkulov

Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad Faculty of Sciences, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

The growing production and extensive use of herbicides have resulted in their frequent detection in various environmental compartments. N-(phosphonomethyl)glycine (glyphosate, GLY) is one of the most widely used herbicides worldwide. Due to its persistence in aquatic environments and its numerous documented negative effects on ecosystems, as well as potential risks to human health, it is considered a highly concerning organic pollutant. Therefore, it is essential to develop efficient and sustainable methods for its removal from water. Among the promising approaches, heterogeneous photocatalysis is a green method characterized by simplicity, environmental friendliness, and the use of renewable energy, which, through simulated solar irradiation and semiconductor materials, such as TiO_2 photocatalyst, successfully degrades organic pollutants in water.

This study investigates two factors affecting the efficiency of the photocatalytic degradation of GLY: the impact of initial pH value of suspension and the influence of hydrogen peroxide concentration. The influence of catalyst loading (0.5 to 2.0 mg/cm^3) on the degradation efficiency was investigated under both acidic and basic conditions, at pH 3 and 10, over a period of 60 min under simulated solar irradiation. The highest removal efficiency was achieved in basic medium with catalyst loading of 2.0 mg/cm^3, when 58% of GLY was removed. The impact of hydrogen peroxide concentration was also investigated in the range of 1.0–10.0 mM at catalyst loading of 0.5 and 2.0 mg/cm^3 in both acidic and basic medium. After 60 min of irradiation in both media, the most efficient system was the one in which the hydrogen peroxide concentration was 3.0 mM. Overall, the results demonstrate that the photocatalytic degradation of GLY is strongly influenced by both of the investigated factors.

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sciforum-167665: Titanate nanotubes for the selective cleavage of lignin inspired β-O-4 linkages towards value-added aromatics under visible light

Fivos Florides [1,*], Athanasia Kotsaridou [2], Dimitrios A Giannakoudakis [1,2] and Konstantinos Triantafyllidis [3,4,5]

[1] Faculty of Chemistry, Maria Curie-Sklodowska University, 20031 Lublin, Poland
[2] Department of Chemistry, Aristotle University of Thessaloniki, University Campus, Thessaloniki, Greece
[3] Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia
[4] Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia
[5] Saudi Aramco Chair in Catalysis and Petrochemicals, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

Rising global demand for chemicals, materials, fuels, and energy demands the adoption of innovative and sustainable technologies. To this end, significant research efforts are focused on the production of value-added chemicals through the catalytic valorization of renewable feedstocks, particularly biomass waste. Moreover, harnessing solar energy to drive selective chemical conversions is regarded as a promising green technology. In this context, the development of novel nanomaterials with improved photocatalytic performance is crucial for efficient biomass valorization. Titanium oxide-based materials have been extensively reported as effective photocatalysts, although they are primarily associated with the non-selective mineralization of organic pollutants. Therefore, novel nanocatalysts are essential to achieve selective photocatalytic activity.

In this study, novel one-dimensional titanium oxides were synthesized from commercially available TiO_2 anatase particles and studied for the selective oxidative cleavage of lignin-inspired *β-O-4* linkages towards value-added aromatics. The resulting material was composed of nanotubes with external diameters 6-10 nm, inner channels between 3-7 nm, and length ranging from 90-200 nm. Furthermore, nanotubes possess a large specific surface area (S_{BET} = 154 m^2/g) and pore volume (V_{total} = 0.80 cm^3/g), significantly higher compared to the commercial precursor TiO_2 Anatase nanoparticles (S_{BET} = 10 m^2/g, V_{total} = 0.03 cm^3/g). The band gap was estimated at 3.12 eV, comparable to that of Anatase (3.2 eV).

The photocatalytic performance of both materials was evaluated either under low intensity UV-A irradiation (370 nm), or monochromatic wavelengths within the range of visible light (427, 440, 525 nm), and combinations thereof. The novel nanomaterial showed the greatest aromatic yield of benzaldehyde (Ph-CHO), enhanced by 2.4 times compared to commercial TiO_2 anatase nanoparticles under combined irradiation of the three monochromatic wavelengths. Mechanistic studies indicated the involvement of multiple reactive species in the photoreaction, with dissolved O_2 playing a pivotal role.

sciforum-162417: Viscoelastic and Thermoreversible study of Water-Based TiO_2 Sol–Gels for High Efficiency Photocatalytic Air Purification

Muhammad Ayyaz [1,*], Maria Vittoria Diamanti [1], MariaPia Pedeferri [1], Maria Jose Mateos [2] and Silvia Suarez [2]

[1] Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Via Mancinelli 7, 20131 Milan, Italy
[2] FOTOAIR-CIEMAT, Energy and Environmental Devices Unit, Energy Department, Avda. Complutense 40, Madrid, Spain

Water-based sol-gel synthesis of TiO_2 is increasingly relevant for sustainable photocatalytic materials, but its strong temperature sensitive hydrolysis-condensation behaviour often leads to poor viscosity control, unpredictable gelation, and non-uniform coatings. These rheological instabilities limit catalyst loading and reduce photocatalytic efficiency, particularly in gas-phase VOC degradation. This work investigates the viscoelastic evolution, thermoreversibility, and structural transitions of fully aqueous TTIP–acetic acid TiO_2 sols to establish processing conditions that yield uniform, high-performance coatings.

TiO_2 sols were aged at ambient temperature (Ta), thermally incubated at 50 °C (Ti), and subsequently cold stored at 4 °C (Tc). Viscosity was monitored using vibro-viscometry, while microstructural viscoelasticity was evaluated through DLS microrheology with 40 nm and 100 nm Au probes. Coatings prepared by dip-coating were examined via FE-SEM, profilometry, XRD, and UV-Vis spectroscopy. Gas-phase formaldehyde (10 ppm) degradation under UV-A irradiation (300–700 mL/min) was used to assess photocatalytic performance.

Ta sols remained weakly condensed (48–60 nm particles; ~1.8 mPa·s viscosity), producing thin, non-uniform coatings with low catalyst loading (0.016 mg/cm^2) and poor HCHO degradation (30%). Thermal incubation induced controlled condensation, optimized viscosity (~8 mPa·s), and generated subdiffusive microrheological behaviour, enabling uniform coatings with 0.106 mg/cm^2 loading and crystallite size ~7 nm. These coatings achieved 100%, 97%, and 78% HCHO degradation under UV-A irradiation at 300, 500, and 700 mL/min, respectively. Cold storage partially reversed the incubation effects, reducing viscosity, thickness, and photocatalytic activity.

Thermally modulated aqueous sol-gel processing enables precise control of TiO_2 sol viscoelasticity and thermoreversibility, allowing the formation of stable, uniform, nanocrystalline coatings with high gas-phase photocatalytic efficiency. The study establishes a rheology-guided pathway for designing sustainable, high-performance water-based TiO_2 photocatalytic materials.

sciforum-167182: Visible Light-Photocatalytic Bioorthogonal Labeling via Strain-Release Cycloaddition

Linghua Wang

School of Life Science and Technology, Xi'an Jiaotong University (Innovation Harbor Campus), Xi'an, ShaanXi Province, 710110, China

The integration of bioorthogonal click chemistry with live-cell fluorescent labeling is of paramount significance for elucidating the spatiotemporal information of biomolecules, which is fundamental to understanding core biological processes and disease pathogenesis. Photoclick chemistry has garnered considerable interest as it circumvents the limitations of metal toxicity and lack of spatiotemporal precision inherent in traditional click reactions. This project addresses the critical challenges of conventional photoclick systems, namely the phototoxicity and poor penetration of UV light, alongside the cytotoxicity of substrates activated by visible light. We conducted a comprehensive investigation, proposing novel reaction mechanisms based on tetrazole compounds and strain-promoted cycloadditions with bicyclo[1.1.0]butanes. By leveraging principles from bioorthogonal chemistry, organic synthesis, and molecular biology, we have translated the concept of spatiotemporally controlled live-cell labeling into the development of new cycloaddition reactions and the synthesis of [3.1.1]propellane scaffolds as saturated aromatic ring bioisosteres. Consequently, we have established a series of novel analytical methods for live-cell fluorescence labeling based on this advanced photoclick chemistry. This work not only opens a new avenue for studying intracellular macromolecules via chemical reactions but also significantly expands the repertoire of bioorthogonal transformations. It thereby fosters a deeper integration of chemistry and life sciences, offering promising new strategies and methodologies for applications in bioimaging and therapeutic monitoring.

Session 2. Photochemistry for Environmental Remediation

sciforum-167478: From Heterojunction Design to Real-Water Performance: Bi_2WO_6@WS_2-PVDF-HFP Sonophotocatalytic Membranes

Dominika Czekanowska [1,2,*], Hugo Salazar [3], Jorge Saiz Galindo [3], Anatolijs Šarakovskis [4], Andrei Kholkin [4,5] and Paweł Głuchowski [1,2]

[1] Division of Optical Spectroscopy, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, 50-422, Poland
[2] Graphene Energy, Ltd., Wrocław, 50-422, Poland
[3] BCMaterials, Basque Center for Materials, Applications and Nanostructures, Leioa, 48940, Spain
[4] Institute of Solid State Physics, University of Latvia, Riga, LV-1063, Latvia
[5] Department of Physics & CICECO–Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-193, Portugal

The persistence of pharmaceutical contaminants in aquatic environments, coupled with their inefficient removal by conventional treatment technologies, poses escalating risks to ecosystems and public health. Herein, we report the development of a hybrid Bi_2WO_6@WS_2-PVDF-HFP composite membrane as an efficient and reusable platform for the sonophotocatalytic degradation of the antibiotic trimethoprim (TMP). The membrane integrates a type-II Bi_2WO_6@WS_2 heterojunction within a piezoelectric PVDF-HFP matrix, enabling synergistic coupling between photocatalytic and sonocatalytic processes.

Comprehensive structural, optical, and electrochemical characterizations confirm strong interfacial coupling, broadened visible-light absorption, enhanced charge separation, and reduced recombination. Under combined light irradiation and ultrasound, the hybrid membrane achieves complete TMP degradation, outperforming membranes containing individual components. Kinetic analyses indicate predominantly pseudo-second-order behavior, while adsorption isotherms suggest favorable, mainly monolayer-type interactions between TMP and the catalytic surface.

Importantly, the membrane maintains high degradation efficiency in complex matrices, including surface water and groundwater, demonstrating robustness beyond model solutions. Reusability tests show 100% degradation efficiency over three consecutive cycles, highlighting excellent structural and functional stability. Liquid chromatography–mass spectrometry analyses indicate that hybrid sonophotocatalysis promotes extensive degradation of trimethoprim, preventing the accumulation of persistent and toxic transformation products.

Overall, this work demonstrates a scalable and environmentally friendly membrane-based strategy that combines photoactivity, piezoelectricity, and material stability, offering a promising solution for the remediation of emerging pharmaceutical contaminants in real water systems.

sciforum-167203: Advances in Excited-State Dynamics: Bridging Small Molecules and Large Systems

Raul Losantos

Chemistry Department, Chemistry Research Institute of University of La Rioja (IQUR), University of La Rioja, Logroño, Madre de Dios, 53. 26006, Spain

Non-adiabatic dynamics govern processes in which the Born–Oppenheimer approximation fails, allowing for strong coupling between electronic and nuclear degrees of freedom. These effects are crucial in photochemistry, where electronic transitions occur on ultrafast timescales. Near conical intersections, the interplay between potential energy surfaces enables efficient radiationless decay and determines reaction pathways, influencing molecular stability and quantum yields.

Recent advances in mixed quantum-classical and fully quantum approaches, such as surface hopping and multi-configurational time-dependent methods, have improved simulations of these phenomena. Non-adiabatic effects are key to understanding photoinduced dynamics in biological chromophores, photovoltaic materials, and catalytic systems, where they impact energy dissipation and functional efficiency. However, as molecular size increases, computational costs become prohibitive, requiring approximations to make such studies feasible.

Surface hopping dynamics emerged as a practical solution, often combining time-dependent methods for systems in which CASSCF and non-adiabatic coupling calculations are expensive. Recently, we introduced the NORA approach, which performs surface hopping dynamics within a molecular mechanics framework. NORA relies on excited- and ground-state parametrization based on quantum mechanical potential energy surfaces, thereby creating accurate force fields that reproduce photostationary states and other photochemical properties. Initially presented as a proof of concept, we aim to expand this methodology through alternative parametrizations and, importantly, to incorporate non-adiabatic coupling terms to achieve truly non-adiabatic dynamics at a classical level.

