Proceedings of the 3rd General Meeting of

DAEMON

COST action

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Editors
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COST ACTION
DAEMON

https://cost-daemon.eu/

DAEMON (Data-driven Applications towards the Engineering of Functional Materials) is a European project focused on transforming how functional materials are developed. Using big data, artificial intelligence, and advanced computational tools, we aim to create innovative materials for energy, technology, and industry worldwide.

DAEMON: Where are we now? What do we miss?

Kevin Rossi
TU Delft, Netherlands

Over the past year, DAEMON has consolidated its methodological and organizational foundations toward an integrated, interoperable ecosystem for atomistic modelling and materials data science. Key achievements include the deployment of standardized data management and sharing workflows aligned with FAIR principles, enabling reproducible pipelines and cross-institutional exchange of simulation and experimental data. Significant progress has been made in uncertainty quantification and propagation, linking model calibration, sensitivity analysis, and confidence metrics to improve predictive reliability. Advances in accounting for long-range and multiscale phenomena have strengthened the treatment of electrostatics, transport, and defect interactions. Tailored case studies across selected materials classes and chemistries have demonstrated the practical value of these approaches. Remaining gaps span both technical and structural dimensions: the development of robust frameworks for benchmarking multimodal methods and addressing multidimensional optimization challenges, alongside implementation of a comprehensive Gender Equality Plan and stronger, practice-oriented engagement with industry and policymakers. Addressing these areas is essential to ensure robustness, inclusivity, and sustained societal impact.

DAEMON: Where are going?

Kevin Rossi
TU Delft, Netherlands

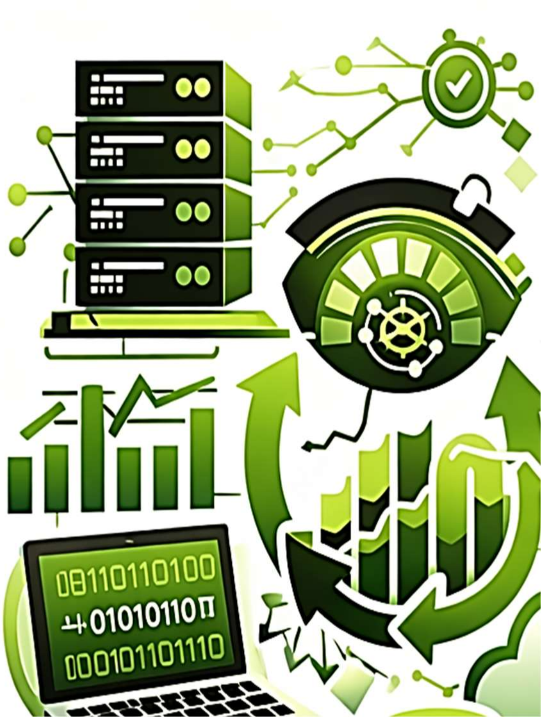
Looking ahead, a co-design process among DAEMON participants has helped articulate a shared vision of the scientific, technical, and societal challenges most likely to shape atomistic modelling and digital materials research in the coming years. This collective scenario analysis highlighted the transformative potential of foundation models trained on heterogeneous simulation and experimental datasets, enabling transferable representations, accelerated discovery, and cross-domain generalization. Participants also identified large language models tailored to materials science as promising tools for knowledge extraction, workflow automation, and human–AI collaboration. Priority needs emerging from the discussion include shared infrastructure, standardized evaluation benchmarks, and open training resources to strengthen community capacity. At the same time, sustainability, supply-chain resilience, and responsible innovation were recognized as key drivers of research direction. Particular care is required for knowledge exchange in security-sensitive domains, balancing openness with governance and compliance.

Talks

RESEARCH DATA POLICY ENCODING ACTIVITY

Lukas Hoermann
Faculty of Physics, University of Vienna, Vienna, Austria

AI-driven molecules and materials design is fundamentally dependent on code and data, where reproducibility, safety, and sustainability are key to scientific progress. Yet, current journal policies on open data and code sharing are highly heterogeneous, limiting the availability of high-quality training data. We develop a framework to encode research data policies and assign a numerical classification to them. This enables analysing open data policies across a representative sample of scientific journals to assess the alignment between publication practices and FAIR principles. We find that journals with higher impact factors are only weakly correlated with stronger data-sharing policies, while journals that embrace open-source practices demonstrate a more consistent adoption of robust policies. Data is generally considered in journal policies, but code sharing and quality control are largely neglected. Furthermore, full compliance with FAIR principles is not yet a standard across journals, creating gaps in accessibility and interoperability. By identifying patterns in journal policies and the factors that promote or hinder FAIR-aligned data sharing, we provide insights for researchers, publishers, and funding agencies.



