CEQPAS

Centennial of Quantum Theory:
Progress in Atomic and Molecular Structure

3–5 November 2025 – Belgrade, Serbia
3–5. новембар 2025 – Београд, Србија

BOOK OF ABSTRACTS
Књига апстраката
CEQPAS 2025

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INTERNATIONAL YEAR OF
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MOLESs
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A welcome to CEQPAS 2025

This year we celebrate a hundred years of the Nobel Prize in Physics awarded to James Franck and Gustav Hertz for their ingenious experimental finding that in collisions of electrons with atoms, the energy is absorbed in a quantized manner and proving the Niels Bohr model of the atom. It is also a year when we honour eighty years of Wolfgang Pauli's acceptance of the Nobel Prize for the discovery of the exclusion principle, named after him, the "Pauli principle", which underpins our understanding of the structure of matter. These two groundbreaking discoveries formed part of the emergence of quantum mechanics as the basis for unravelling the nature of the atomic and molecular world. Accordingly, 2025 was declared by the United Nations as the "International Year of Quantum Science and Technology (IYQ)", recognising 100 years since the initial development of quantum mechanics. Hence, we are organising the conference "Centennial of Quantum Theory: Progress in Atomic and Molecular Structure (CEQPAS)" to present the advancements of quantum physics in diverse fields such as:

- Atomic and molecular spectroscopy and its applications to atmospheric sciences and astronomy;
- Collisions and their applications in plasma physics;
- Studies in Chemical physics & physical chemistry;
- The application of quantum science to our wider understanding of phenomena, including radiation sciences;
- The use of Artificial Intelligence (AI) and Machine Learning (ML) for atomic and molecular data analysis and generation.

We are delighted to organise this conference in Belgrade, the capital of the Republic of Serbia, at two institutes of national importance: the Institute of Physics Belgrade and the Institute of Chemistry, Technology and Metallurgy. During the conference, more than 25 speakers will present the state of the art across the different topics represented in the conference; summaries of these talks are presented in this Book of Abstracts.
Immediately after the CEQPAS conference, we will hold the inaugural meeting of the MOLecular Excited State spectroscopy (MOLESs) Consortium. This consortium has been established to review the status of our knowledge of the electronic spectroscopy of molecules, revising and extending the classic series of Melvin Robin's three-volume books on "Higher Excited States of Polyatomic Molecules". A series of reviews of the electronic state spectroscopy of different molecular series in different phases —

gaseous, liquid and solid — will be presented together with reviews of different experimental and theoretical methods used to collect this data and a discussion of relevance to important applications.

We hope all participants enjoy the scientific content of the conference, allowing new collaborations to be formed. We also hope participants will take the opportunity to explore Belgrade.

Finally, we wish to thank all who have contributed to the success of the CEQPAS and MOLESs meeting and who will help to celebrate the IYQ.

On behalf of the Scientific Committee,

Nigel J. Mason & Bratislav P. Marinković

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ATOMIC AND MOLECULAR SPECTROSCOPY AND ITS APPLICATIONS TO ATMOSPHERIC SCIENCES AND ASTRONOMY

Spectroscopy and Quantum Mechanics – Intertwined and Entangled

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Abstract: Spectroscopy and quantum mechanics are inherently interlinked, both being essential to understanding atomic and molecular properties. Spectroscopy played a key role in the development of quantum mechanics and thus, in this centenary year, in which we celebrate the emergence of quantum theory it is necessary to both recognize the role of spectroscopy in the development of quantum mechanics and the importance of continuing spectroscopic studies that underpin many aspects of modern science in fields such as quantum computing, astrophysics and astronomy, environmental and atmospheric chemistry, and nanotechnology, to name a few.

In this opening talk, I will briefly review the historical interconnections of spectroscopy and quantum mechanics before reviewing the state of the art – both experimental and theoretical – whilst highlighting several fields in which spectroscopic data is essential in both understanding the 'foundation' science that underpins such fields and allows them to develop.

I will also discuss the challenges we face, both scientifically and politically, in retaining the spectroscopic community we need for the future, thereby ensuring the retention of skills and expertise.

Keywords: Spectroscopy; Quantum Mechanics; Atomic and Molecular Spectra.