This contribution reviews the progression from high-cost CASSCF non-adiabatic molecular dynamics to more affordable methods under development. Examples include CASSCF NAMD on mycosporine-like amino acids and ongoing studies using TD-DFT-based surface hopping, where energetic gaps are used to approximate hopping events in regions that TD-DFT cannot fully describe. Finally, I present NORA as an entry point for excited-state dynamics in biological systems using classical molecular mechanics

sciforum-162426: Comparative photocatalytic performance of asphaltene-tuned photocatalyst and Pd/g-C_3N_4 for degradation of 2,5-dichlorophenol

Ammar Haider * and Grzegorz Boczkaj

Department of Sanitary Engineering, Faculty of Civil and Environmental Engineering, Gdańsk University of Technology, Gdańsk, Poland

The efficient degradation of halogenated organic compounds is a major challenge in advanced water treatment processes. This study reports the synthesis and evaluation of an asphaltene-tuned photocatalyst under two different photochemical reactors for degradation of 2,5-dichlorphenol, which is not only persistent and toxic but also declared as a pollutant of priority concern. Based on photocatalytic efficiency, graphitic carbon nitride was selected as a support material for immobilization of asphaltenes and for optimization of degradation parameters. Palladium-loaded graphitic carbon nitride (Pd/g-C_3N_4) nanocomposites were also synthesized. Photocatalytic performance of both synthesized photocatalytic materials was evaluated in two different photoreactor systems, i.e., an UV photoreactor and Xe-lamp photoreactor. Asphaltenes-tuned g-C_3N_4 exhibited significant photocatalytic activity under both irradiation sources which revealed the potential of asphaltenes as a promising and effective component of photocatalysts and highlighted the potential of transforming problematic petroleum fractions into functional materials that can be used for sustainable water treatment. The synergistic interactions between Pd nanoparticles with g-C_3N_4 matrix and effective generation of reactive species under irradiation accounts for a higher degradation rate for Pd/ g-C_3N_4 in both photoreactor systems. The comparative analysis revealed the role of loading metal on degradation kinetics. Overall, this study revealed that asphaltenes-tuned graphitic carbon nitride and palladium-loaded graphitic carbon nitride are efficient and promising photocatalysts for effective degradation and dehalogenation of halogenated phenols in diverse irradiation environments.

sciforum-167707: Design and Synthesis of Next Generation of UV Filters with Enhanced Efficacy, Safety and Antioxidant Properties

Leonardo López-Cóndor *, Víctor Pozo-Gavara, Raúl Losantos and Diego Sampedro

Department of Chemistry, University of La Rioja, Logroño, 26007, Spain

Solar radiation contains ultraviolet (UV) radiation (100 - 400 nm) and is classified into UVC, UVB and UVA regions. While UVC radiation is blocked by the ozone layer, UVA and UVB reach the Earth's surface. Although this radiation is essential for life, it is also responsible for acute and chronic skin damage, including erythema, permanent pigmentation, and skin cancer. Skin cancer is currently one of the most prevalent cancers worldwide, with its incidence steadily increasing over recent decades as a consequence of excessive and prolonged exposure to solar radiation. According to the American Cancer Society, more than three million new cases are diagnosed each year.

Sunscreens remain the most effective strategy to mitigate the risks associated with solar exposure; however, many commercially available UV filters have not evolved sufficiently to meet current safety, efficacy, and environmental standards. Moreover, several widely used UV filters raise concerns regarding photostability, photoreactivity, potential toxicity, and environmental persistence. To address these limitations, there is an urgent need for the development of next-generation of UV filters that combine strong UV absorption with robust photoprotection mechanisms and improved safety profiles. Ideal UV filters should exhibit high chemical and thermal stability, efficient and non-reactive energy dissipation pathways, low phototoxicity, and biodegradability.

Inspired by naturally occurring molecules, our research group has rationally designed a new family of photoprotective compounds featuring enhanced photoprotective performance. Their efficacy has been evaluated through detailed studies of UV absorption, photostability, antioxidant capacity and toxicity. The results demonstrate improved stability, enhanced photoprotection, and increased safety, highlighting the potential of these compounds as a new generation of UV filters.

sciforum-167790: Detection of Microplastics Using Fluorescent Probes

Dóra Hessz *, Gergő Kovács, Ádám Mező and Miklós Kubinyi

Department of Physical Chemistry and Materials Science, Budapest University of Technology and Economics, Budapest, Hungary

Nowadays, environmental pollution represents a global-scale problem. During the environmental degradation of plastic waste, micro- and nanosized plastic particles are formed, which pose potential health risks; at the same time, their detection and characterization constitute a significant analytical challenge.

Currently, the detection of microplastics is carried out primarily using microscopic techniques. The most commonly applied fluorescent dye, Nile Red [1], does not bind, or binds only under more intensive staining conditions, to several frequently occurring plastic types (such as PVC, PA, and PET), which makes the development of new, more efficient fluorescent labeling agents necessary.

In the present study, various solvatochromic dyes have been tested as tools for the quantification and visualization of microscopic plastic fragments. Since different plastic types possess distinct dielectric constants, these dyes may be suitable for the qualitative characterization of microplastics by exhibiting plastic-type-dependent changes in their fluorescence emission. The applicability of DANS (4-dimethylamino-4′-nitrostilbene) has already been demonstrated in the literature [2]; in our own research, we developed this approach further. Due to the apolar nature of many plastics, their dielectric constant values are relatively close to one another, resulting in significant overlap in the fluorescence emission spectra for certain plastic types (such as PE and PP). However, even in such cases, the fluorescence decay times may be significantly different, which can be exploited as a secondary selectivity parameter for qualitative discrimination. The measurement method was also extended to additional solvatochromic fluorescent probes.

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sciforum-124345: Enhanced Visible-Light-Driven Photocatalytic Degradation of Organic Pollutants by a Novel MgO/g-C_3N_4/Bi_2O_3 Ternary Nanocomposite

Pandurangan Vijayalakshmi

Centre for Global Health Research, Saveetha Institute of Medical and Technical Sciences, Chennai, Tamil Nadu, India

In the present investigation, a novel ternary nanocomposite, MgO/g-C_3N_4/Bi_2O_3, was successfully fabricated via a wet impregnation technique. The photocatalytic efficacy of this hybrid system was thoroughly assessed for the degradation of various organic pollutants, namely the antibiotic amoxicillin (AMX), the pesticide chlorpyrifos (CPF), and the dye methylene blue (MB), under visible light irradiation in an aqueous medium. Extensive physicochemical characterizations were performed employing XRD, SEM, TEM, EDS, XPS, UV-DRS, PL, BET, and EIS analyses. XRD patterns confirmed the coexistence of crystalline phases corresponding to hexagonal g-C_3N_4, monoclinic Bi_2O_3, and cubic MgO, with their respective characteristic planes distinctly discernible in the composite. Morphological investigations using SEM and TEM illustrated a hybrid structure composed of nanosheets interspersed with nanorods. Optical studies revealed enhanced visible light harvesting and a reduced bandgap energy of 2.3 eV, promoting efficient photoexcitation. Under optimized conditions - 10 ppm pollutant concentration, pH 6, 100 mg catalyst dosage, and 90 minutes of visible light illumination - the nanocomposite achieved remarkable degradation efficiencies of 96.2% (MB), 74.2% (CPF), and 62.7% (AMX), substantially surpassing the performances of its individual components (g-C_3N_4, Bi_2O_3, and MgO). Radical quenching experiments identified photoinduced holes (h^+) and superoxide radicals ($O_2^{\cdot -}$) as the primary reactive species orchestrating the degradation pathways. Importantly, the photocatalyst exhibited excellent structural robustness and maintained high photocatalytic activity over three consecutive cycles, demonstrating superior reusability and stability. These findings establish the MgO/g-C_3N_4/Bi_2O_3 nanocomposite as a highly efficient, visible-light-responsive photocatalyst for the sustainable remediation of organic contaminants in aquatic systems.

sciforum-162076: First highly efficient degradation and dechlorination of herbicides by photocatalytic hydrogenation: Advanced reduction processes (ARP) approach

Bakhtiar Ali Samejo * and Grzegorz Boczkaj

[1] Department of Sanitary Engineering, Faculty of Civil and Environmental Engineering, Gdansk University of Technology, Gdansk, G. Narutowicza St. 11/12, 80-223, Poland
[2] School of Civil, Environmental, and Architectural Engineering, College of Engineering, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Republic of Korea

The widespread use of phenylurea herbicides (PUHs) such as chlorotoluron (CHL) has caused important environmental and human health concerns due to their persistence, bioaccumulation and resistance to conventional wastewater treatments. Until now, the degradation and transformation of PUHs have been the subject of numerous research. Adsorption, microbial degradation, chemical oxidation, biodegradation, and radical-based advanced oxidation processes (AOPs) have all been shown to be effective in the removal of PUHs. These methods do have some serious disadvantages, though, including poor kinetics, the production of hazardous byproducts, and high costs of treatment. On the other hand, ARPs could be an effective alternate to degrade impurities and yield non-harmful byproducts unlike AOPs and other approaches.

In this paper, we have studied the degradation of a phenylurea herbicide (CHL) contaminant in an aqueous environment by the first highly effective process based on UV based sulfite (S), palladium on activated carbon (Pd-C), and hydrogen gas (H_2) (UV/S/Pd-C/H_2) using an ARP approach. The developed process provides CHL's complete reduction within 1 hour of treatment along with >90% dechlorination at ambient temperature. Also, we observed excellent resistance of the reaction system to the presence of inorganic anions, and the system performed well across a wide pH range.

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sciforum-162425: Investigating the Photooxidation of $CHBr_3$: Matrix-Isolation, Gas-Phase, and DFT Study

Michelle Tatiana Custodio Castro * and Rosana Mariel Romano

Department of Chemistry, Faculty of Exact Sciences, Center for Inorganic Chemistry "Dr. Pedro J. Aymonino" (CEQUINOR), National University of La Plata (UNLP), CCT-CONICET La Plata, associated with CIC-PBA, La Plata, B1900, Argentina

Bromoform ($CHBr_3$) is a very short-lived substance (VSLS) present in the troposphere, originating mainly from natural sources (e.g., phytoplankton and macroalgae)[1]. It contributes to the formation of reactive bromine species that participate in ozone depleting and other atmospheric reactions[2]. The aim of this work is to investigate the evolution of $CHBr_3$ in the presence of O_2 under UV-vis irradiation and to elucidate the mechanism involved in the photoreaction.

Different $CHBr_3$:O_2:Ar mixtures (1:1:400 and 1:20:400) were prepared on a vacuum line using standard manometric techniques. The mixtures were deposited on a CsI window cooled at 10 K using a pulse-deposition technique. A Xe(Hg) arc lamp was operated at 800 W. To reproduce atmospheric conditions, selected spectral intervals were used: $400 \leq \lambda \leq 800$ nm for visible radiation; $350 \leq \lambda \leq 450$ nm and $280 \leq \lambda \leq 320$ nm, corresponding to portions of the UV-A and UV-B regions, respectively; and $200 \leq \lambda \leq 800$ nm to include UV-C, UV-B, UV-A, and visible radiation. Complementarily, we investigated the reaction mechanism between $CHBr_3$ and O_2 in the gas phase using a home-built cell that allows simultaneous irradiation and FTIR acquisition.

The initial spectra of the matrix-isolated samples showed only the bands of $CHBr_3$. After irradiation with broadband UV-vis light and using the $350 \leq \lambda \leq 450$ nm filter, new bands appeared in the absorption region of CO, HBr, and CO_2. These bands exhibited the same growth kinetics and increased their intensity after annealing. CO, HBr, and CO_2 were detected as photoproducts in gas phase experiments.

The structures of the possible intermolecular complexes formed among the photoproducts were theoretically simulated using the B3LYP-D3/6-311++G(d,p) approximation. At the molecular level, we detected, via FTIR-matrix isolation techniques, new complexes involving CO, HBr, and Br_2, in agreement with theoretical calculations.

(1) Villamayor et al. *Nat. Clim. Chang.* 13 (**2023**) 554–560.

(2) Tinel et al. *Elem. Sci. Anthr.* 11:1 (**2023**) 00032.

sciforum-162389: Investigation of bimetallic Pt-Co and Pt-Ni catalysts in the photoreduction of nitrate

Anca Vasile *, Florica Papa, Veronica Bratan, Crina Anastasescu, Irina Atkinson and Ioan Balint

"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 Spl. Independentei, 060021 Bucharest, Romania

Photocatalytic nitrate (NO_3^-) reduction represents a novel and transformative technology that has the potential to produce harmless gaseous byproducts. The photocatalytic denitrification process is frequently accompanied by the creation of undesirable nitrite (NO_2^-) or ammonium (NH_4^+), resulting in poor selectivity for dinitrogen (N_2). The catalytic reduction of NO_3^- ions utilizing bimetallic catalysts necessitates the presence of a noble metal, alongside a promoting transition metal. The transition metal facilitates the reduction of NO_3^- to NO_2^- ions through a redox mechanism, which subsequently results in its oxidation. Furthermore, the noble metal's function is to maintain the transition metal in its lower oxidation states via hydrogen spillover. Among oxide photocatalysts, titanium dioxide (TiO_2) has found significant application in photocatalysis and the cleanup of environmental contaminants.