MACHINE LEARNING INTERATOMIC POTENTIALS BENCHMARK ACTIVITY

Venkat Kapil
University College London, London, United Kingdom

A number of so-called foundational machine-learning interatomic potentials (MLIPs) have recently emerged, and their development has been guided by established benchmarks. However, most existing benchmarks focus indirectly on zero kelvin behaviour of materials. This working group is developing finite-temperature benchmarks for foundation models. We present updates on a dataset of reference ab initio trajectories and preliminary benchmarks of diagnostics aimed at predicting the accuracy of the resulting simulated ensembles.

SELECTED AB INITIO STUDIES OF MAGNETISM AND REACTIVITY AT CRYSTALLINE SURFACES

Željko Šljivančanin

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Pristine and functionalized crystalline surfaces host atomic sites whose coordination numbers are substantially reduced compared to their bulk counterparts. This reduced coordination leads to distinctive magnetic properties and the emergence of surface atoms with markedly enhanced chemical reactivity. In this talk, I will present examples spanning a range of systems, including structural defects and nanostructures on metal surfaces; adatoms on two-dimensional materials such as graphene and hexagonal boron nitride; ultrathin oxide films; and substitutional impurities in two-dimensional MXenes.

EMERGENT AND UNCONVENTIONAL MAGNETISM IN QUANTUM MATERIALS

Srđan Stavrić

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Altermagnets are an emerging class of magnetic materials characterized by a collinear compensated arrangement of magnetic moments and a momentum-dependent spin splitting in the band structure. This peculiar combination, arising from specific crystal symmetries, merges the most desirable traits of antiferromagnets - such as ultrafast dynamics without stray fields - with the strong time-reversal-symmetry-breaking responses characteristic for ferromagnets [1]. Found in a diverse range of materials from metals to insulators, altermagnets offer a versatile new platform for next-generation spintronics, paving the way for high-density magnetic memory and terahertz nano-oscillators [2]. This talk will explore the fundamental principles and significant potential of this exciting new class of materials. A special focus will be on recent observation of p-wave magnetism in a spin-spiral type-II multiferroic NiI_2 [3]. We will explore how the symmetry-protected coupling between chirality and polar order enables electrical control of a primarily non-relativistic spin polarization in this material. Finally, we will examine the role of spin-orbit coupling in two-dimensional altermagnets, where this relativistic interaction cannot be neglected as it is the source of the magnetic anisotropy which is crucial for stabilizing long-range magnetic order at finite temperatures [4].

[1] L. Šmejkal, J. Sinova, T. Jungwirth: Phys. Rev. X 12, 031042 (2022)
[2] C. Song, H. Bai, Z. Zhou et al.: Nat. Rev. Mater. 10, 473 (2025)
[3] Q. Song, S. Stavrić, P. Barone, et al.: Nature 642, 64 (2025)
[4] M. Milivojević, M. Orozović, S. Picozzi, M. Gmitra, S. Stavrić: 2D Mater. 11, 035025 (2024)

PD@C HYBRID MATERIAL FOR ENHANCED H_2O_2 REDUCTION: TOWARD DATA-DRIVEN INSIGHTS INTO SURFACE–INTERFACE DESIGN STRATEGY OF ELECTROCATALYSTS

Marjan Ranđelović

University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry

Understanding complex surface–interface phenomena is crucial for the rational design of functional electrocatalytic materials. This presentation introduces a Pd@C hybrid material, synthesized via a simple hydrothermal route, and discusses its performance as an efficient electrocatalyst for the hydrogen peroxide reduction reaction (HPRR) in alkaline media. Structural and morphological characterization confirmed the formation of graphene-supported palladium nanoparticles with uniform and catalytically favorable dispersion, providing a well-defined platform for studying adsorption-driven electrochemical mechanisms. Electrochemical analysis reveals that the enhanced catalytic activity is accompanied with adsorption of both H2O2 and O2 on palladium nanoparticles and their intricate interplay through adsorption equilibria, disproportionation reactions, and coupled electron-transfer processes. The resulting mechanism represents a catalytic cycle, where the initial reactant dynamically generates an electroactive intermediate, leading to intertwined reaction pathways manifested as a single voltammetric response. Beyond the specific Pd@C system, this presentation aims to motivate future efforts toward integrating detailed electrochemical datasets with data science and machine learning methodologies as a promising pathway for advancing the understanding of electrode process kinetics and electrocatalysts design. Such approaches hold the potential to assist in explanation of complex and overlapping reaction pathways, extracting meaningful descriptors of catalytic performance, and guiding the rational design, discovery and optimization of electrocatalysts for sensing and energy-related applications.

RAPID PROTOTYPING AND EXPERIMENTAL VALIDATION OF DIGITAL TWINS

Aleksandar Sedmak, Miloš Milošević

Innovation Centre of Faculty of Mechanical Engineering, University of Belgrade

This presentation introduces an integrated approach to rapid prototyping and experimental validation of digital twins. By combining additive manufacturing with optical measurement and advanced testing methods, digital models are quickly transformed into physical prototypes and experimentally verified under different type of loadings. The approach enables fast feedback, iterative improvement, and increased confidence in digital twin accuracy. Practical examples demonstrate how this workflow accelerates engineering development and reduces risk.