Fully Differential Studies of Single Ionization of Atoms and Small Molecules by Electron Impact

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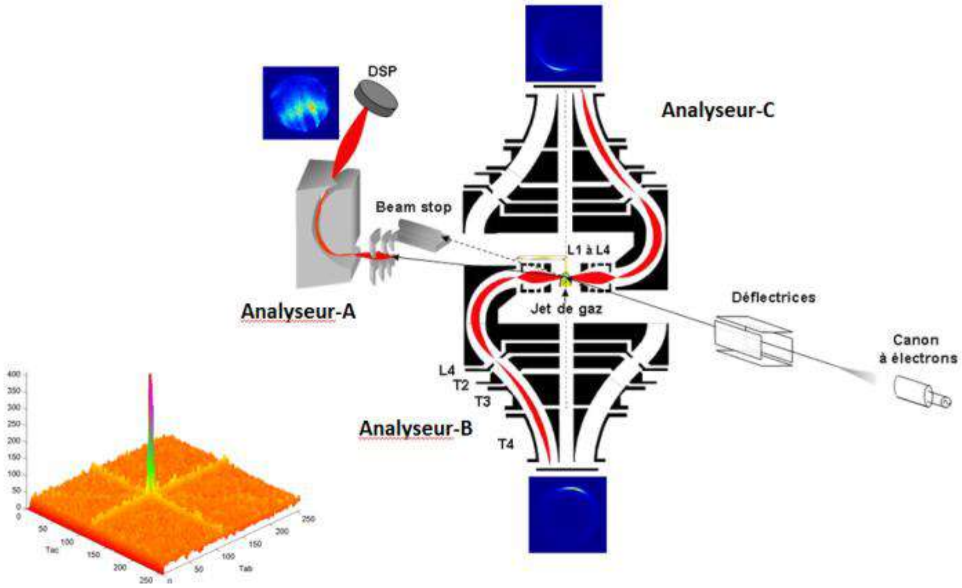
Abstract: Particle scattering experiments play a fundamental role in the study of matter. By directing a beam of incident particles onto a target that generates a short-range potential, and by analyzing the characteristics of the scattered particles, one can extract fundamental information about interaction dynamics, target structure, and internal motion.

Our (e,2e) and (e,3e) experiments constitute powerful tools for investigating the dynamics of single and double ionization of small atomic and molecular systems by electron impact, and more generally for deepening our understanding of many-body interactions.



Recently, we have performed experiments in a largely unexplored kinematic domain, where the momentum transfer to the residual ion is significant. In this regime, the ion plays an active role in the projectile–target interaction. The experimental results are compared with the predictions of advanced theoretical models.

We review a selection of recent experimental results on atoms and small molecules that reveal distinctive physical features of the (e,2e) ionization dynamics. These findings provide deeper insight into correlation and interference effects governing electron–impact ionization processes.

Keywords: TDCS; Ionization; Toroidal Analyzer.

The Quest for Gravitational Atoms on the Sky: Expanding 2D Spectroscopy and Quantum Neural Processes for Supermassive Black Holes

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Abstract: We present the innovative extension of 2D-correlation spectroscopy from molecular physics (Kovačević, 2024 and references therein), combined with Quantum Neural Processes (QNPs; Kovačević et al., 2025), for time-domain studies of supermassive black holes (SMBHs). We showcase pilot results from the Legacy Survey of Space and Time Data Preview 1 (NSF-DOE Vera C. Rubin Observatory, 2025), demonstrating how the extended version of 2D-correlation spectroscopy can probe SMBH populations in upcoming time-domain big data to test the hypothesis of ultralight-boson–coupled SMBHs, gravitational atoms—macroscopic analogs of the hydrogen atom—on a population level (Du et al., 2022). We show that both classical and quantum neural process models reproduce SMBH emission variability within a latent probabilistic manifold that directly encodes the transfer function of the plasma accretion disk and SMBH mass (Raju et al., submitted), providing interpretability beyond conventional deep learning. With this, we hope to invite discussion and collaboration on new synergies between atomic physics, quantum learning, and forthcoming large space- and ground-based astronomical surveys, aiming to explore gravitational atoms as natural laboratories for emergent quantum phenomena in the Universe.