In this report, we present the deposition of platinum (Pt), cobalt (Co), and nickel (Ni) onto the surface of TiO_2 powder through a successive impregnation method. The influence of non-noble metal incorporation over Pt-TiO_2 catalyst was studied by means of powder X-ray diffraction (XRD), diffuse reflectance UV-Vis, and temperature programmed reduction in hydrogen (H_2-TPR) analyses and photoluminescence spectroscopy (PL). The initial activity evaluation focused on the catalytic reduction of NO_3^- with H_2. The following stage involved the evaluation of the photocatalytic activity of the catalysts by monitoring the reduction of NO_3^- under the illumination of a UV lamp. A primary goal is to assess these materials for their optimal selectivity in generating benign end products (such as N_2). In the tests conducted under UV light irradiation, the selectivity toward N_2 was around 68%, which is approximately 1.5 times greater than the values obtained during denitrification without light exposure. A preliminary test for water splitting using the Pt-Ni/TiO_2 sample yielded hydrogen. It is hypothesized that hydrogen is generated, yet it is utilized in the process of nitrate photoreduction.

sciforum-161158: Investigation of the Photocatalytic Degradation Efficiency of Methylene Blue Using TiO_2:Sm^{3+} Luminescent Nanoparticles

Badis Kahouadji [1,*], Lamine Mebarki [2], Federico Locardi [3], Stefano Alberti [3] and Benchikh Abdelkader [4]

[1] Department of Technology (El Kseur Campus),), Laboratory Electrochesitry,Corrosion and Energy Valorization (LECVE), University of Bejaia, Bejaia, 06000, Algeria
[2] Exact science faculty, Laboratory of Physical-chemistry, University of Bejaia, Bejaia, 06000, Algeria
[3] Department of Chemistry and Industrial Chemistry, Nanostructures for Energy and Environment Lab, University of Genova, Genoa, Italy
[4] Department of Technology (El Kseur Campus), Laboratory Electrochesitry,Corrosion and Energy Valorization (LECVE), University of Bejaia, Bejaia, 06000, Algeria

The extensive use of synthetic dyes in industrial sectors such as textile, leather, and paper manufacturing generates large volumes of colored wastewater, posing serious risks to human health and the environment. Semiconductor photocatalysis has emerged as an efficient and environmentally friendly strategy for the degradation of organic pollutants in water. Among semiconductor materials, TiO_2 nanoparticles have attracted considerable attention due to their chemical stability, low cost, and non-toxicity; however, their photocatalytic efficiency is often limited by rapid electron–hole recombination and limited light absorption. Rare-earth ion doping has been proposed to overcome these limitations.

In this study, pure TiO_2 and Sm^{3+}-doped TiO_2 nanoparticles were successfully synthesized via a sol–gel method. The structural, morphological, textural, optical, and photoluminescent properties of the nanoparticles were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), Brunauer–Emmett–Teller (BET) surface area analysis, UV–Vis absorption spectroscopy, and photoluminescence (PL) spectroscopy. Photocatalytic activity was evaluated by the degradation of methylene blue (MB) in aqueous solution under UV irradiation. Experiments were conducted using 50 mL of MB solution with an initial concentration of 20 $mg{\cdot}L^{-1}$, while photolysis tests confirmed that no degradation occurred in the absence of a photocatalyst.

The results indicate that Sm^{3+} doping significantly enhances the photocatalytic activity of TiO_2 nanoparticles. After 90 min of irradiation, pure TiO_2 achieved a degradation efficiency of approximately 20%, corresponding to an apparent quantum yield (AQY) of **0.7%**, whereas Sm^{3+}-doped TiO_2 nanoparticles reached about 80% degradation, with an AQY of **2.8%** under identical conditions. The enhanced photocatalytic performance is attributed to improved light absorption and reduced electron–hole recombination induced by Sm^{3+} incorporation. These findings demonstrate that Sm^{3+}-doped TiO_2 nanoparticles are promising photocatalysts for efficient wastewater treatment applications.

sciforum-166628: Low-Dimensional Structures and Composite Materials for Environmental Remediation

Pawel Gluchowski [1,2,*], Dominika Czekanowska [1,2], Daniela Kujawa [1,2], Hugo Salazar [3], Anna Grzegórska [4], Anna Zielinska-Jurek [4], Ermelinda Falletta [5], Melissa Galloni [5], Vincenzo Fabbrizio [5], Qianqian Chen [6], Carsten Blawert [6] and Maria Serdechnova [6]

[1] Department of Optical Spectroscopy, Institute of Low Temperature and Structural Research, Polish Academy of Sciences, Okólna 2, Wrocław, 50-422, Poland
[2] Graphene Energy Ltd, Okólna 2, Wrocław, 50-422, Wroclaw, Poland
[3] BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, Leioa, 48940, Spain
[4] Department of Process Engineering and Chemical Technology, Faculty of Chemistry, Gdańsk University of Technology, G. Narutowicza 11/12, Gdańsk, 80-233, Poland
[5] Department of Chemistry, Università degli Studi di Milano, via C. Golgi 19, Milan, 20133, Italy
[6] Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck Strasse 1, Geesthacht, 21502, Germany

Low-dimensional structures, including one-dimensional (1D) carbon dots and two-dimensional (2D) materials, are intensively studied as catalysts for environmental remediation due to their excellent optical and electronic properties and highly developed surface areas. Carbon dots with sizes below 10 nm are characterized by photostability, low toxicity, tunable emission, and easy surface functionalization, enabling effective pollutant degradation and water purification. Meanwhile, 2D materials, such as graphene and transition metal dichalcogenides, offer a high surface area and tunable energy gaps, which promote improved adsorption, photocatalysis, and charge separation, thereby contributing to the elimination of pollutants such as dyes, drugs, and pesticides.

This presentation discusses our recent results on the synthesis of low-dimensional materials and their composites, including coatings, membranes, and hybrid photo and sonocatalysts. In photocatalytic systems, carbon dots (1D) structures are used to enhance light harvesting, charge separation, and overall energy conversion efficiency. In piezoelectric 2D materials such as Bi_2WO_6, WO_3 or MoS_2, mechanical deformation induces an internal electric field that promotes charge separation and reduces recombination, improving catalytic performance. 2D materials are also effective in sonocatalysis, where ultrasonic waves generate cavitation, producing localized high-energy conditions that activate catalyst surfaces, enhance mass transfer, and generate reactive species. Coupling light with ultrasound in sono-photocatalysis provides synergistic effects, enabling efficient pollutant degradation and water purification. The combination of photo and sonocatalysts yields synergistic effects, improving remediation efficiency, selectivity, and stability under real-world conditions. Addressing challenges related to synthesis, performance optimization, and scalability, the presentation provides insights into the use of 1D and 2D composites in sustainable environmental technologies, paving the way for practical applications in wastewater treatment.

Acknowledgements

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sciforum-162659: Removal of ethidium bromide from aqueous waste using advanced oxidation processes via heterogeneous photocatalysis

Raúl Mendoza-Ruiz [1,*], Gabriela Rivadeneyra-Romero [2], Rocio Guadalupe Franco-Fabian [3], Adolfo Amador-Mendoza [4] and Nelda Xanath Martínez-Galero [1]

[1] Organic Synthesis Laboratory, Scientific Research Center, Applied Chemistry Institute, Universidad del Papaloapan, Tuxtepec, 68301, México
[2] Studies of Energy Institute, Universidad del Istmo, Tehuantepec, 70760, México
[3] Preventive Health, School of Medicine, Universidad del Papaloapan, Tuxtepec, 68301, México
[4] Agroengineering Institute, Universidad del Papaloapan, Loma Bonita, 68400, México

Ethidium bromide (EB) is a compound used as an intercalating agent in molecular biology for the visualization of nucleic acids in agarose gels. Its high mutagenic and carcinogenic properties, along with its potential for bioaccumulation, raise concerns regarding its release into aqueous effluents from research, diagnostic, and teaching laboratories. In this context, advanced oxidation processes (AOPs), particularly heterogeneous photocatalysis, are presented as an alternative for the complete degradation or mineralization of recalcitrant organic contaminants. In these processes, a radiation-activated semiconductor generates highly reactive radicals (•OH, $•O_2^-$, h^+) capable of breaking aromatic bonds and removing contaminants that escape conventional treatments. The objective of this protocol is to propose an experimental methodology for the removal of EB from laboratory wastewater using heterogeneous photocatalysis and to optimize operating parameters.

Based on the preliminary results obtained, the use of advanced oxidation processes, specifically heterogeneous photocatalysis with TiO_2, is a viable method for removing ethidium bromide (EB) from laboratory wastewater. It is expected that, under optimized conditions (pH, catalyst dosage, irradiation, aeration), removal rates greater than 80% can be achieved within reasonable operating times, with kinetic constants on the scale of 10^{-3} min^{-1}. Furthermore, it is essential to consider minimizing byproducts, evaluating mineralization (TOC/COD), and transitioning to continuous or scalable systems. In this regard, the findings support the integration of this technology into biotechnological effluent treatment flows, promoting environmentally responsible management and reducing the risk associated with EB release into aquatic environments.

Keywords: Advanced oxidation processes; ethidium bromide; heterogeneous photocatalysis; contaminant degradation

sciforum-161554: Shining Light on Ciprofloxacin Removal: How Reaction Conditions Shape Photodegradation Efficiency

Nina Finčur *, Dušica Jovanović, Daniela Šojić Merkulov, Vesna Despotović and Sabolč Bognar

Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Novi Sad, Serbia

The growing production and extensive use of pharmaceuticals have resulted in their frequent detection in various environmental compartments. Ciprofloxacin (CIP), a fluoroquinolone antibiotic used for treating respiratory, urinary tract, and gastrointestinal infections, is increasingly present in aquatic environment due to its intensive medical application and incomplete removal in conventional treatment systems. In response to the tightening of environmental regulations aimed at reducing pollutant emissions, the development of efficient and sustainable methods for eliminating pharmaceutical contaminants has become a priority. Among promising approaches, advanced oxidation processes stand out for their ability to generate highly reactive radicals under relatively mild operating conditions, enabling effective degradation of persistent pollutants.

In this study, the photodegradation of CIP was investigated under simulated sunlight using heterogeneous photocatalysis. Degradation kinetics was monitored with particular attention devoted to several operational parameters: catalyst type (ZnO and TiO_2), catalyst loading (0.5–5.0 mg/mL), initial CIP concentration (0.025–0.125 mmol/L), and photoreactor design. Complete removal of CIP was achieved within 60 min using both photocatalysts. The results indicate that increasing catalyst loading slightly decreases removal efficiency within the tested range, with the highest performance obtained at 0.5 mg/mL. Similarly, increasing initial CIP concentration led to a moderate reduction in degradation efficiency, with the most effective removal observed at 0.025 mmol/L. The higher photocatalytic performance observed with the xenon lamp reactor was attributed to its UVA light intensity, which was 26.1 times greater than that of the reactor with the halogen lamp. Finally, the reusability of ZnO was assessed over three successive cycles under identical conditions. A gradual decline in efficiency was observed, likely due to the adsorption of degradation products blocking active sites on the photocatalyst surface.

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sciforum-162366: Sustainable photolytic and photocatalytic removal of antibiotic and antipsychotic from the aquatic medium in the presence of H_2O_2, $KBrO_3$, and $(NH_4)_2S_2O_8$

Dušica Jovanović *, Daniela Šojić Merkulov, Vesna Despotović, Sabolč Bognar and Nina Finčur

Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad Faculty of Sciences, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

The continuous growth of the population calls for the production and consumption of pharmaceuticals in large quantities. However, these compounds do not disappear after excretion. Instead, they enter the aquatic environment through wastewater from households, hospitals and pharmaceutical industries, as well as from agriculture and livestock. For instance, antibiotics can foster the development of antibiotic-resistant bacteria, while antipsychotics can interfere with the brain chemistry of non-target organisms.

Advanced oxidation processes, such as photolysis and photocatalysis, are defined as eco-friendly processes based on the formation of reactive species that participate in the degradation/removal of various (in)organic pollutants present in (waste)waters.

Therefore, the efficiency of indirect photolysis and heterogeneous photocatalysis in removing one antibiotic (ciprofloxacin, CIP) and one antipsychotic (sulpiride, SUL) from an aquatic medium, in the presence of H_2O_2, $KBrO_3$, and $(NH_4)_2S_2O_8$, was investigated. Moreover, the influence of selected photosensitizers on CIP and SUL removal was examined under ultraviolet (UV) and simulated solar irradiation (SSI). Lastly, the effect of three initial molar H_2O_2 concentrations on SUL removal efficiency was explored under SSI.

Regarding indirect photolysis, after 60 min of irradiation, the $(NH_4)_2S_2O_8$/UV system removed 97.8%, while the $(NH_4)_2S_2O_8$/SSI system removed 97.3% of CIP. Furthermore, complete SUL removal was reached with the $(NH_4)_2S_2O_8$/UV, $(NH_4)_2S_2O_8$/SSI, and H_2O_2/SSI systems. Additionally, the highest SUL removal efficiency was observed with 3.0 mmol/dm^3 of H_2O_2.

Finally, the results of the heterogeneous photocatalysis, conducted under 60 min of SSI using ZnO as a photocatalyst, revealed no significant difference in CIP and SUL removal in the case of all three studied electron acceptors.

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sciforum-162362: Tailored Co- and Sn-Doped $YMnO_3$ Perovskites for Sustainable Removal of 17α-Ethinylestradiol

Szabolcs Bognár [1,*], Paula Sfirloaga [2], Predrag Putnik [3], Vesna Despotović [1], Nina Finčur [1], Dušica Jovanović [1] and Daniela Šojić Merkulov [1]

[1] Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad Faculty of Sciences, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[2] National Institute of Research and Development for Electrochemistry and Condensed Matter, Dr. A. Paunescu Podeanu Street, No. 144, 300569 Timisoara, Romania
[3] Department of Food Technology, University North, Trg dr. Žarka Dolinara 1, 48000 Koprivnica, Croatia

The widespread occurrence of organic pollutants in water has prompted research into advanced purification strategies. 17α-ethinylestradiol (EE2), a synthetic estrogen widely used in contraceptives and hormone therapies, poses serious health risks, including prostate cancer and reduced sperm production. Heterogeneous photocatalysis, an advanced oxidation process, offers an efficient and sustainable solution for removing such contaminants.