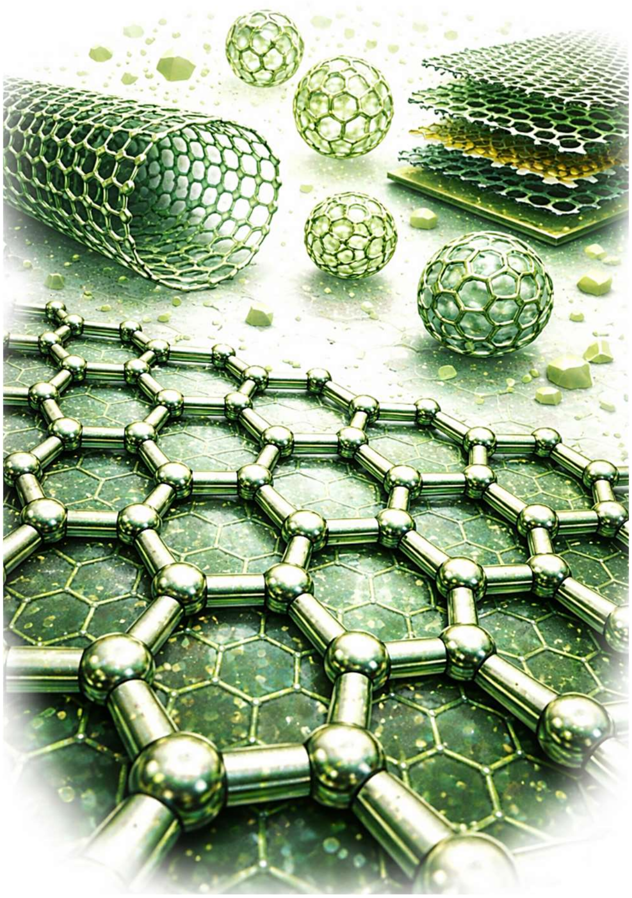
PERIODIC TRENDS AND DEFECT SELECTIVITY IN TWO-DIMENSIONAL MATERIALS: A SYSTEMATIC DFT PERSPECTIVE

Igor Pašti

University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia

Serbian Academy of Sciences and Arts, Belgrade, Serbia

Density functional theory (DFT) is widely used to study two-dimensional (2D) materials, yet many published results remain difficult to compare due to differences in computational protocols and limited chemical scope. In this lecture, I will present a series of systematic DFT studies on graphene and hexagonal boron nitride that demonstrate how large, internally consistent datasets enable reliable benchmarking and trend extraction. By examining adsorption of broad classes of elements on pristine and defect-engineered 2D surfaces within a unified framework, clear relationships emerge between defect type, adsorption strength, cohesive energy scaling, and electronic-structure modification. The lecture highlights how such systematic approaches provide a robust foundation for predictive modeling, shared databases, and collaborative data-driven research.



SAIFA - SERBIAN ARTIFICIAL INTELLIGENCE FACTORY ANTENNA

Marija Mitrović-Dankulov, Dušan Vudragović

Scientific Computing Laboratory, Institute of Physics, Belgrade

The Serbian Artificial Intelligence Factory Antenna serves as Serbia's national hub within the EuroHPC AI Factory ecosystem, supporting the full lifecycle of AI innovation. It provides coordinated access to advanced EuroHPC computing resources, AI tools, curated datasets, and expert consulting for academia, public administration, startups, and industry. By bridging high-performance computing and artificial intelligence, SAIFA enables scalable AI research, domain-specific solutions, and deeper integration of Serbia into the European AI and HPC ecosystem.

A COMPUTATIONAL FRAMEWORK FOR THE ERK2/HDAC4 INHIBITORS DEVELOPMENT

Branislav Stanković

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

In this lecture, we analyze the design of multi-target inhibitors as a basis for future cancertherapies. Specifically, we focus on the development of compounds that simultaneously target ERK2 (extracellular signal-regulated kinase 2) and HDAC4 (histone deacetylase 4). The research integrates machine learning–based QSAR models, molecular docking, and fragment-based drug design using state-of-the-art deep learning approaches, along with quantum chemical calculations and molecular dynamics simulations to validate the findings. Finally, we evaluate ADMET (absorption, distribution, metabolism, excretion, and toxicity) properties as well as synthetic accessibility.