Keywords: Quantum Neural Processes; Supermassive Black Holes; Two-dimensional Spectroscopy; Large Astronomical Surveys; Gravitational Atoms.

Acknowledgement

A.B.K. acknowledges funding provided by the University of Belgrade - Faculty of Mathematics (the contract 451-03-136/2025-03/200104).

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Infrared spectroscopy and VUV photochemistry of molecular ices relevant for Titan

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Abstract: The lower atmosphere and surface of Titan, Saturn's largest moon, host a chemically rich environment where hydrocarbons and nitrogen-bearing molecules condense and are likely to undergo energetic processing. Thus, investigating the spectroscopic and reactive behaviour of such molecular ices is essential for understanding their chemical evolution and interpreting data from past and future missions, such as the upcoming NASA's Dragonfly mission. In this contribution, we present a combined study using infrared (IR) spectroscopy, periodic-DFT calculations, vacuum ultraviolet (VUV) irradiation, and temperature-programmed desorption experiments to investigate phase-dependent photochemistry of Titan-relevant ices, including diacetylene (C_4H_2), pyridine (C_5H_5N), the co-crystal between C_5H_5N and acetylene ($C_5H_5N:C_2H_2$), and a potential novel co-crystal, $C_5H_5N:C_4H_2$.

IR spectra of these ices reveal distinct phase-dependent features. The transition from amorphous to (co)crystalline ices is characterised by narrowing of absorption bands and frequency shifts, reflecting enhanced molecular ordering and changes in intermolecular interactions. When exposed to VUV irradiation, we observe phase-dependence in molecular depletion and photoproduct formation, suggesting that intermolecular interactions and molecular packing alter the efficiency of molecular diffusion and recombination. Our results provide reference IR data and photochemical insights for Titan-relevant molecular systems, demonstrating how phase and co-crystallization influence the stability and reactivity of organic ices.

Keywords: Titan; Planetary Ices; Infrared Spectroscopy; Photochemistry.

Acknowledgement

This work was supported by an AINSE Ltd. Postgraduate Research Award (PGRA) and the Marsden Fund Council from Government of New Zealand, managed by Royal Society Te Aparangi (Proposal: 21-UOO-123). We thank New Zealand eScience Infrastructure (NeSI) for access to high performance computing resources (Project UOO03077). We thank contributions from Dr. Robert Hodyss, Dr. Morgan Cable, Dr. Tuan Vu, Dr. Edith Fayolle, Dr. Ellen Czaplinski, Dr. Samuel Dyuker and Prof. Brendan Kennedy.

Accurate Theoretical Prediction of Vibrational and Electronic Spectra of Fullerenes and Derivatives

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Abstract: This study establishes reliable and cost-effective computational protocols for predicting the vibrational and electronic spectra of fullerenes (C_{60}, C_{70}), their hydrogenated derivatives ($C_{60}H$, $C_{70}H$, $C_{60}H_{18}$, $C_{60}H_{36}$), and related ions. We systematically evaluated various Density Functional Theory (DFT) methods, performing geometry optimizations and vibrational frequency calculations. Electronic spectra were computed using time-dependent DFT (TD-DFT). Comparison of theoretical and experimental vibrational frequencies identified the r2SCAN-D3/def2-tzvp method with a scaling factor of 0.977 as optimal for predicting vibrational frequencies and infrared spectra. For electronic transitions and UV-Vis spectra, the most accurate results were achieved with the TD-DFT/M06-2X/def2-tzvp method applied on r2SCAN-optimized geometries. These recommended protocols offer a balanced blend of accuracy and computational efficiency for studying these complex molecular systems.

Keywords: Fullerenes; Infrared; UV-Vis; Spectra; DFT.

Acknowledgement

The financial support by Ministry of Education, Science and Technological Development of Republic of Serbia Contract number: 451-03-137/2025-03/200146

Ejected electron spectra from N_2O molecule obtained by OHRHA electron spectrometer

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Abstract: Electron spectrometer OHRHA (Jureta et al. 2025) is used to obtain ejected electron spectra from nitrous oxide (N_2O) molecule. The spectrum at 101.05 eV incident electron energy and in the range of kinetic energies from 5 eV to 9 eV is shown in Figure 1. The assignments of the peaks should be provided by TD-DFT calculations.