The aim of this study was to investigate new (un)doped perovskite materials ($YMnO_3$, Sn-doped $YMnO_3$, and Co-doped $YMnO_3$) in the photocatalytic degradation of EE2, under different experimental conditions (catalyst type, initial pH) using simulated solar irradiation (SSI), as well as a reusability test.

The obtained results showed that the highest photocatalytic efficiency was achieved in the presence of the Co-doped $YMnO_3$, where 70% of EE2 was successfully removed after 120 min of SSI. The higher activity of the doped material compared to the pristine $YMnO_3$ was explained by the sponge-like morphology and the higher surface area. Since the highest removal efficiency was recognized for Co-doped $YMnO_3$, the experiments regarding the influence of initial pH on the photocatalytic activity were carried out in the presence of this newly prepared material. The obtained findings demonstrate that the highest removal efficiency was achieved without modifying the initial pH value of ~9. This behavior was explained by the favorable electrostatic interactions between YMO-Co and EE2. Moreover, photocatalyst reusability was assessed over three consecutive cycles in the presence of Co-doped $YMnO_3$, under SSI conditions, at pH 9 in ultrapure water. Only a slight decrease in photocatalytic efficiency (≤5%) was observed, indicating that the catalyst retained high activity even after three successive runs.

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sciforum-162650: Treatment of effluents contaminated by synthetic dyes using heterogeneous photocatalysis

Nelda Xanath Martínez-Galero [1,*], Miguel Angel García-Muñoz [1], Raúl Mendoza-Ruiz [1], Gabriela Rivadeneyra-Romero [2], Adolfo Amador-Mendoza [3] and Rocio Guadalupe Franco-Fabian [4]

[1] Organic Synthesis Laboratory, Scientific Research Center, Applied Chemistry Institute, Universidad del Papaloapan, Tuxtepec, 68301, México
[2] Studies of Energy Institute, Universidad del Istmo, Tehuantepec, 70760, México
[3] Agro-Engineering Institute, Universidad del Papaloapan, Loma Bonita, 68400, México
[4] Preventive Health, School of Medicine, Universidad del Papaloapan, Tuxtepec, 68301, México

The treatment of industrial effluents represents one of the most significant challenges in contemporary environmental engineering due to the presence of persistent organic compounds, synthetic dyes, pharmaceuticals, and endocrine disruptors that are not removed by conventional methods. Therefore, advanced oxidation processes (AOPs) are effective alternatives for the complete mineralization of recalcitrant pollutants through the generation of highly reactive species capable of degrading complex molecules into carbon dioxide, water, and inorganic salts. The objective of this work is to degrade five dyes using heterogeneous photocatalysis. The AOP study was carried out using DOE 2k and UV-Vis spectroscopic monitoring (Perkin-Elmer, Spectrum 100). The five model pollutants (AM, AT, RB, RM, and VM) (Sigma-Aldrich) were degraded under controlled conditions of pH, H_2O_2, and TiO_2. The response variables included the percentage of pollutant removal (%ERD), the apparent rate constant (kapp), and the final pH.

The optimized AOP achieved degradation efficiencies exceeding 99% for various aromatic organic compounds, demonstrating the high oxidative capacity of the generated radicals. AOPs constitute a versatile and highly efficient environmental technology capable of transforming persistent organic compounds into less toxic byproducts or completely mineralizing them. Their implementation contributes to reducing the pollutant load in effluents, promoting compliance with environmental regulations, and the reuse of treated water.

Session 3. Photocatalytic Energy Conversion

sciforum-155162: Machine Learning Guided Design of Metal–Ligand Complexes for Photocatalysis

Connor Jackson

Department of Chemistry, University of York, York, YO10 5DD, United Kingdom

The efficiency of photocatalytic reactions depends critically on the ability of a catalyst to absorb photons with energies that match the activation barrier of the desired chemical process. However, identifying metal–ligand complexes that can absorb a specific photon energy (Ea) remains a major challenge due to the vast diversity of possible combinations and the nonlinear relationship between molecular structure and electronic excitation energy. In this work, we present a machine learning framework that performs inverse design of photoactive complexes—accepting a target energy input (Ea) and predicting metal–ligand combinations capable of absorbing photons with that energy to catalyze a specified transformation.

The model leverages patterns learned from computational and experimental data to identify how structural and electronic features influence photon absorption. By reversing this relationship, the algorithm can suggest promising complexes tailored to the energy requirements of a given reaction. This approach enables a rational, data-driven route to photocatalyst discovery, reducing reliance on empirical screening and expensive quantum chemical calculations. Beyond identifying suitable complexes for specific activation energies, the framework offers a foundation for designing light-responsive materials across a range of catalytic and energy-conversion processes. It represents a step toward fully automated materials discovery, where machine learning can translate energetic requirements directly into molecular design strategies.

sciforum-153169: Di-nuclear water-soluble oxovanadium (V) Schiff base complexes: Electrochemical properties, catalytic oxidation, and Photovoltaic applications.

RAHHOU Abd elaziz [1,*], HASNAOUI Ali [2], ROCHDI Nabil [3] and AIT ALI Mustapha [2]

[1] IMED-Lab, Faculty of Sciences and Techniques, Cadi Ayyad University, Bd Abdelkrim Al Khattabi, BP 549, 40000, Marrakech, Morocco
[2] Molecular Chemistry Laboratory, Faculty of Sciences Semlalia, Cadi Ayyad University, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco
[3] MED-Lab, Faculty of Sciences and Techniques, Cadi Ayyad University, Bd Abdelkrim Al Khattabi, BP 549, 40000, Marrakech, Morocco

Two dinuclear oxovanadium(V) complexes with water solubility, $[(L1H)VO(\mu\text{-}O)]_2$ (C1) and $[(L2H)VO(\mu\text{-}O)]_2$ (C2), were successfully synthesized via the reaction of $VOSO_4$ with their respective tetradentate Schiff base ligands, namely [N-(2-hydroxyethylamino)ethyl]-5-methoxysalicylaldimine (L1H) and 2-[(2-(2-hydroxyethylamino)ethylimino)methyl]phenol (L2H), under reflux in methanol. The synthetic procedure afforded the complexes in good yields and with high purity, as confirmed by spectroscopic analyses and elemental composition. These dinuclear Schiff base oxovanadium complexes were systematically evaluated for their catalytic activity in the oxidation of olefins using water as a green and environmentally benign solvent in combination with various oxidizing agents. The experimental results demonstrated high catalytic efficiency, excellent product yields, and remarkable reusability, highlighting the potential of these complexes as sustainable catalysts in aqueous media. Beyond their catalytic applications, these oxovanadium(V) complexes possess significant photophysical and electrochemical properties, including strong absorption in the visible region and tunable redox potentials. These characteristics render them promising candidates for photovoltaic applications, particularly in dye-sensitized solar cells (DSSCs) and other solar energy conversion devices, where efficient light harvesting and electron transfer are essential. The combination of water solubility, catalytic performance, and photophysical features makes these complexes versatile functional materials for both chemical and energy-related applications.

sciforum-162393: Enhanced photocatalytic hydrogen production over TiO_2–based composites modified with ferroelectric BST, MXenes, and metal co-catalyst

Sonia Díaz Moral *, Xavier Vendrell and Jarosław Serafin

[1] Department of Inorganic and Organic Chemistry, Inorganic Chemistry Section, University of Barcelona, Martí i Franquès 1-11, 08028, Barcelona, Spain
[2] Institute of Nanoscience and Nanotechnology (IN2UB), University of Barcelona, C/ Martí i Franquès, 1, 08028, Barcelona, Catalunya, Spain

The global rise in energy demand and the continuous increase in atmospheric CO_2 emissions have underscored the urgent need to develop cleaner and more sustainable energy technologies. Among the different strategies under study, photocatalytic hydrogen production is especially attractive, as it enables the conversion of solar energy into a carbon-free fuel. Titanium dioxide (TiO_2) is one of the most widely investigated photocatalysts owing to its stability, low cost, and non-toxicity. However, its practical efficiency remains limited by rapid electron–hole recombination and weak absorption in the visible region. In this work, we synthesized novel TiO_2-based composites modified with ferroelectric BST perovskites ($Ba_{1-x}Sr_xTiO_3$), conductive MXene ($Ti_3C_2T_x$), and metallic co-catalysts (Ni/Cu). The samples were using X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), UV–vis diffuse reflectance spectroscopy, photoluminescence spectroscopy (PL), and Brunauer–Emmett–Teller (BET) surface area analysis to evaluate their structural, optical, and morphological properties. Photocatalytic tests revealed a clear enhancement in hydrogen photoproduction. While pure TiO_2 generated around 0.5 mmol $h^{-1} \cdot g_{cat}^{-1}$, the best-performing TiO_2/BST/MXene/Cu composite reached values equal to ~60 mmol $\cdot h^{-1} \cdot g_{cat}^{-1}$. This improvement can be attributed to the synergistic contribution of each component. BST helps to separate charges more efficiently thanks to the internal electric field within its ferroelectric structure, which reduces the chance of electron–hole recombination. At the same time, MXenes act as highly conductive pathways, facilitating efficient electron transfer to the metal co-catalyst sites. As a result, charge recombination is suppressed, leading to a significant increase in hydrogen evolution activity. Overall, the obtained results demonstrate that combining TiO_2 with BST, MXene, and Cu metal co-catalysts is a high effective strategy for enhancing photocatalytic performance and supports the development of renewable hydrogen technologies.

sciforum-167792: Investigation of new Additive Manufacturing DED application for waste-to-hydrogen conversion

Svetlana Boshnakova

Center of Competence “Intelligent Mechatronic, Eco- and Energy-Saving Systems and Technologies”, Technical University Sofia, branch Plovdiv, 4000 Plovdiv, Bulgaria

Relatively low-cost Titanium Carbide (TiC) materials and Metal Matrix Composites (MMC) are proposed for waste-to-hydrogen conversion. Two type of steels are used as bases prepared from EN 10088 flat products, namely X2CrTi12 (1.4512, AISI 409) and X5CrNi18-10 (1.4301, AISI 304). TiC is mixed with TRIBALOY® T-800 alloy in powder form and applied via Laser Directed Energy Deposition (DED-LB) over the substrates. For the powder mixture, Fourier transform infrared spectroscopy (FT-IR) and Differential Scanning Calorimety (DSC) are performed. The raw materials are investigated for the processes that occur in them under heating. After the solidification of the molten mixture, grinding and polishing are performed to achieve a thin layer. The studies of the obtained MMC include interface zones assessment, hardness and Young's modulus distribution, microstructural analysis, and visual defect evaluation. Advanced sensors for Acoustic Emission (AE) and Electrical Contact Resistance (ECR) gave characterization together with micro-scratch testing. The use of Photoluminescence Spectroscopy is proposed for the new composite materials. The electron transfer pathway can be studied with time-resolved spectroscopy. Renewable energy production by breaking down waste into hydrogen-rich syngas can be achieved through pyrolysus, followed by steam reforming and purification. The obtained novel materials show promising application solutions with increased durability, corrosion, and wear resistance.

sciforum-167693: Light-Assisted CO_2 Conversion on Electrodeposited Cu_2O-Based Composite Layers

Krzysztof Mech [1], Patrycja Kolbusz [1,*], Andrzej Sławek [1], Mateusz Marzec [1] and Edit Csapó [2]

[1] AGH University of Krakow, Academic Centre of Materials and Technology, al. Mickiewicza 30, Krakow 30-059, Poland
[2] Interdisciplinary Excellence Center, Department of Physical Chemistry and Materials Science, University of Szeged, Rerrich B. sqr. 1, Szeged H-6720, Hungary

Light-assisted electrochemical conversion of carbon dioxide is widely investigated as a potential pathway toward sustainable energy and carbon utilization technologies. Cu_2O-based materials remain central to these studies due to their ability to facilitate complex CO_2 reduction processes. In this contribution, we focus on the relationship between electrodeposition conditions and the photoelectrocatalytic performance of copper-based composite layers during light-assisted CO_2 conversion. The composite layers were prepared by electrodeposition from alkaline electrolytes based on copper(II) lactate complexes, containing dispersed reduced graphene oxide (rGO). The layers were electrodeposited at different potentials in order to optimize their selectivity and efficiency toward ethylene formation. The electrodeposited layers were examined under dark and under illumination in CO_2-saturated aqueous electrolyte to assess the influence of synthesis parameters on their photoelectrochemical performance in the conversion of CO_2 to hydrocarbons. The analysis highlights qualitative trends linking electrodeposition conditions with changes in the photoelectrochemical performance of the obtained layers. Differences observed between materials obtained at varied deposition potentials point to the role of material composition in the modification of charge-transfer processes during light-assisted CO_2 reduction. The presence of rGO further contributes to modulation of the photoelectrochemical response, indicating its influence on interfacial charge transport under illuminated conditions. The results emphasize electrodeposition as a versatile method of synthesis of composite layers for PEC CO_2 conversion. Obtained results provide insight into how controlled adjustment of electrodeposition parameters can guide the design of materials for light-assisted electrochemical CO_2 conversion.

sciforum-165355: Synthesis and Photoelectrochemical Characterisation of Indole–Based Organic Dyes

Vanam Hariprasad [1,*], Praveen Naik [1], Prashanth Vishwa [2] and Sakthivel Kandaiah [2]

[1] Department of Chemistry, Nitte Meenakshi Institute of Technology, Yelahanka, Bengaluru 560064, Karnataka, India
[2] Department of Chemistry, REVA University, Bengaluru 560064, Karnataka, India

Two novel donor–acceptor (D–A)-type indole-based organic dyes, In-C8-BA and In-C8-TBA, were synthesized and thoroughly characterized for advanced photoactive applications. These dyes integrate indole as a robust electron-donating moiety with either barbituric acid (BA) or thiobarbituric acid (TBA) as strong electron-withdrawing acceptors, facilitating pronounced intramolecular charge transfer (ICT). Comprehensive structural validation was performed using $^{1}H/^{13}C$ NMR, FT-IR, and mass spectrometry, confirming successful molecular construction. Optical studies revealed broad and intense absorption bands in the visible region, with In-C8-TBA exhibiting a red-shifted profile due to the enhanced electron affinity of the sulfur-containing acceptor. Thermal gravimetric analysis (TGA) demonstrated high thermal stability, crucial for device integration. Cyclic voltammetry established well-aligned HOMO–LUMO energy levels suitable for both p- and n-type semiconductor interfaces, enabling versatile photosensitization capabilities. Photoelectrochemical measurements in protic electrolytes (e.g., aqueous phosphate buffer) yielded stable, reproducible photocurrents, suggesting active participation in proton-coupled electron transfer (PCET)—a key mechanism in solar fuel generation. Density functional theory (DFT) computations and molecular electrostatic potential (MESP) maps corroborated experimental data, revealing asymmetric charge distribution favoring directional ICT from indole to the acceptor. These combined attributes underscore In-C8-BA and In-C8-TBA as promising candidates for dye-sensitized solar cells, organic photodetectors, and photocatalytic systems, where efficient light harvesting and interfacial charge dynamics are paramount.