MULTIMODAL DEEP LEARNING FOR ENHANCED MATERIAL PROPERTY PREDICTION: INTEGRATING CHEMICAL COMPOSITION, CRYSTAL STRUCTURES, AND X-RAY DIFFRACTION

Patrícia Ramos[1,2], José Oliveira[1,3]

[1]INESC TEC - Institute for Systems and Computer Engineering, Technology and Science, Porto, Portugal; [2]CEOS.PP, ISCAP, Polytechnic of Porto; [3]School of Economics and Management, University of Porto

Multimodal machine learning offers a promising approach to advance materials design by integrating diverse data types, including chemical compositions, 2D crystal structure visualizations, and X-ray diffraction (XRD) patterns, to predict complex properties such as band gap, formation energy per atom, energy above hull per atom, total energy per atom, magnetic moment per volume, volume per atom, and density of states per atom. This presentation outlines a scalable architecture that fine-tunes pre-trained foundation models, Google's Electra-base for textual composition encoding and Timm's CaFormer-b36 for image-based structure and XRD processing, to extract domain-specific embeddings, which are fused via a late multimodal strategy using a multi-layer perceptron for enhanced property prediction. Key challenges addressed include data alignment across heterogeneous sources, feature integration, computational demands, data scarcity, and model interpretability. The framework leverages tools like pymatgen and Crystal Toolkit for generating standardized inputs from 1,000 materials in the Alexandria dataset, split into 80% training, 10% validation, and 10% test sets. Training employs simultaneous encoder fine-tuning and AdamW optimization with mean squared error loss, achieving considerable scaled mean absolute error reductions across all properties compared to unimodal baselines, demonstrating multimodal superiority through complementary insights from elemental interactions, symmetry-driven patterns, and long-range crystallographic order. The robust, flexible design supports efficient data-driven discovery for energy, electronics, and advanced materials applications. Future directions include incorporating graph neural networks, comparing with materials-specific models, and advancing fusion techniques with attention mechanisms for improved interpretability and performance.

Posters

Integrating Data Science in the Design of Biowaste Derived Functional Carbon Materials

Mirjana Medić Ilić, Bojana Paskaš Mamula, Bojana Kuzmanović, Danilo Kisić, Katarina Batalović

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Carbon materials derived from processed organic waste represent a sustainable and multifunctional platform for environmental remediation and electrochemical energy applications. Their performance is governed by a complex interplay between synthesis conditions, pore architecture, and surface chemistry, making conventional trial-and-error optimization inefficient. Here, we demonstrate how a descriptor-based, data-driven approach enables the systematic identification of key structural and chemical features that control material functionality and process efficiency. In water purification, these descriptors govern adsorption efficiency, kinetics, and selectivity toward aqueous pollutants. Simultaneously, high specific surface area, hierarchical porosity, and tunable surface functionalities enable biowaste-derived carbons to function as electrode materials for supercapacitors and as conductive supports in fuel cell systems, where efficient ion transport, charge storage, and electronic conductivity are critical. By linking synthesis parameters to both adsorption and electrochemical performance through shared descriptors, this approach highlights the potential of bio-derived carbon materials as a unifying platform connecting sustainable waste valorization, environmental technologies, and advanced energy storage and conversion.

Altermagnets or weak ferromagnets: the curious cases of 2D fluorides

Marko Orozović[1], Timon Moško[2], Marko Milivojević[3,4], Martin Gmitra[2,5], Srdjan Stravrić[1]

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[2] Institute of Physics, Pavol Jožef Šafarik University in Košice, Slovakia,

[3] Institute of Informatics, Slovak Academy of Sciences, Slovakia,

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The spin group formalism classifies altermagnets as a new type of collinear magnets with compensated magnetization, based on the assumption of decoupled spin and lattice symmetries. This condition is violated under strong spin-orbit coupling (SOC), an effect especially important in 2D magnets, where magnetic order is stabilized by magnetic anisotropy. Here, we study 2D fluorides (VF4, RuF4, OsF4) and demonstrate their non-relativistic altermagnetic nature, with spin splittings up to 200 meV. However, SOC induces spin canting, transforming these systems into weak ferromagnets. The degree of canting is governed by interplay of Dzyaloshinskii-Moriya interaction and single-ion anisotropy. Our work uncovers a fundamental link between altermagnetism and weak ferromagnetism mediated by SOC, emphasizing that spin-orbit effects must be carefully considered in altermagnetic materials, especially those with heavy elements.