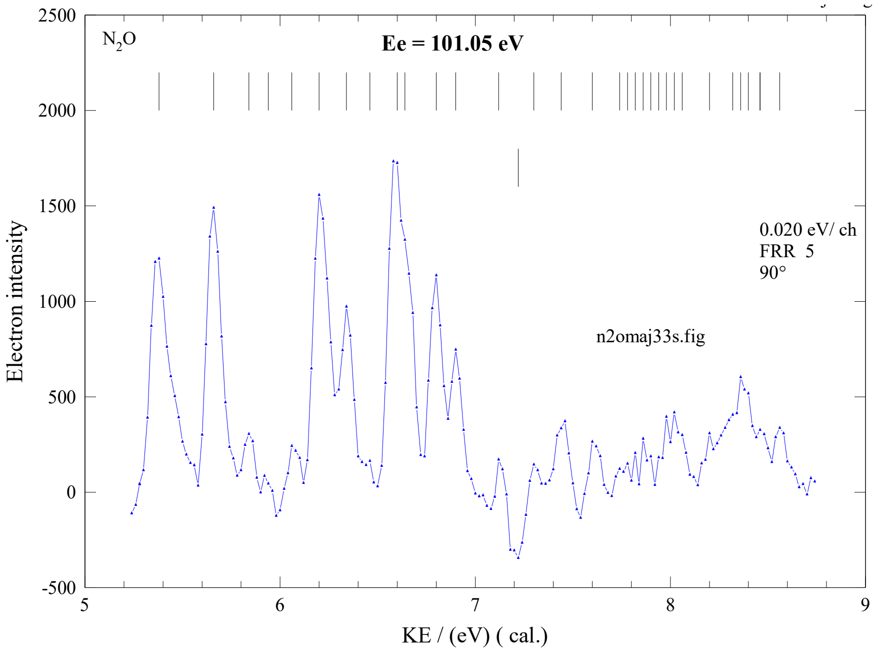

Figure 1 Ejected electron spectrum from N_2O molecule at 90° angle and101.05 eV impact electron energy. Kinetic energy range is from 5 eV to 9 eV. The most prominent peaks are at the KE=5.38; 5.66; 5.84; 5.94; 6.06; 6.20; 6.34; 6.60; 6.80; 6.90; 7.12; 7.22 (dip); 7.3; 7.44; 7.6 eV.

Keywords: Nitrous Oxide; Ejected Electron Spectra.

Acknowledgement

This research was supported by the Science Fund of the Republic of Serbia, Grant No. 6821, Project title – ATMOLCOL

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Jureta J. et al., Adv. Space Res. (2025) doi: 10.1016/j.asr.2025.05.043

Study of Elastic Electron Scattering Cross Section for Desflurane at 200 eV in the Gaseous Phase

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Abstract: Motivated by the environmental impact of halogenated anesthetics, we investigated elastic electron scattering from desflurane ($C_3H_2F_6O$) at an incident energy of 200 eV using both experimental and theoretical approaches. The measurements were performed with a crossed-beam setup employing the relative-flow normalization method with argon as the reference gas. Theoretical differential cross sections were calculated within the IAM-SCAR+I (Independent Atom Model combined with the Screening Corrected Additivity Rule and interference effects) framework and compared with the experimental data, showing good overall agreement. Since desflurane, like other volatile anesthetics, is largely exhaled unchanged and contributes to greenhouse gas emissions, these results provide useful parameters for atmospheric modeling and assessing its environmental impact.

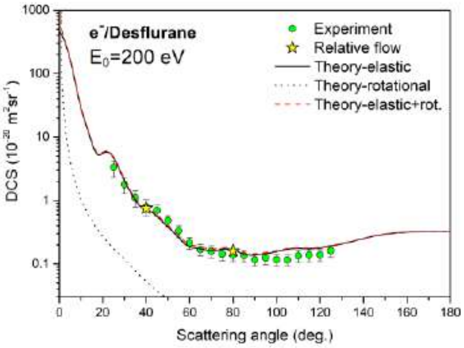

Figure 2. Differential cross section for elastic electron scattering from desflurane molecule.

Keywords: Electron Scattering; Desflurane; IAM-SCAR+I.