Session 4. Photodynamic and Photothermal Therapy

sciforum-162400: A photocontrollable conjugate of a natural chlorin and a chemotherapeutic agent for combined photodynamic therapy.

Vladimir Sorokin *, Petr Ostroverkhov, Ekaterina Plotnikova and Mikhail Grin

Department of Chemistry and Technology of Biologically Active Compounds, Medicinal and Organic Chemistry, Institute of Fine Chemical Technologies, MIREA – Russian Technological University, 119571 Moscow, Russia

PDT is known as a non-invasive technique for the treatment of tumors of epithelial tissues. One of the main directions in the development of PDT methods is to increase their cytotoxicity. For this purpose, a combined therapy strategy is being implemented, which consists of the simultaneous use of a photosensitizer and cytotoxic agent [1]. Doxorubicin is one of the most commonly used chemotherapeutic agents. In order to reduce its off-target toxicity and implement the principle of combination therapy, guided delivery systems need to be developed [2]. Light is a convenient external stimulus, and conjugates of therapeutic agents through photocleavable linkers have been shown to be effective for combined PDT [3].

In our work, we obtained a conjugate of the derivative of natural chlorin, anthracycline antibiotic doxorubicin and a photocleavable linker. The mechanism of photochemical destruction was studied both experimentally using light irradiation, UV-Vis spectrophotometry, and fluorescence spectroscopy, as well as computationally using density functional theory (DFT) calculations. We conducted biological tests on a human breast cancer cell line MCF-7 and tried to interpret the results obtained in vitro using in silico docking methods.

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sciforum-162405: Amphiphilic Phthalocyanines as Dual-Mode Photo- and Sonosensitizers for Antimicrobial Applications

Aleksandra Pawska [1,2,*], Marcin Wysocki [1], Jakub Szymczyk [1], Marianna Szczepaniak [1], Daniel Ziental [1], Jolanta Długaszewska [2], Emre Güzel [3] and Łukasz Sobotta [1]

[1] Department of Inorganic and Analytical Chemistry, Poznan University of Medical Sciences, Rokietnicka 3, 60-806 Poznan, Poland
[2] Department of Genetics and Pharmaceutical Microbiology, Poznan University of Medical Sciences, Rokietnicka 3, 60-806 Poznan, Poland
[3] Department of Engineering Fundamental Sciences, Faculty of Technology, Sakarya University of Applied Sciences, 54050, Sakarya, Turkey

A newly developed series of amphiphilic and cationic phthalocyanines was designed to determine how quaternization, peripheral substituents, and metal coordination govern photodynamic and sonodynamic performance. All derivatives displayed characteristic Q-band absorption between 673 and 705 nm and fluorescence quantum yields spanning Φ_f = 0.01–0.26. Quaternization markedly increased emission in Zn(II) complexes (Φ_f: 0.02 → 0.17), while reducing it in metal-free and In(III) analogues. Singlet oxygen formation was efficient across the series, with Φ_Δ = 0.63 for both InPc and QInPc and a twofold increase for ZnPc upon quaternization (Φ_Δ: 0.27 → 0.51). The unsubstituted ZnPc was used as a reference. Photodecomposition quantum yields (10^{-5}–10^{-4}) indicated that quaternization enhanced photostability for metal-free and Zn(II) derivatives, while minimally affecting the In(III) complex.

The quaternized phthalocyanines demonstrated high antimicrobial potency. In methicillin-resistant *Staphylococcus aureus* (MRSA) and ESBL-producing *Escherichia coli*, inactivation reached 4.6 logs, while Gram-negative strains showed 4.5-log reductions. Activity against fluconazole-resistant *Candida albicans* demonstrated the following: QH_2Pc, QInPc, and QZnPc achieved 3.2-log reductions.

Sonodynamic evaluation confirmed strong ROS formation. Non-quaternized sensitizers accelerated DPBF decay around 4.5-fold, with ZnPc showing the fastest kinetics (k = 0.152 min^{-1}; $t_{0.5}$ = 4.55 min). Quaternized derivatives remained sonodynamically active; QZnPc has the potential to generate ROS efficiently (k = 0.130 min^{-1}) and displayed improved ultrasound stability ($t_{0.5}$ = 59.7 min vs. 11.2 min for ZnPc).

These results establish this family of amphiphilic phthalocyanines as potent, multimodal sensitizers, capable of achieving high-log photodynamic reduction and showing potential for strong sonodynamic ROS output. Their performance, together with clear structure–property relationships, highlights their promise for next-generation antimicrobial therapy.

sciforum-162403: Comparative Evaluation of Human serum Albumin Conjugation and Micellization for the Delivery of Chlorin-based Photosensitizers

Nikolay Dmitrievich Govorov [1,*], Anastasia Sergeevna Pukhova [1], Nikita Sergeevich Kirin [1], Petr Vasilievich Ostroverkhov [1], Olga Alekseevna Bezborodova [1,2] and Mikhail Alexandrovich Grin [1]

[1] Federal State Budgetary Educational Institution of Higher Education "MIREA - Russian Technological University", Moscow, Russian Federation
[2] Moscow Hertsen Research Institute of Oncology-Branch of the National Medical Radiology Research Center, Ministry of Health of the Russian Federation, Moscow, Russian Federation

In this study, conjugation with human serum albumin (HSA) was explored as an alternative to micellar formulations for improving aqueous solubility and modulating the delivery profiles of chlorin-based photosensitizers (PSs) intended for photodynamic therapy (PDT).

A comparative analysis was performed for chlorin e6, HSA conjugates of chlorin derivatives and their unconjugated micellar formulations using *in vitro* assays on the A431 carcinoma cell line. Intracellular accumulation kinetics were quantified by flow cytometry at multiple incubation times, and photoinduced cytotoxicity was evaluated following 2 h, 4 h, and 8 h incubation in the presence and absence of a washout step.

Chlorin e6 demonstrated relatively slow intracellular uptake and correspondingly lower photoinduced cytotoxicity. In contrast, the non-conjugated PSs exhibited rapid and pronounced accumulation, accompanied by high levels of phototoxicity. HSA-conjugated PSs displayed a distinctly different uptake profile: intracellular accumulation increased gradually and continuously over time, yielding cytotoxicity values that approached those observed with unconjugated PSs at longer incubation periods. This behavior reflects the altered transport mechanisms imposed by albumin binding and suggests sustained cellular delivery rather than rapid saturation.

Micellar PS formulations showed the highest uptake rates and phototoxicity *in vitro*; however, their non-specific endocytic internalization may limit their biological selectivity *in vivo*. Although HSA conjugation resulted in comparatively slower uptake *in vitro*, albumin is an endogenous long-circulating carrier capable of passive tumor targeting and receptor-mediated cellular uptake, suggesting potential advantages for *in vivo* biodistribution, reduced systemic toxicity, and improved tumor selectivity compared to micellar systems.

These findings highlight that HSA conjugation provides a tunable delivery strategy that balances solubility enhancement and photodynamic efficacy, thereby representing a promising alternative to micellar formulations for PDT applications.

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sciforum-162218: Conjugates of photosensitizers and doxorubicin with cleavable linkers for controlled release

Daniil Durnev [1,*], Dmitry Medvedev [1,2], Petr Ostroverkhov [1], Ekaterina Plotnikova [1,3] and Mikhail Grin [1]

[1] Department of Chemistry and Technology of Biologically Active Compounds, Medicinal and Organic Chemistry, Institute of Fine Chemical Technologies, MIREA – Russian Technological University, 119571 Moscow, Russia
[2] Frumkin Institute of Physical Chemistry and Electrochemistry of Russian Academy of Sciences, 119071 Moscow, Russia
[3] National Medical Research Radiological Centre of the Ministry of Health of the Russian Federation, P.A. Hertsen Moscow Oncology Research Institute, 125284 Moscow, Russia

Introduction: Chemotherapy as a method of fighting cancer has a number of significant limitations, so the search for new drugs to increase the effectiveness of this type of therapy and reduce side effects is relevant. Another therapeutic approach is less invasive photodynamic therapy with minimal side effects, however, its spectrum of action does not go beyond the treatment of superficial tumors due to the low depth of light penetration into tissues. The objective of the work was to synthesize and study the biological activity of conjugates of derivatives of natural chlorines and doxorubicin containing thioketal (ROS-sensitive) and disulfide (GSH-sensitive) linkers designed for controlled release directly in tumor cells and the tumor microenvironment.

Methods: NMR spectra were recorded on a Bruker DPX300 spectrometer. Absorption and fluorescence spectra of photosensitizers solutions were recorded using a UV1800 spectrophotometer. Bioavailable micellar emulsions of the test compounds were analyzed and characterized using dynamic light scattering. Chromatography-mass spectrometry was carried out using a Dionex UltiMate RS 3000 ultra-high-performance liquid chromatograph with a mass spectrometry system.

Results: In this work, a number of compounds for combined photodynamic therapy were obtained. The structures of the conjugates obtained and the fragments formed during their cleavage under various conditions were analyzed using high-resolution chromatography-mass spectrometry. The destruction of labile linkers was studied with chromatograph mass spectrometric monitoring. Biological studies *in vitro* were performed on the MCF-7 human breast adenocarcinoma cell line.

Conclusions: A strategy for the synthesis of chlorin-doxorubicin conjugates containing various linker molecules was proposed and developed. Studies of photoinduced and cytotoxic activity *in vitro* on human MCF-7 cells have demonstrated the high efficiency of synthesized compounds. The results of confocal microscopy demonstrated that for conjugates with labile linkers, chlorin internalization is observed in the cytoplasm, and doxorubicin in the nucleus, which indicates the effectiveness of the chosen strategy.

sciforum-161697: Evaluation of nano-formulation of Pheophorbide-a-mediated photodynamic therapy against 3D Lung cancer cells

Kave Moloudi *, Heidi-Abrahamse and Blassan P George

Laser Research Centre, Faculty of Health Sciences, University of Johannesburg, P.O. Box 17011, Johannesburg 2028, South Africa

Pheophorbide-a (PPBa) is a potent photosensitizer (PS) with some limitations such as poor water solubility, low bioavailability, etc. [1]. As a strategy, liposomes can provide a platform in co-delivery of drugs in cancer therapy [2]. In this study, we synthesized two nanocomplexes (Lipo@AuNPs@PPBa) from PPBa and gold nanoparticles (AuNPs) for photodynamic therapy (PDT) purposes using a 660 nm laser on A549 lung cancer spheroid cells. The thin-film hydration method was used to synthesize Lipo@AuNPs@ PPBa and characterization was carried out using UV-VIS spectroscopy, FTIR, DLS, EDS, and SEM. Thereafter, the cytotoxic effects of nanocomplexes in PDT on A549 spheroid cells were evaluated by morphological changes, MTT, ATP, amd LDH assays and then the apoptotic rate was determined with immunofluorescence (IF), flow cytometry, and real-time PCR.