Experimental Data across Synthesis, Characterization, and Application

Zorica Mojović, Nataša Jović-Jovičić

University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Department of Catalysis and Chemical Engineering, Njegoševa 12, 11000 Belgrade, Republic of Serbia

Our group in the Department of Catalysis and Chemical Engineering at the Institute of Chemistry, Technology and Metallurgy focuses on the synthesis, modification, characterisation, and application of aluminosilicate materials, including clays, zeolites, and alumina. These materials are applied in catalysis, adsorption, and electrochemistry, where structure–property relationships critically determine performance. Experimental studies on these materials generate large and diverse datasets from structural, physicochemical, and functional characterisation. Traditionally, conclusions are drawn using classical data interpretation methods, which are effective when datasets are limited in size and complexity. However, as the number of experimental variables increases, identifying dominant parameters and meaningful correlations becomes increasingly challenging. Principal component analysis (PCA) is commonly used to provide initial insights into parameter influence, yet it often offers only partial or qualitative guidance. Recent advances in artificial intelligence (AI) and machine learning (ML) present new opportunities for deeper and more systematic data analysis. These tools can uncover hidden patterns, nonlinear relationships, and synergistic effects that are inaccessible to conventional methods. Nevertheless, effective implementation of AI and ML requires a shift in research strategy. In particular, data-driven approaches demand larger, more structured, and more diverse datasets than those produced by traditional experimental setups. Therefore, there is a growing need to design new experimental frameworks tailored to AI-assisted analysis. Establishing such workflows will enable more efficient knowledge extraction and accelerate the development of functional aluminosilicate-based materials.

Battery research for innovative growth in high energy technologies: lithium-sulfur and redox flow systems

Milica Vasić

University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia

The growing needs for advanced energy storage systems, with better efficiency, sustainability and high-performance, necessitate the development of new materials for battery technologies. The main objective of this project involves the preparation and characterisation of high-efficiency, low-cost and environmentally harmless electrode materials for lithium-sulphur(Li-S) batteries and redoxflow (RFBs) systems. The conditions for preparation of advanced electrode materials will be optimized, including incorporation of various low-cost additives. The project will be realized through multidisciplinary approach, applying various experimental techniques and data processing, through collaboration among three teams with different research skills, from Slovakia, Serbia and Czech Republic.

Acknowledgements This research was supported by the Ministry of Science, Technological development and Innovation, Republic of Serbia: Multilateral Scientific and Technological Cooperation Projects in the Danube Region: project No.003614304 2025 13440 003 000 000 001 01 008. Authors also acknowledge COST Action DAEMON CA22154.

Exploring Metal Hydride Stability through Charge Density Descriptors and Machine Learning Modeling

Bojana Paskaš Mamula, Mirjana Medić Ilić, Bojana Kuzmanović, Katarina Batalović

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Ongoing efforts toward cleaner energy sources promote hydrogen as a promising energy carrier, making its safe and efficient storage in metal hydrides a key challenge in materials design. Recent advances in machine learning enable reliable prediction of metal hydride properties by leveraging data from diverse materials databases.

In this work, we employ a transfer learning strategy based on atomic embeddings derived from the graph neural network MEGNet to develop a model for predicting hydride formation enthalpy. The model is constructed using the atomic composition and crystal structure of the parent intermetallic compounds, allowing efficient screening of candidate materials. To further enhance physical interpretability and predictive capability, we investigate charge density–based descriptors that capture both electronic and geometric characteristics of metal–hydrogen interactions. By linking these descriptors to machine learning modeling, we explore their influence on the stability of binary and ternary metal hydrides, providing additional insight into the underlying factors governing hydride formation and stability.

Design of Polyaniline-Based Composites for Electrochemical Applications

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[1]Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Serbia

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[3]The University of Texas at San Antonio, One UTSA Circle, San Antonio TX

Polyaniline (PANI)-based hybrid composites are promising pseudocapacitive materials for electrochemical energy storage due to their high capacity, good conductivity, and tunable interfacial properties. Combining PANI with 2D materials or structured surfaces leads to improved stability and device performance. For PANI–TiO_2 systems, spectroscopic analyses, electrochemical measurements, and density functional theory calculations revealed strong inorganic–organic interfacial interactions that promote electron delocalization and enhanced charge transport. We address the design of MXene–PANI composites using a multimodal machine learning framework based on DFT-derived databases and uMLIPs and word2vec embeddings to identify stable and high-performance combinations that avoid critical row materials. The combined experimental and data-driven approach highlights interfacial engineering and machine learning as effective strategies for optimizing PANI-based composites for supercapacitors and related electrochemical devices.

Acknowledgements This research was supported by the Science Fund of the Republic of Serbia (Grant No. 372, Harnessing Machine Learning for Green Energy Materials: Insights into MXene/Polyaniline Composite Surface – GEMComp). Authors also acknowledge COST Action DAEMON CA22154.