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COLLISIONS AND THEIR APPLICATIONS IN PLASMA PHYSICS

Quantum phenomena in cold scattering and molecular rocking

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It is 100 years since Schrödinger and Heisenberg formulated quantum mechanics, a theory which may claim to be the most successful of the past century. We would like to highlight how we may understand some aspects of quantum scattering, specifically those which have little or no analogue in classical mechanics. To do this we will describe the topic of low energy electron scattering by atoms and molecules in which the wave character of electrons is strongly dominant. For example the de Broglie wavelength of a 10 meV electron is 12.3 nm. Collisions between electrons and molecules at thermal energy play a key role in the chemistry and physics of plasmas, ranging from those in space to the chemically active plasmas used for thin film and microcircuit fabrication. In addition we should like to explore a currently classical theory of 'molecular rocking' in solids and its possible extension to a quantum description.

The examples that we give are based on experimental measurements performed at the synchrotron laboratories at Daresbury SRS (UK), Orsay (ACO, Super-ACO, France) and Aarhus (ASTRID and ASTRID2). We will talk about dissociative attachment to CCl_4, to highlight superposition, as well as the Ramsauer-Townsend effect – the grandaddy of quantum scattering. We will mention how high resolution VUV spectroscopy and other techniques, coupled with the spontelectric nature of thin solid films of dipolar molecules (see reference below), can be used to describe the electric field in which constituent molecules experience. We will show that this enables estimates of the angles through which molecules in the solid state, such as nitrous oxide or water ice, may undergo rocking motion of fractions of a degree to tens of degrees. The anomalous case of solid ammonia will also be described.

Keywords: Collisions; Cold Electrons: Dissociative Attachment; the Ramsauer-Townsend Effect; Molecular Rocking in Solids.

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We thank the Villum Foundation and the Danish National Research Foundation for recent funding of these projects

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Time-dependent vibrational distribution function of N_2 in DC-pulsed plasma

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Abstract: Vibrational distribution population of the N_2 gas molecules in the condition of low temperature and low pressure DC-pulsed plasma has been theoretically investigated. The calculation was performed by using an extended Monte Carlo simulation of electron transport trough the N_2 gas merged with master equations solver for tracking V-V and V-T vibrational kinetic due to gas collision processes. The simulation includes the processes of vibrational excitation and de-excitation induced by collisions of accelerated electrons in DC-pulsed electric field and the gas molecules. The processes of fast V-V redistribution during the molecule-molecule collisions are also tracked together with relatively slow V-T energy transition processes. All of these processes mutually dictate the temporary state of vibrational distribution population of the N_2 molecules in low temperature and low pressure plasmas. The DC-pulsed plasma parameters, like value of electric field strength, pulse time and pulse pause time determine the dynamic of vibrational distribution development. Also, number of the pulses in a burst has influence to final population distribution. All of these parameters are varied in the simulation and results show a high impact of these modulated parameters on development and discharge evolution of vibrational distribution. A special attention was dedicated to vibrational distribution quenching at post discharge time. Also, the influence of different electron concentration to vibrational distribution is analyzed and different physical mechanisms which contribute to spreading of vibrational distribution were revealed.

Keywords: Vibrational Excitation; V-V and V-T Kinetic; DC-pulsed Plasma; Low Temperature Plasma.

The quantum collision theory of electron scattering

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Abstract: Electron scattering from atoms, molecules, and ions underpins electron-induced chemistry in low-temperature plasmas, semiconductor fabrication, astrophysical spectroscopy, and radiation biology. Reliable, highly accurate electron scattering cross sections are therefore essential inputs to advances in science and technology. This presentation will summarize recent progress and outlines a roadmap showing how developments in quantum theory and computation have reshaped collision theory in general. We trace the roadmap from Schrödinger-based partial-wave scattering to fully *relativistic* Dirac formulations that include spin effects.

The discussion surveys methods across energy regimes and the problems they were built to solve. In the low electron energy domain (around ~0 to 20 eV), close-coupling approaches like R-matrix variants—provide detailed treatment, especially considering exchange and polarization effects and can resolve resonances due to the formation of a transient excited state. In the intermediate to high-energy region (~20 to 5000 eV), beyond which excitation and ionization channels become prominent, methods such as optical potential, Born approximations, distorted-wave models, etc. offer efficient and practical predictions of various cross sections with relatively less computational power. For heavier targets and spin-resolved observables, relativistic Dirac-based formulations incorporating spin–orbit coupling further refine thresholds and angular distributions. All these methods have delivered *high-accuracy* integral, differential, and momentum-transfer cross sections across wide energy ranges.