UV-VIS spectroscopy, FTIR, EDS, and DLS results showed successful co-loading of PPBa and AuNPs in liposomes at 6 µM and 10 µg/mL concentrations, respectively. SEM and TEM images showed the shape of Lipo@AuNPs@ PPBa was a rod-like and the size was 87 nm. Cellular response indicated that IC_{50} of Lipo@AuNPs@ PPBa was 60 µg/mL and caused significant cellular death, ATP reduction, LDH release, and spheroid shrinkage post-PDT (15 J/cm^2). Additionally, IC_{50} of Lipo@AuNPs@PPBa post-PDT caused 46.4% and 21.4% of early and late apoptotic rates, respectively. Moreover, Lipo@AuNPs@PPBa nanocomplexes induced activation of apoptotic proteins such as BAX, Cyt c, and CASP9 in A549 spheroids post-PDT. Additionally, IF and real-time PCR showed that the nanoformulation of PPBa caused up-regulation of apoptotic proteins and genes more than in its free form post-PDT. In conclusion, AuNPs demonstrated a synergistic effect on PPBa in PDT. Hence, liposomes can provide a remarkable platform for the co-delivery of PPBa and AuNPs.

sciforum-167138: Extracellular vesicles for improved intracellular accumulation of photosensitizers

Daria Prilutskaya [1,2,*], Maria Mollaeva [2], Nikita Yabbarov [2], Maria Sokol [2], Margarita Chirkina [2], Maksim Klimenko [2], Ivan Gulyaev [2], Yulia Bortnevskaya [3], Natal'ya Bragina [3], Kseniya Zhdanova [3] and Elena Nikolskaya [2]

[1] Faculty of Chemical and Pharmaceutical Technologies and Biomedical Products, D. Mendeleev University of Chemical Technology of Russia, Moscow, 125047, Russia
[2] Laboratory of Quantitative Oncology, Institute of Biochemical Physics NM Emanuel, Moscow, 119991, Russia
[3] Department of Chemistry and Technology of Biologically Active Compounds, Medicinal and Organic Chemistry, MIREA – Russian Technological University, Institute of Fine Chemical Technology, Moscow, 119454, Russia

Introduction. Photodynamic therapy (PDT) is based on the use of photosensitizers (PS) that generate cytotoxic reactive oxygen species (ROS) upon light exposure. The efficacy of PDT depends on the efficient PS intracellular accumulation and preservation of their photodynamic activity. However, the limited solubility and poor pharmacokinetics of many PS necessitate the development of efficient delivery systems. Extracellular vesicles (EVs) have been proposed as promising nanocarriers for PS delivery.

Materials and methods. EVs were isolated from human embryonic kidney (HEK293) cells using ultrafiltration. The photosensitizer 5,15-bis(3-methoxy(4-(6-pyridylhexyloxy)phenyl)-10,20-di(ethynylphenyl)porphyrinato zinc (ZnP) was loaded in EVs by sonication, followed by removal of non-encapsulated ZnP by size-exclusion chromatography. Photodynamic activity of ZnP-EVs was assessed using the MTT assay on A549 cells after irradiation with red light (660 nm). ZnP-EVs induced ROS formation in A549 (human lung adenocarcinoma) cells was evaluated by flow cytometry. ZnP release was studied in a model medium (phosphate-buffered saline supplemented with 10% fetal bovine serum, pH 7.4).

Results. After ZnP-loading, EVs recovery rate was approximately 40%. ZnP encapsulation resulted in a slight increase in EVs size and zeta potential, consistent with membrane incorporation. Both free ZnP and ZnP-loaded EVs showed no dark toxicity in A549 cells at tested concentrations. Photoactivity assay confirmed that ZnP remains functional within EVs, while flow cytometry revealed that ZnP-EVs generate ROS more efficiently than free ZnP. Analysis of ZnP release from EVs demonstrated that only 16% of ZnP was released within the first 24 h, suggesting more selective PS accumulation in target tissues.

Conclusions. The results demonstrate that EVs derived from HEK293 cells preserve the photodynamic properties of the encapsulated PS, enable controlled release under biologically relevant conditions and enhance ROS generation compared to free ZnP.

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sciforum-162359: Photodynamic Activity of Hypericin-Loaded Liposomes in Breast Cancer Cells

Alicja Makarec [1,2,*], Marta Woźniak [2] and Jerzy Gubernator [1]

[1] Department of Lipids and Liposomes, Faculty of Biotechnology, University of Wroclaw, Wroclaw, 50-383, Poland
[2] Department of Clinical and Experimental Pathology, Division of General and Experimental Pathology, Wroclaw Medical University, Wroclaw, 50-368, Poland

Introduction:

Photodynamic therapy (PDT) is based on the photochemical activation of a photosensitizer to generate reactive oxygen species (ROS) that induce cell death. Hypericin is a natural photosensitizer, but its clinical utility is restricted by poor solubility and limited intracellular accumulation. Liposomal encapsulation improves its stability, delivery, and phototoxic performance. This study evaluates cellular uptake, photocytotoxicity, and migration inhibitory effect following PDT using a liposomal hypericin formulation in breast cancer models.

Methods:

Liposomal hypericin was prepared by the thin-film hydration method. Breast cancer cell lines MCF-7 and MDA-MB-231 cells were incubated with free or liposomal hypericin, and cellular uptake was quantified by flow cytometry based on intrinsic hypericin fluorescence. PDT was performed using orange-light irradiation, followed by assessment of cell viability using the MTT assay. The effect of PDT on cancer cell migration was examined with a wound healing assay by observing scratch closure over time.

Results:

Flow cytometry showed time-dependent changes in intracellular hypericin uptake in both cell lines. Despite the lower fluorescence intensity of liposomal hypericin compared to the free compound, the liposomal formulation produced effective and reproducible light-dependent cytotoxicity with minimal dark toxicity, demonstrating high phototoxicity and low toxicity in the absence of light. PDT with liposomal hypericin also significantly reduced cancer cell migration, reflecting ROS-mediated effects.

Conclusions:

Liposomal encapsulation enhances the photochemical safety and therapeutic applicability of hypericin by enabling controlled delivery and effective PDT responses. These findings support liposomal hypericin as a promising photosensitizer with improved translational potential for photodynamic cancer therapy.

sciforum-162503: Reduced imide derivatives of natural chlorins

Viktor Pogorilyy *, Julia Sergeevna Kartava, Tanaka Tandare and Mikhail Grin

Department of Chemistry and Technology of Biologically Active Compounds, Medicinal and Organic Chemistry, Institute of Fine Chemical Technologies, MIREA-Russian Technological University, 86 Vernadsky Avenue, 119571 Moscow, Russia

Introduction. For photodynamic therapy (PDT), special attention is paid to photosensitizers (PS) based on chlorins and their derivatives, synthetic analogues of natural pigments that combine powerful photoactivity with the possibility of subtle chemical modification. The main advantages of chlorin photosensitizers are their intense absorption in the long-wavelength region of the spectrum (650-750 nm), providing deep penetration of light into biological tissues, high quantum yield of singlet oxygen generation and the ability to selectively accumulate in pathological foci. Reduced derivatives of chlorin imides are of particular interest in this context, as they have greater stability under physiological conditions.

Methods. *N*-hydroxy and *N*-methoxy derivatives of purpurinimide-18 methyl ester were selected as the starting compounds. The obtained derivatives were purified by preparative chromatography. The structures of the obtained compounds were confirmed by a complex of modern physico-chemical analysis methods: electron and fluorescence spectroscopy, mass spectrometry, ^{1}H- and ^{13}C NMR spectroscopy.

Results. In this work, strategies for the reduction of the “exocycle E” *of N* -methoxy purpurinimide-18 were developed. The resulting derivative had an absorption maximum in the long-wave region of the visible spectrum (656 nm), as well as a three-fold higher quantum yield of singlet oxygen generation compared to the original compound.

Conclusions. The resulting reduced imide derivative combines absorption in the therapeutic window (656 nm) and high photoactivity (compared to the parent compound). The reduction of carbonyl groups of exocycle E can lead to an improvement in pharmacokinetic parameters and a more effective modification of the nitrogen atom. This compound is a promising candidate for the development of new effective drugs for PDT.

The work was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation (government assignment №075-00727-25-05 dated 20/03/2025; FSFZ-2024-0013).

sciforum-162401: Visual readout-enabled systems: Merocyanine–β-Cyclodextrin complexes as photo-controlled material actuators

Andreea Neacsu [1,*], Stela Minkovska [2], Valentin Alexiev [2] and Viorel Chihaia [1]

[1] Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, 202 Splaiul Independentei, 060021, Bucharest, Romania
[2] Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bldg.11, Sofia 1113, Bulgaria

The interaction between beta-cyclodextrin (β-CD) and the merocyanine form of 4-[(2E)-1,1-dimethyl-2-({[(1Z)-2-oxo-1,2-dihydronaphthalen-1-ylidene]amino}methylidene)-1H,2H,3H-benzo[e]indol-3-yl]butane-1-sulfonic acid (MC) was investigated to elucidate host–guest complexation dynamics and stability, in order to develop applications such as photoswitches for imaging and therapy. These applications are possible due to MC's absorption changes upon isomerization; therefore, the β-CD environment can provide a consistent, water-compatible platform and potentially targetable coatings. β-CD is a cyclic oligosaccharide that is well known for its ability to form "inclusion complexes" with other molecules, changing the properties of the guest molecule upon binding. Spironaphthoxazines belong to the class of organic photochromic compounds. In this work, MC's Open Photomerocyanine form was used in the investigations and complex formation. Aqueous solutions of MC in the presence and absence of β-CD were irradiated at the corresponding wavelength, and their spectroscopic behavior was analyzed. Binding constants were calculated, and the continuous variation method (Job's plot) demonstrated that stoichiometries other than 1:1 were present. Not only were 2:1 and 3:1 complexes observed, but many other possible intermediate stoichiometries (e.g., between 1:1 and 3:1) may also be present in the solution. Dynamic light scattering measurements were used to characterize the β-CD/MC nanoparticles. The thermal behavior of the complexes was investigated using solution calorimetry. Docking studies combined with DFT calculations were done to evaluate the stability of β-CD/MC complexes with different stoichiometries. Interestingly, the 2:1 complex shows a slightly higher stability compared to the 1:1 and 3:1 complexes, aligning well with experimental findings. The results have shown that the inclusion of MC within the β-CD cavity influences the rate and direction of isomerization between different MC forms, also affecting MC solubility and stability. The interaction between MC and β-CD can be used for further applications to create controlled optical switches that respond to external stimuli like light, temperature, or pH.

Session 5. Photoluminescent Materials

sciforum-152818: Development of Sulfur- and nitrogen-doped carbon dots (S,N-CDs) dual biosensor from *Ricinus communis* (castor) seeds for the estimation of Protamine and Uric acid in biological samples

Rutu Patel and Vasanti Suvarna *

Department of Pharmaceutical Analysis, SVKM's Dr. Bhanuben Nanavati College of Pharmacy, Mumbai, Maharashtra 400056, India

Introduction: Sustainable, biocompatible fluorescent probes are increasingly needed for clinically relevant analytes. Protamine, the only clinically used antidote for heparin overdose, and uric acid, a key biomarker for metabolic, renal, and cardiovascular disorders, both require reliable quantification in biological fluids for effective clinical management.

Methods: Sulfur- and nitrogen-doped carbon dots (S,N-CDs) were synthesized via a one-step hydrothermal method using Ricinus communis (castor) seeds as a carbon source and thiourea as the nitrogen and sulfur dopant. Finely ground castor seed powder was mixed with thiourea in distilled water and heated in a sealed autoclave at 180 °C for 6 h to obtain S,N-CDs suitable for fluorescence-based sensing.

Results: The S,N-CDs showed uniform spherical morphology (2–8 nm), green emission (λ_em = 520 nm), and good stability toward pH variation, ionic strength, and photobleaching. Surface functional groups enabled a fluorescence turn-off response to both targets. Protamine was quantified over 3.2–7.2 µM (limit of detection 0.45 µM), with recoveries of 98.9–103.1% in spiked human serum. Uric acid was detected over 50–124.8 µM (limit of detection 16.7 µM), with recoveries of 94.9–101.8% in serum and 92.6–95.3% in urine. These results indicate that the probe can operate in complex biological matrices using a simple, low-cost fluorescence readout.

Conclusion: Castor seed–derived S,N-CDs function as an application-focused fluorescent probe for dual detection of protamine and uric acid in biological fluids. The study demonstrates a sustainable synthesis route and links the surface functionality of the CDs to their fluorescence response, supporting their utility for applied biosensing rather than mechanistic photophysical advancement.

sciforum-162334: White-Emitting Dy^{3+}/Eu^{3+} Co-Doped Fluorapatite Nanoparticles for Multispectral Biomedical Applications

Dušan V. Milojkov

Sector for Metallurgical Technology and Environmental Protection, Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, 11000, Serbia

Engineering luminescent nanomaterials capable of emitting stable multispectral visible light remains a key challenge in the development of advanced bioimaging technologies. While white-light emission from rare-earth co-doped phosphors has been widely explored, most existing systems rely on multi-component architectures, high-temperature synthesis routes, or host matrices with limited biocompatibility, restricting their applicability in biomedical environments. Achieving multispectral emission within a single, biocompatible, and structurally stable host therefore remains an open challenge.

In this work, a simple and low-energy room-temperature co-precipitation route (≈25 °C) is reported for the synthesis of spherical Dy^{3+}/Eu^{3+} co-doped fluorapatite ($Ca_5(PO_4)_3F$) nanoparticles, establishing fluorapatite as an efficient single-host platform for multispectral emission. Owing to its intrinsic biocompatibility and structural flexibility, fluorapatite enables the simultaneous incorporation of multiple rare-earth ions without compromising phase purity or crystallographic integrity. Structural characterization confirms successful Dy^{3+} and Eu^{3+} substitution within the apatite lattice, while FESEM analysis reveals uniformly distributed spherical nanocrystalline particles.