Transforming Waste into Advanced Carbon Materials for Water Remediation

Tamara Terzić [1], Vedran Milanković [1], Igor A. Pašti [2,3], Tamara Lazarević-Pašti [1]

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[2] Faculty of Physical Chemistry, University of Belgrade, Serbia

[3] Serbian Academy of Sciences and Arts, Serbia

The development of sustainable and cost-effective materials for water remediation has motivated increasing interest in the valorization of bio-waste as a resource for functional carbon adsorbents. The research activities presented here focus on the systematic transformation of diverse waste streams, including spent coffee grounds, viscose fibers, immature walnuts, walnut liqueur pomace, and spent mushroom substrate, into engineered carbon materials for the removal of a broad spectrum of water contaminants, such as organophosphorus pesticides, synthetic dyes, antibiotics, and toxic metals. A range of synthetic approaches, including pyrolytic carbonization, chemical activation, hydrothermal carbonization, and hybrid processing routes, has been employed to achieve precise control over pore architecture, surface chemistry, and adsorption selectivity. Structure-function relationships identified across multiple material systems indicate that microporosity predominantly governs the adsorption of small hydrophobic molecules such as chlorpyrifos. At the same time, mesoporosity is critical for the efficient uptake of bulkier contaminants, including dyes. Adsorption mechanisms involve pore filling, π-π interactions between aromatic pollutants and sp^2 carbon domains, electrostatic effects, and surface complexation mediated by heteroatom-containing functional groups. Across the studied carbon materials, adsorption kinetics are consistently described by pseudo-second-order models, while equilibrium behavior is well captured by Langmuir or Sips isotherms, reflecting the presence of well-defined sorption sites even on heterogeneous surfaces. Several waste-derived carbons demonstrate pronounced selectivity, excellent regenerability over multiple adsorption-desorption cycles, and substantial reductions in pollutant-associated toxicity. In addition, a successful application under dynamic filtration conditions highlights the scalability and practical relevance of these systems. Waste-derived carbon materials represent versatile, tunable, and sustainable platforms for advanced water remediation, effectively aligning materials engineering with circular-economy principles and real-world environmental needs.

From Smoke to Soil: AI-Optimized Clay for Environment Clean Air, and Circular Value

Sanja Milošević Govedarović, Tijana Pantić

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Industrial air pollution remains a critical challenge for sustainable development, requiring solutions that combine efficiency, adaptability, and circular value. The SMG Filtration System introduces a patented clay-based technology optimized through artificial intelligence to absorb hazardous smoke components. AI-driven approaches—including random forest and XGBoost models—enable optimization of thermal treatments and design of hybrid materials. Digital twins and fluid simulations allow customization of filtration recipes tailored to industrial client needs, while advanced modeling and real-time sensor analytics ensure accurate lifespan prediction and continuous performance monitoring. By integrating molecular dynamics with machine learning, this innovation bridges environmental protection. Authors acknowledge support from COST Action DAEMON CA22154.

Exploring Single-Element Additions in $(Mg_{1/5}Ni_{1/5}Zn_{1/5}Co_{1/5}Cu_{1/5})O$ High-Entropy Oxides via Universal MLIPs

Tanja Asanović Antonić, Katarina Batalović

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

High-entropy oxides (HEOs) are crystalline solid solutions containing five or more metal cations distributed over a common sublattice, whose thermodynamic stability is partly governed by configurational entropy. Universal machine-learned interatomic potentials (uMLIPs), such as CHGNet and MatterSim, offer a computationally efficient alternative to density functional theory (DFT) for exploring the high-dimensional compositional and structural space of HEOs. We investigate the effect of Mn incorporation in the rocksalt $Mg_{1/5}Cu_{1/5}Ni_{1/5}Co_{1/5}Zn_{1/5}O$ system, starting from the equimolar $Mn_{1/6}Mg_{1/6}Cu_{1/6}Ni_{1/6}Co_{1/6}Zn_{1/6}O$ composition. Mixing enthalpy and the standard deviation of cation–oxygen bond lengths are employed as structural–thermodynamic descriptors to quantify stability and local lattice distortions. Decreasing the Mn concentration drives the system toward a single-phase solid-solution regime, whereas increasing Mn content progressively shifts the mixing enthalpy toward the MnO end member and promotes multiphase behavior at high Mn concentrations, consistent with thermodynamic expectations. Ongoing work will extend this framework to additional dopants (e.g., Mo and Ti) and will explore advanced machine-learning strategies, including fine-tuning of uMLIPs, to systematically analyze HEO structures, defect energetics, and vacancy stability. Ultimately, this approach aims to establish composition–structure–property relationships relevant for the design of HEO-based electrode materials. Authors acknowledge support from COST Action DAEMON CA22154, TUBITAK project 123M886 and Karadeniz Techincal University Scientific Research Projects FBA-2023-10632; FBA-2022-10352.