Previous bottlenecks, including restricted target descriptions and challenges in benchmarking unstable species, have been alleviated through enhanced electronic-structure inputs (such as DFT-optimized geometries), refined continuum bases, scalable solvers and software ecosystems, and curated databases that facilitate comparison and data reutilization. Other significant problems encompass scalable relativistic methodologies for complex polyatomic systems, integration of nuclear dynamics and dissociative pathways in the calculation, forward-angle scattering, excited-state targets, and comprehensive end-to-end uncertainty quantification.

At the time of the meeting, we will present the most recent results obtained using optical potential and R-matrix methods. However, there are various difficulties that are being encountered presently when investigating complex systems (like heavy, cyclic, polar, etc.), which will also be discussed during the meeting.

Keywords: Quantum Collision; Electron Scattering; Optical Potential; R-matrix; Cross Section.

Low-energy electron beam-induced dissociation of molecules mediated via symmetry lowering

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Abstract: In many cases, upon electron or photon interaction with a molecule, direct dissociation without geometric distortion is not possible due to symmetry constrain. For example, chlorobenzene, a planar molecule, π^* resonance cannot dissociate without geometric distortion [Burrow 1986].

We will discuss the effect of geometric distortion and resulting symmetry lowering in low-energy electron molecule collision studies. We used an electron energy loss spectrometer (EELS) and dissociative electron attachment – quadrupole mass spectrometer (DEA-QMS) setup to study vibrational excitation and N—H bond cleavage in pyrrole molecule. Whereas a DEA-VMI (dissociative electron attachment – velocity map imaging) spectrometer to study low-energy electron beam induced dissociation of four unsaturated chlorohydrocarbons, vinyl, allyl benzyl chloride and chlorobenzene.

We experimentally showed that in pyrrole molecule the N−H bond cleavage following resonant electron attachment is allowed and controlled by the motion non-dissociating carbon-attached hydrogen atoms [Kumar 2022].

The dissociation of the four above-mentioned chlorohydrocarbons is mediated via formation of the lowest shape resonance. In the planar compounds, vinyl chloride and chlorobenzene, due to symmetry constraint the anions (π^* resonances) cannot dissociate without a geometry distortion [Burrow 1986]. Whereas for the non-planar molecules, allyl chloride and benzyl chloride, the shape resonance has a mixed $\pi^* - \sigma^*$ character and can dissociate without any geometric distortion. We have measured the angular distributions of the Cl^- fragments produced from all the above-mentioned unsaturated chlorohydrocarbons. Our goal was to find out the imprints of the dynamical situation on the angular distribution of the Cl^- fragments [Nag 2021]. We found all the four molecules show distinct angular distributions. We have interpreted our results with the help of a single-electronic-state model in the axial recoil approximation.

Keywords: Dissociative electron attachment; Symmetry Lowering; Velocity Map Imaging; Electron Energy Loss.

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Nag P. *et al* 2021 *Phys. Rev. A.* **103** 032830.

Stark effect in low temperature plasma

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Abstract: Historically, Stark effect has been one of the bedrock phenomena for the quantum theory of atoms. Today it is well explained, though its precise calculation is mathematically demanding, except for hydrogen. It was firstly observed in specially designed experiments with a strong electric field but it also occurs in laboratory plasma, and even in some cases in astrophysical plasmas. Specifically, in plasma discharges, the charge density from ions and free electrons is governed by the Poisson equation, and at the boundary always exist a thin layer, so called 'sheath' region. This sheath is a consequence of charge separation and is characterized by a strong macroscopically directed electric field. Examples are near-electrode spaces and plasma streamer heads. Since atoms in the sheath undergo Stark effect, their spectral lines are split and shifted according to the electric field strength. Therefore, Stark effect can be used as a diagnostic tool for measuring one of the most important plasma parameters, the field that regulates particle fluxes. It was found that the ab-initio bases and nonprotrusive nature of this spectroscopic emission method is perfect for examination of spatiotemporal development of plasma. Initially, Hydrogen Balmer series were the most used lines (Ganguly 1991, Videnovic 1996, Cvetanovic 2017). Helium, being a more complicated system, requires a hydrogen-like potential approximation for higher levels, giving a linear effect (Foster 1927, Kuraica 1997, Cvetanovic 2015). Recently, helium Stark spectroscopy has found new application in nonthermal atmospheric pressure discharges that are the most investigated and most promising type of laboratory plasma sources in the last two decades (Obradovic 2017).