Under near-UV excitation at 380 nm, the co-doped nanoparticles exhibit combined visible emission arising from the characteristic Dy^{3+} blue/yellow transitions and Eu^{3+} red emission, resulting in an overall white-light appearance. This combined multispectral emission enables the collection of spectral signals from multiple regions of the visible spectrum using a single nanomaterial, which is particularly advantageous for multispectral bioimaging and multiplexed detection. Importantly, this multispectral luminescence is achieved using a single excitation wavelength and a single biocompatible host matrix, eliminating the need for hybrid or multi-phase phosphor systems and reducing spectral cross-talk.

The combination of room-temperature synthesis, intrinsic biocompatibility, spherical morphology, and single-host multispectral emission positions Dy^{3+}/Eu^{3+} co-doped fluorapatite nanoparticles as a versatile platform for multispectral biomedical imaging and related applications requiring stable luminescent probes.

sciforum-162744: Aggregation-induced emission (AIE) dye-polymer nanoformulations via electrostatic complexation

Michaila Akathi Pantelaiou [1,2,*], Georgios Rotas [3] and Stergios Pispas [1]

[1] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., 11635 Athens, Greece
[2] Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece
[3] Section of Organic Chemistry and Biochemistry, Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece

Introduction

Aggregation-induced emission (AIE) dyes are a newly discovered class of molecules that has gained significant research attention. AIE dyes present enhanced emission intensity upon their aggregation with other molecules.

Methods

In this research, the sodium tetraphenylethylene 4,4′,4″,4‴-tetrasulfonate dye was electrostatically complexated with a series of poly(2-(diisopropylamino)ethyl methacrylate-co-2-(dimethylamino)ethyl methacrylate-co-oligoethylene glycol methyl ether methacrylate), P(DIPAEMA-co-DMAEMA-co-OEGMA) multiresponsive terpolymers. Different ratios of terpolymers to dye were utilized in order to investigate the aggregation-induced emission phenomenon and its dependence on dye concentration. All experiments were performed in aqueous solutions, while interaction with fetal bovine serum (FBS) proteins was also tested.

Results

Dynamic light scattering (DLS) measurements and Attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy confirmed the successful complexation of dye with all terpolymers and their stability. Ultrasmall nanoparticles with a 5-7 nm hydrodynamic radius were achieved for various formulations. As the polymers utilized are thermoresponsive, temperature-induced DLS measurements showcased the thermoresponsiveness of the polymer-dye nanosystems. Photophysical studies via Ultraviolet-visible absorption (UV-Vis) and fluorescence (FS) spectroscopy revealed the aggregation-induced emission phenomenon and enhanced emission intensity compared to pure dye. All nanoformulations presented no significant interactions with FBS. Finally, the fluorescence emission intensity of nanoformulations in FBS medium was retained.

Conclusions

Polymer-dye thermoresponsive nanoformulations presenting the AIE phenomenon were fabricated via an easily scalable method. Further biocompatibility and in vivo tests can confirm the stealthiness and the ability of such nanoparticles to penetrate the blood-brain barrier. These promising ultrasmall nanosystems can find applications in photochemistry and bioimaging, where enhanced emission intensity is required.

sciforum-163819: Deciphering Bio-Interfacial Interactions of photoactive Imidazo-Pyrimidine Derivatives: Linking Photophysics, SAR, and Molecular Dynamics Simulations.

Debosreeta Bose

Department of Basic Science and Humanities, Institute of Engineering and Management, School of University of Engineering and Management, Newtown, Kolkata, 700160, India

Imidazo-pyrimidine derivatives are promising biologically relevant fluorophores due to their structural similarity with nucleic acids and pronounced photophysical response in biologically relevant microenvironments. These imidazo-pyrimidine derivatives present well defined photophysical characteristics exhibiting fluorescence. In this work, we present a unified spectroscopic and computational investigation to elucidate the structure–function relationship and interaction dynamics of novel bio-imperative imidazo-pyrimidine derivatives with serum proteins and biomimicking micellar systems. Steady-state spectroscopic studies demonstrate strong binding interactions between one such derivative (SB1) and serum proteins, with a markedly higher affinity toward human serum albumin (HSA) compared to bovine serum albumin (BSA). These findings are corroborated by quenching and denaturation experiments as well as molecular docking analyses, which reveal preferential localization of the probe within a more hydrophobic binding pocket of HSA stabilized by π–π and alkyl interactions. Extending the investigation to self-assembled systems, with another imidazo-pyrimidine derivative (BFIP) examining probe–micelle interactions in cationic CTAB and anionic SDS micelles using UV–visible spectroscopy, fluorescence measurements, dynamic light scattering, and molecular dynamics simulations. The surface charge of the micelles plays a decisive role in governing the interaction mechanism, with the probe forming a stable, hydrophobically driven complex within the CTAB micellar core, while remaining largely solvent-exposed and weakly associated in the pre-micellar regions of SDS. Density functional theory calculations encompassing FMO analysis, ESP mapping and polarity statements further validate the structure–activity relationship of the probe and their propensity to interact with biomimicking systems. Collectively, this multiscale study provides comprehensive insights into how microenvironmental polarity, charge, and hydrophobicity modulate the binding and photophysical behaviour of imidazo-pyrimidine derivatives, in diverse biomimetic systems highlighting their potential as sensitive molecular probes for such systems paving their applications in biomedical and pharmaceutical domains. This mainly highlights the novelty statement of the work.

sciforum-166041: Development of 3D-Printed Parts for Photonic Applications

Fernando Rivera-López [1,*], Christian Hernández-Álvarez [2], Inocencio R. Martín [2] and Rubén Sahuquillo Redondo [1]

[1] Departamento de Ingeniería Industrial, Escuela Superior de Ingeniería y Tecnología, Universidad de La Laguna. Apdo. 456. E-38200 San Cristóbal de La Laguna, Santa Cruz de Tenerife, Spain
[2] Departamento de Física, Instituto de Materiales y Nanotecnología and MALTA- Consolider Team, Universidad de La Laguna. Apdo. Correos 456, E-38206, San Cristóbal de La Laguna, Santa Cruz de Tenerife, Spain

The development of advanced functional materials through additive manufacturing has opened new opportunities in photonic applications [1,2]. In this work, we report the fabrication of 3D-printed parts using a photo-curable resin doped with rare-earth ions, enabling the production of optically active structures with tailored luminescent properties. By incorporating rare-earth elements into the resin formulation, the resulting manufactured components exhibit characteristic optical emissions when illuminated under appropriate excitation conditions.

The primary objective of this research is the development of 3D-printed parts for information encoding and visual communication. Specifically, structures such as QR codes and ASCII-based patterns are fabricated, in which the encoded information is revealed through luminescent responses arising from the optically active ions. This approach enables secure and contactless information retrieval, with potential applications in anti-counterfeiting, data storage and smart labeling. In addition, the versatility of the printing process allows the fabrication of customized photonic elements for signaling and safety applications.

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Acknowledgmens

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sciforum-167287: Dy3+, Mn4+ co-doped Sr4GaNbO8 materials towards dual-mode thermometry, anti-counterfeiting and information encryption applications

Kai Li [1,*], Zhenyu Huang [1], Zhiyu Zhang [1], Jianing Liu [1] and Daiman Zhu [2]

[1] School of Science, China University of Petroleum, Beijing, 102249, China
[2] Department of Energy Power and Mechanical Engineering, North China Electric Power University, Beijing, 102206, China

Herein, we reported a novel multi-function phosphor Sr4GaNbO8:Dy3+/Mn4+ with excellent performance. Under different UV excitations, the phosphor simultaneously exhibited characteristic emissions of Dy3+ around 490 and 578 nm and Mn4+ around 712 nm, realizing the tunable luminescence from yellow to red. Moreover, there is energy transfer between Mn4+ and Dy3+ in the co-doped phosphor. Based on the fluorescence intensity ratio (FIR) technique, maximum relative sensitivities (Sr) and absolute sensitivity (Sa) were achieved to be 14.12% K-1@298 K and 2.33 K-1@473K for Sr4GaNbO8:0.04Dy3+ ,0.005Mn4+, and 13.92% K-1@298 K and 1.68 K-1@473K, respectively, and for Sr4GaNbO8:0.04Dy3+,0.007Mn4+, which were much higher

than most reported results. Remarkably, we proposed an innovative fluorescence lifetime ratio (FLR) prototype approach based on the opposite change of temperature-dependent lifetime behaviors for Dy3+ and Mn4+ under 285 nm excitation, achieving maximal Sr and Sa values of 34.08% K-1@298 K and 5.22 K -1@393 K for the Sr4GaNbO8:0.04Dy3+,0.005Mn4+ sample, which is higher than those obtained using FIR technology, demonstrating its high potential in future design of fluorescent thermometers with higher sensitivity. Moreover, an anti-counterfeiting and information encryption model was designed based on the tunable luminescence properties related to excitation wavelength (250 - 420 nm) and temperature (298 - 473 K) of as-prepared materials. The results enable breakthrough applications in optical sensing, optical encryption and dynamic anti-counterfeiting systems, providing innovative solutions for non-contact thermometry and information security.

Keywords: dual-mode temperature sensing; fluorescent lifetime ratio (FLR); Dy3+/Mn4+ co-doping; optical anti-counterfeiting; information encryption

sciforum-167847: Exploring photochemical potential of a new Cd(II) complex with pyrazole derivative

Marijana Regojevic [1,*], Mirjana Radanovic [1], Berta Barta Holló [1], Kende Attila Béres [2,3], Zsolt Dürvanger [4] and Spiros Gardelis [5]

[1] Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, 21000 Novi Sad, Serbia
[2] Research Centre for Natural Sciences, Institute of Materials and Environmental Chemistry, Magyar Tudosok Krt. 2, Budapest 1117, Hungary
[3] György Hevesy PhD School of Chemistry, Institute of Chemistry, Eötvös Loránd University, Pázmány Péter S. 1/A, Budapest 1117, Hungary
[4] Laboratory of Structural Chemistry and Biology, Institute of Chemistry, Eötvös Loránd University, Pázmány Péter S. 1/A, Budapest 1117, Hungary
[5] Department of Physics, National and Kapodistrian University of Athens, Athens, Greece

Organic ligands containing conjugated C=N bonds can significantly enhance photophysical behavior [1]. While Ag(I) coordination polymers exhibit intriguing photophysical properties [2], Ag(I) is more reactive and less stable than Cd(II), motivating the exploration of Cd(II)-based systems as viable alternatives. In this work, we report the synthesis, photochemical, and photoluminescent properties of a new Cd(II) complex, $[CdL_2I_2H_2O]$, L = ethyl-5-amino-1-methyl-1H-pyrazole-4-carboxylate.

The obtained compound was characterized by ATR-FTIR, molar conductivity in DMF, and X-ray diffraction. Room temperature fluorescence of the samples was measured using a 355 nm UV solid-state pulsed laser.

White crystals of the complex $[CdL_2I_2H_2O]$ were obtained by reacting CdI_2 with L in methanol and in its mixture with other solvents as MeCN, Me_2CO, and H_2O. In the obtained complex, L coordinates through the unsubstituted nitrogen atom of the pyrazole ring. The asymmetric unit of this mononuclear complex comprises one Cd(II), two N-coordinated pyrazole ligands, two iodido ligands, and one coordinated water molecule. The Cd(II) center adopts a distorted trigonal-bipyramidal geometry.

Complex shows strong near-UV to blue fluorescence. The compound emits at 393 nm (powder/pellet) with FWHM 72/80 nm; intensity rises from 44,600 to 151,687 a.u.

A novel mononuclear Cd(II) complex pyrazole derivative ligand was synthesized and characterized. With its simple and accessible synthesis, $[CdL_2I_2(H_2O)]$ represents a promising candidate for advancing existing Cd(II)-based luminophores and exploring structure–property relationships in photoluminescent materials.

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sciforum-166649: Facilitating Tunable Near-Infrared Persistent Luminescence through Chemical Unit Co-Substitution

Jiaren Du *, Siyi Wei and Xiaomeng Wang

International Joint Research Center for Photoresponsive Molecules and Materials, School of Chemical and Materials Engineering, Jiangnan University, Wuxi 214122, China

Persistent luminescence (PersL) is an extraordinary optical phenomenon defined by the prolonged emission of light lasting from several seconds to hours following the removal of excitation sources. At present, afterglow materials are extensively utilized in security signage, anti-counterfeiting measures, information storage, bioimaging, and nocturnal vision applications due to their long-lasting luminescence after excitation. In comparison to traditional visible afterglow, near-infrared (NIR) PersL provides enhanced tissue penetration, reduced background noise, and superior biocompatibility, rendering it particularly advantageous for biomedical and security purposes. Moreover, since NIR light remains undetectable to the human eye in low-light conditions, such materials facilitate critical nocturnal monitoring activities, including aerial drone detection, vehicular tracking on highways, and surveillance of moving pedestrians. Although advancements have been made in steady-state NIR luminescence, the development of materials exhibiting tunable NIR afterglow and dynamically adjustable emission properties continues to pose significant challenges.