Macrocyclic Perylene-dimiide Relaxation and Exciton Dynamics

Nikola Fišić and B. Milovanović

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Understanding the impact of molecular structure and thermal fluctuations on exciton formation and relaxation dynamics in macrocyclic perylene diimide (PDI) systems is essential for the rational design of next-generation optoelectronic materials. In this work, we examine two macrocyclic PDI dimers exhibiting distinct degrees of π–π overlap (high and low), which serve as model systems to unravel the fundamental photophysical mechanisms governing exciton coupling, localization, and energy dissipation. Exciton delocalization occurs on markedly different timescales depending on the degree of interchromophoric coupling and structural arrangement. In the strongly coupled system (high degree of overlap), exciton delocalization is achieved only after approximately 170 fs, whereas in the weakly coupled counterpart (low degree of overlap) it occurs within 15 fs. This disparity mirrors the contrasting relaxation dynamics, where stronger coupling leads to slower population decay and more persistent electronic coherence. The results indicate that in systems with enhanced excitonic interactions, exciton localization on individual chromophoric units requires more time than transitions between adiabatic states, reflecting the intricate interplay between electronic and nuclear degrees of freedom. Conversely, in weakly coupled assemblies, rapid localization and energy dissipation are facilitated by reduced electronic coupling and narrower distributions of nonadiabatic coupling terms. Overall, these findings demonstrate how the strength of excitonic coupling and structural flexibility govern the ultrafast evolution of excited states and the transition from delocalized to localized excitonic behavior—an essential insight for understanding and tuning exciton transport in molecular aggregates and optoelectronic materials.

Variability and Reliability of Word Embeddings as Feature Vectors for Machine Learning in Materials Design

Jana Radaković, Katarina Batalović, Bojana Paskaš Mamula, Nikola Novaković

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Serbia

Natural language processing models have attracted attention in materials science and chemistry for generating high-dimensional vector representations of domain-specific terms, i.e., word embeddings of chemical elements and compounds, which can serve as materials' innate, task-agnostic feature vectors in machine learning applications. When word embeddings representing chemical elements are combined to form composite embeddings representative of chemical compounds, the resulting composite embeddings can serve as composition-based predictors, which encode physicochemical knowledge directly derived from the scientific literature. However, static word embeddings are known to exhibit variability due to the heterogeneity of training corpora, which raises concerns about their reliability in automated materials discovery pipelines, where precision and reproducibility are paramount.

The extent of variability in materials science-affiliated word embeddings trained across three distinct environments is investigated using publicly available research manuscripts from chemistry, physics, and materials science. The substantial variability observed in individual atomic embeddings is strongly influenced by the vocabulary terms selected during language modelling. Despite its extent, the variability does not impair the transfer of encoded physicochemical information when composite embeddings were employed as feature vectors in regression models predicting materials' potential stability. Furthermore, the predictive performance and encoded information remain robust following feature vector calibration through dimensional reduction. These findings offer deeper insight into the reliability and generalizability of text-derived representations of chemical elements and compounds in computational materials design, thus informing strategies to control variability and strengthen the use of word embeddings as autonomous predictors in high-throughput screening and automated materials discovery workflows.

UNDP Serbia

United Nations Development Programme (UNDP) in Serbia supports innovation in green and circular transition, in collaboration with the Ministry of Environmental Protection, the Global Environment Facility (GEF), the European Union, the European Investment Bank (EIB), and the Governments of Switzerland and Sweden. Over 120 circular innovations were financially supported since 2022, in the total amount of over 4 million dollars, in collaboration with the public, private and academic sectors. These innovations increased resource and energy efficiency, promoted digital and AI-powered solutions, and identified and deployed advancements that brought transformative changes to the entire products' lifecycle.
UNDP provides no-strings-attached funding for early-stage innovations, making them more appealing to other investors, and provides hands-on mentoring and guidance to participants, equipping them with the skills and knowledge needed to carry out sustainable and financially viable initiatives.
Some of the supported solutions were impactful enough to spur amendments of Serbian waste regulations, e.g. the procedures for using waste for scientific and research purposes are now simpler, and registration of end-of-waste and by-product status is easier, allowing treated waste to be returned to the market and used in new production processes. This enables systematic application of circular innovations in the real economy, and advances in innovative materials development and testing.

Image: Presentation of Serbian Circular Economy Innovations at the World Circular Economy forum 2024 in Brussels

Serbia was among the first countries in the world having adopted and fully implemented strategic framework for circular transition - Circular Economy Development Programme with Action Plan 2022-2024. With quantified measures, actions and indicators and clear monitoring and evaluation framework, this document set the pathway for circular transition.

Circular Round-Table with Female Entrepreneurs in Impact Hub in Belgrade, 2025

The new strategic framework is under development, with the aim to develop a circular economy platform focused on prevention of waste generation, and support sustainable management of food waste, application of circular principles in the textile industry and sustainable tourism.
Finally, social inclusion and strengthening of local communities remains in the center of the green and circular transition. The fight for a cleaner environment and more efficient economic model requires not just innovation, funding and improved policies, but also empowerment of women, youth and disadvantaged groups, for the joint action and shared benefits.
UNDP organized specific challenged Calls and supported 13 ideas for integrating informal waste collectors into formal waste management systems, as well as 20 female entrepreneurs and innovators in the fields of textiles, architecture, cosmetics and food production, to strengthen their circular economy businesses.
UNDP will continue to work with the government, development partners, businesses, civil society, academia, citizens, women, youth and disadvantaged groups, to support tackling of solid waste pollution, promote the circular economy and (re)use of innovative, highly efficient materials.

More information can be seen here:
cirkularnezajednice.rs
zelenatranzicija.undp.org.rs

Image: Circular Round-Table in the Ethnographic Museum in Belgrade, 2023

Talks

ARTIFICIAL INTELLIGENCE AND ROBOTICS IN THE SERVICE OF SUSTAINABLE AGRICULTURE (AGROAI)

Marija Radmilović, Jelena Ilić

Mihajlo Pupin Institute, Belgrade

The agricultural sector is embracing the digital and AI revolution driven by precision agriculture and increased automation. Precision agriculture uses multi-sensor systems and advanced data processing to monitor, detect, treat and intervene in plant health issues. As a country known for its agricultural potential but modest level of technological development, the goal of this project is to: significantly contribute to the adoption of robotics and artificial intelligence in Serbian agriculture, address the labor shortage in seedling care, increase efficiency and productivity in the field, reduce CO2 emissions and provide tools for pesticide-free organic production. The project aims to develop a fully automated seedling production process using robots and automated systems supported by artificial intelligence.

MATERIALS IMPLEMENTED INTO COSMETIC PRODUCTS GUIDED BY THE PRINCIPLES OF THE CIRCULAR ECONOMY

Miljana Mirković

Vinča Institute of Nuclear Sciences –National Institute of the Republic of Serbia, University of Belgrade, Serbia

Materials obtained through green technology principles enable the innovative repurposing of waste, such as producing completely pure activated carbon from organic coffee grounds via pyrolysis. The green synthesis of hydroxyapatite provides a material with exceptional filtering and antimicrobial properties, while the ethanol remaining from its synthesis is reused for cultivating acetic acid bacteria to produce bacterial cellulose. The materials obtained this way have demonstrated superior performance in skin protection and care. As a result of these projects, three new cosmetic products have been developed following specific technical solutions: Vida sunscreen lotion, Nura skin cleansing milk, and B3iocEll facial masks.

BACTERIAL BIOPOLYMERS IN FUNCTIONAL MATERIAL DEVELOPMENT

Marijana Ponjavić

Group for Eco-biotechnology and Drug Development, Institute of Molecular Genetics and Genetic Engineering, University of Belgrade

Bacterial biopolymers such as bacterial nanocellulose (BNC) and polyhydroxyalkanoates (PHAs) have emerged as versatile, sustainable materials with wide-ranging applications in biomedicine, packaging, and advanced functional systems. Increasing the usage of the bacterial biopolymers as an alternative to commonly used plastic will not only decrease the reliance on fossil-based feedstocks but also reduce the environmental impact and accumulation of resistant plastic waste. Their unique physicochemical properties, high purity, tunable mechanical properties, biocompatibility, and biodegradability, position bacterial biopolymers as the greenest alternatives to conventional synthetic polymers. BNC offers exceptional potential in wound healing, tissue engineering, and flexible electronics, while PHAs provide a biodegradable solution for drug delivery systems and packaging. Recent advancements and efforts have been made in modifying and activating the structure and surface properties of BNC and PHA to boost mechanical properties, improve biodegradability and compatibility with biological systems. Combination of BNC and PHA with biomolecules (such as prodigiosin and actynomycin, pomegranate peel extract) resulted in the new, functional biomaterials of tailored performances beneficial for targeted drug delivery systems, smart packaging and functional food. The integration of machine learning, metabolic modeling, and bioprocess optimization will play a pivotal role in overcoming current limitations for broader application such as production costs, yield variability, and property customization. Supporting the innovations in PHA and BNC based materials are key pillars of the circular bioeconomy in the next-generation functional materials.

Hydrogen fuel cell integration into the modular solar trigeneration system for heating, cooling and electricity - Energy Cube

Marko Mančić

Faculty of Mechanical Engineering, University of Niš

Rising energy-price volatility and tightening decarbonization targets are increasing demand for distributed energy solutions that can reliably provide electricity alongside heating and cooling with minimal on-site complexity. Yet many commercially available hybrid systems remain site-fixed and fragmented, requiring bespoke design and installation, dedicated indoor space, and can exhibit performance sensitivity to ambient conditions—factors that raise cost and reduce user adoption across household, public, and remote-use cases. This work presents the Energy Cube concept: an outdoor, modular “plug-and-play” trigeneration monoblock that integrates solar PV (optionally with tracking), heating and cooling via a heat-pump-based approach, and an optional hydrogen fuel-cell module, coordinated through a single IoT control layer. The architecture emphasizes transportability through a foldable design and standardized interfaces to support flexible operation in grid-connected, backup, or off-grid modes while aiming to simplify deployment and improve operational robustness under varying environmental and load conditions.

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