This study introduces a series of NIR PersL solid solutions achieved through the modification of the chemical composition via unit cosubstitution, which enables the modulation of emission characteristics in the deep-red and NIR spectral ranges. These solid solutions were systematically analyzed to clarify the relationship between their structural attributes and luminescent behaviors, as well as to investigate the variations in trap distribution and density induced by compositional changes. This research evaluates the advantages and limitations of chemical unit cosubstitution in the enhancement of NIR persistent phosphors, thereby encouraging further investigation into luminescent materials with unique properties.

sciforum-162414: Photoluminescence Tuning in Sonochemically Synthesized CdS Nanostructures via Controlled Cd:S Stoichiometry

Shafiga Safar Alakbarova and Lala Gahramanli

Nano Research Laboratory, Excellence Center, Baku State University, Z. Khalilov Street 23, Baku AZ1148, Azerbaijan

Understanding how composition controls photoluminescence is essential for improving semiconductor nanomaterials used in optical sensing and light-emitting technologies. In this work, cadmium sulfide (CdS) nanostructures were synthesized using a sonochemical method with different Cd:S molar ratios (1:0.1, 1:0.25, 1:0.5, 1:0.75, and 1:1), and their structural and emission properties were systematically investigated. Ultrasound-driven nucleation produced nanocrystals ranging from irregular Cd-rich aggregates to well-defined, uniform particles at stoichiometric compositions. XRD analysis revealed a controlled phase transition from purely hexagonal CdS to mixed hexagonal–cubic structures, with crystallite sizes between ~6 and 35 nm.

Photoluminescence measurements demonstrated two characteristic emission regions: near-band-edge (≈420 nm) and deep-level defect-related bands (≈540–560 nm). Emission intensity and spectral position were strongly dependent on precursor stoichiometry. The 1:1 sample showed the highest PL intensity with a dominant emission around 547 nm, indicating enhanced defect-assisted radiative recombination. In contrast, intermediate compositions, particularly 1:0.5, exhibited broadened PL bands and suppression of higher-order Raman modes, consistent with phonon confinement and increased surface defect activity. UV–Vis absorption confirmed composition-dependent band gap modulation, reflecting quantum confinement and defect state evolution.

These results show that tuning the Cd:S ratio provides a simple and effective strategy for controlling crystal phase, defect density, and photoluminescent behavior in CdS nanomaterials. This approach is promising for light-emitting devices, UV photodetectors, and photochemistry-driven optoelectronic applications.

sciforum-162384: Photoluminescent sulfur quantum dots stabilized by pillar[5]arenes containing amide and amino groups

Inna Tanaeva *, Dmitry Shurpik, Olga Mostovaya and Ivan Stoikov

A. M. Butlerov Chemical Institute, Kazan (Volga Region) Federal University, Kazan, Russia

Sulfur quantum dots (SQDs) have gained significant attention due to their tunable photoluminescence, high photostability, and low toxicity, offering an eco-friendly alternative to heavy-metal-based QDs. However, their application as independent sensory platforms is limited by the absence of intrinsic receptor groups.

This study presents a novel synthesis of SQDs using decasubstituted amide- and amino-functionalized pillar[5]arenes (P[5]As), addressing three key challenges. Firstly, the P[5]As act as effective surface passivation agents. The high density of electron-donating amino groups ensures their stable anchoring to the SQD surface, suppressing defect formation and aggregation. Secondly, these amino groups generate an alkaline medium necessary for sulfur dissolution and nanoparticle formation, eliminating the need for traditionally used NaOH in SQD synthesis, thereby reducing the number of reagents. Finally, P[5]As are capable of forming host-guest inclusion complexes, which imparts molecular recognition functionality to the SQDs. The sensory potential of the resulting nanomaterials was evaluated by studying their interaction with a series of antitumor drugs (tegafur, floxuridine, 5-fluorouracil, dacarbazine, and lomustine).

The following methods were applied to achieve the goal: NMR, IR, UV-vis, and fluorescence spectroscopy, MALDI-TOF mass spectrometry, elemental analysis, DLS, and TEM.

For the first time, SQDs were synthesized in the presence of P[5]As serving as both surface passivation agents and alkaline medium providers. The resulting P[5]As-SQDs exhibit high-intensity blue fluorescence, average sizes of up to 10 nm, and a spherical morphology. UV-vis spectroscopy demonstrated the selective binding of 5-fluorouracil to the P[5]As-SQDs, confirming the key role of the macrocyclic ligand in recognition. Binding constants (lgK_{as}) determined by UV-vis and fluorescence titration were 2.42 and 2.06, respectively.

Thus, functionalization with amide- and amino-functionalized P[5]As provides a validated single-step strategy to create stable, recognition-capable SQDs. This approach opens promising avenues for developing SQD-based sensors, particularly for detecting specific bioactive molecules such as 5-fluorouracil.

sciforum-162641: Spectral Response of a Styryl Dye Confined in 1:2 Cucurbit[7]uril Inclusion Complexes

Olga P. Kolesnikova [1,2,*], Denis A. Ivanov [2], Igor V. Kryukov [2] and Nikolai Kh. Petrov [1,2]

[1] Moscow Center for Advanced Studies, Moscow, Kulakova Str, 20, 123592, Russia
[2] National Research Center Kurchatov Institute, Moscow, Akademika Kurchatov Square, 1, 123182, Russia

The formation of 1:2 inclusion complexes between the styryl dye DASPI and cucurbit[7]uril (CB[7]) in aqueous solution leads to changes in the absorption and fluorescence spectra of the dye. While similar spectral effects were previously attributed to protonation processes [1], direct pH measurements demonstrate that the addition of CB[7] does not alter acidity under the conditions used [2]. Instead, the observed spectral transformations arise from the specific geometry of triple complexes [3]. Key spectroscopic evidence is provided by a comparative analysis with the isolated donor fragment of DASPI.

Aqueous solutions of DASPI (C = 10-5 M) were studied in the free form, in the presence of CB[7], and under acidic conditions, while the donor fragment was investigated separately to establish a reference spectrum. Absorption spectra were recorded using a Shimadzu UVmini-1240, and fluorescence spectra were recorded on a Fluorolog-3 Tau.

In the 1:2 complex, two negatively charged portals of CB[7] are located on opposite sides of the π-conjugated bridge of DASPI. This arrangement creates an electrostatic field that disrupts the intramolecular charge transfer between donor and acceptor fragments of the dye. As a result, the characteristic long-wavelength band at 450 nm, associated with charge transfer, disappears, and a new band emerges at 330 nm. This new band coincides with the absorption of the isolated donor fragment, which confirms the localization of excitation on the donor part.

Thus, the use of the donor fragment as a spectroscopic reference allowed us to directly demonstrate the mechanism of electrostatic control. The results suggest that tuning the stoichiometry of complexes with cucurbiturils may provide a powerful approach for regulating the optical properties of organic dyes, and can be potentially extended to other supramolecular platforms or sensing applications.

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sciforum-163692: Structure–Property Relationships in Triphenylamine-Based p-Type Organic Dyes for Dye-Sensitized Solar Cells: A Theoretical Study

Praveen Naik

Department of Chemistry, Nitte Meenakshi Institute of Technology, Nitte (Deemed to be University), Bengaluru, 560064, India

The design of efficient organic sensitizers for dye-sensitized solar cells (DSSCs) depends critically on understanding their electronic structure and optical absorption behavior, as these properties directly influence light harvesting, charge separation, and electron injection efficiency. Triphenylamine-based p-type organic dyes are promising sensitizers owing to their strong electron-donating nature, molecular stability, and structural versatility. In this work, a systematic theoretical investigation is performed to elucidate the electronic and optical properties of a series of triphenylamine-derived organic dyes using density functional theory (DFT) and time-dependent density functional theory (TD-DFT).

Ground-state geometries are optimized at the B3LYP/6-31G* level to determine the highest occupied and lowest unoccupied molecular orbital (HOMO–LUMO) energies and their spatial distributions, which are crucial for effective charge transfer and energetic alignment in DSSCs. The analysis shows that structural modifications within the triphenylamine framework strongly affect orbital localization and energy gaps, thereby influencing intramolecular charge-transfer characteristics. TD-DFT calculations are employed to simulate optical absorption spectra, focusing on absorption intensity and spectral position in the visible region. The results demonstrate that extending π-conjugation and enhancing molecular planarity lead to red-shifted absorption bands with increased oscillator strengths, improving overlap with the solar spectrum and suggesting enhanced photocurrent generation.

Molecular electrostatic potential surface analysis further reveals the distribution of electron-rich and electron-deficient regions, providing insight into the role of functional groups in facilitating donor–acceptor interactions and charge redistribution. Overall, this study establishes clear structure–property–performance relationships and offers practical design guidelines for developing triphenylamine-based organic dyes with improved light-harvesting capability and potential DSSC efficiency.

sciforum-167079: Theoretical Study on the Design and Optical Properties of a Carbon Nanoring System

Xiao Huang [1,*], Fengwei Gao [1] and Zhong-min Su [2]

[1] School of Chemistry and Environmental Engineering, Changchun University of Science and Technology, 7989 Weixing Road, Changchun, 130012, China
[2] State Key Laboratory of Supramolecular Structure and Materials, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130021, China

The rational design of supramolecular assemblies enables precise modulation of molecular optical properties through controlled intermolecular interactions. This study employs density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations to investigate the structure–property relationships governing the second-order nonlinear optical (NLO) responses in host–guest complexes formed between C_{60} and carbon nanoring derivatives (B-PLY-CPP and N-PLY-CPP). The optimized geometries of B-PLY-CPP@C_{60} and N-PLY-CPP@C_{60} confirm stable convex–concave π–π stacking, with interaction energies of approximately –35 kcal/mol. The static first hyperpolarizability (β_{tot}), calculated at the CAM-B3LYP/6-31G(d) level, reveals that the N-doped complex (N-PLY-CPP@C_{60}) achieves a β_{tot} value of 1.01×10^4 au, which is significantly higher than that of its B-doped analogue and is competitive with classic push–pull NLO chromophores. This enhancement correlates directly with a more efficient intermolecular charge transfer from the nanoring host to the C_{60} guest, as evidenced by a substantial red-shift in the calculated low-energy absorption band. Analysis using a two-level model confirms that the superior NLO response originates from a lower transition energy and a larger transition dipole moment associated with this charge-transfer excitation. The results provide comparative mechanistic insights into how heteroatom doping and supramolecular organization can be used to tailor charge-transfer excited-state characteristics and enhance second-order NLO activity in carbon-based materials, highlighting a viable supramolecular strategy for property modulation.

sciforum-162148: Unexpected Photoluminescence Enhancement upon Epoxidation of Coronene: A DFT/MRCI Study

Dmitry Romanov [1,*], Anatoly Lavrentyev [1] and Igor Ershov [2]

[1] Department of Electrical Engineering and Electronics, Don State Technical University, Rostov-on-Don 344000, Russia
[2] Department of Physics, Don State Technical University, Rostov-on-Don 344000, Russia

Due to their pronounced fluorescence in the near-UV and visible spectral regions, polycyclic aromatic hydrocarbons (PAHs) are widely regarded as model photoluminescent systems. The attachment of heteroatoms or functional groups generally reduces fluorescence intensity, primarily due to structural distortions and the emergence of additional non-radiative relaxation pathways. However, the photoluminescent response critically depends on the type, position, and number of substituents.

This work focuses on quantifying the photoluminescent contribution of an epoxide group attached to peripheral sites of coronene. Owing to the high symmetry of coronene (D6h), two distinct edge positions were identified and selected for functionalization. Geometry optimization and the calculation of absorption and emission edge wavelengths for both pristine and functionalized structures were performed using the density functional theory multireference configuration interaction method (DFT/MRCI).

For pristine coronene, the calculated absorption and emission edges are 300 nm and 397 nm, respectively, in good agreement with experimental data. When the epoxide bridges two carbon atoms within a single benzene ring, the absorption edge undergoes a redshift, while the emission wavelength is slightly blueshifted—a trend consistent with typical substituent effects. In contrast, epoxidation across two adjacent benzene rings induces a pronounced bathochromic shift in both absorption and emission bands and, unexpectedly, an increase in the oscillator strength of the S1 → S0 transition.

These findings underscore that the substitution position is a critical factor governing the optical properties of PAHs. They further suggest that precise control over functionalization sites can not only mitigate fluorescence quenching but also enable deliberate tuning—and potentially even enhancement—of photoluminescence efficiency in functionalized carbon-based materials.

sciforum-177200: One-pot amination-arylation synthesis and structure-property relationships of luminescent and redox-active aryl-triarylamines and -phenothiazines

Thomas J.J. Müller

Institut für Organische Chemie und Makromolekulare Chemie der Universität Düsseldorf, Universitätsstr. 1 (Geb. 26.43.00), 40225 Düsseldorf, Germany

Triarylamines and phenothiazines are electron-rich Π-systems and, therefore, as donor components omnipresent in organic electronics, organic photonics, and organic photovoltaics.1 For establishing design principles of donor systems, the interplay between modelling and experimental studies are fruitful and, therefore, a concise access to substance libraries of functional Π-systems by multicomponent reactions2,3 is highly desirable. Employing Pd-catalyzed sequences allow for efficiently concatening elementary steps with a maximum of functional group tolerance in a one-pot fashion.4,5,6 These synthetic methodological advances allow for establishing extensive physical organic structure-property correlations in the electronic ground state (oxidation potential) as well as in the electronic excited state (absorption, emission). Concatenating Suzuki arylation and Buchwald-Hartwig amination in a consecutive three-component fashion7 sets the stage for comprehensive physical-organic correlation studies on the redox, absorption and emission properties of 3,10-diaryl phenothiazines8 and p-,m- and o-aryl triarylamines9,10

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MDPI AG
Grosspeteranlage 5
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