Keywords: Stark Effect; Plasma, Spectroscopy; Electric Field.

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Processes in atmospheric pressure plasma used for application in water treatment – dynamics of reactive species

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Abstract: Non-thermal Atmospheric Plasmas (NAPs) have ability to create a chemically reactive plasma volume (containing ions, radicals, excited species etc.) with overall gas temperature at ambient temperature. In the last decades, interactions between NAPs and liquids (mainly water) have gained tremendous importance in the context of applications in environmental remediation, decontamination and, more recently, medical, and agricultural applications (Kumar, 2021; Puač and Škoro, 2025). In such systems reactive species created in plasma in collisions with electrons and heavy particles interact further with the liquid. For all applications it is important to understand the dependence of concentrations of reactive species deposited in water (e.g. H_2O_2, NO_2^-, NO_3^-) on plasma conditions - entangled task due to complexity of the system (Bruggeman, 2016). So, in this work, we employed experimental measurements and modeling to study a creation and dynamic of reactive species in a system where NAP was in contact with water. The study aimed to gain deeper insight into the reaction pathways: of the reactions initiated in the gas phase, with special focus to OH radicals, and also of liquid-phase processes responsible for the formation of long-lived species significant for applications. We used an atmospheric-pressure plasma jet in a pin-electrode configuration operating with addition of Ar at kHz frequency range of excitation signal that produced a streamer-like discharge which was in contact with a water sample. We performed electrical characterization, optical emission spectrometry and obtained spatial emission profiles of important reactive species in the discharge. In order to comprehend interaction between plasma and liquid a zero-dimensional gas–liquid model was developed and results were compared with measurements of concentrations of reactive species in the treated water.

Keywords: atmospheric pressure plasma, reactive species, water treatment, gas–liquid model

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Collisions of electrons, photons and ions with atoms and (bio)molecule systems - ATMOLCOL project

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Abstract: The core of ATMOLCOL project is to study collisional processes involving atoms and (bio)molecules, especially focusing on very short time scales. Elastic scattering (Vukalović 2024) of electrons on atom/molecule, autoionization (Jureta 2024,), Ionization (Srećković 2025), photoionization (Delibašić 2024), electron autodetachment and dissociative electron attachment (Kopyra 2025) are accompanied processes that are examined. The planned experimental methodology is based on the cross-beam technique that provides conditions for the binary collision events (Vukalović 2024, Kopyra 2025), while the theoretical is based on first- and second-order theories (Delibašić et al). Both methodologies are supported with the numerical calculations and methods (IAM method, Gauss-Legendre and Gauss-Mehler quadratures). ATMOLCOL is bringing together experimental and theoretical knowledge which may lead to further technological developments and direct and indirect impacts on climate change, the environment science and human health.

Keywords: Electrons; Molecules; Collisions.

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STUDIES IN CHEMICAL PHYSICS AND PHYSICAL CHEMISTRY

What is a Chemical Bond?

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Abstract: The chemical bond is one of the central yet most elusive concepts in chemistry. Despite more than a century of quantum theory, its fundamental nature remains debated. In this presentation, I revisit the quantum mechanical foundations of chemical bonding and challenge long-held assumptions such as electron-pair sharing, spin pairing, and potential-energy lowering as the defining criteria of bond formation. To this end, I introduce the interference energy analysis (IEA) (Cardozo et al., 2024), a framework that quantitatively partitions the total electronic energy into quasi-classical and interference components. Using spin-coupled generalised valence-bond (SCGVB) wavefunctions (Dunning et al., 2021), atomic-like, monoelectronic, non-orthogonal orbitals are self-consistently optimised, enabling quantification of the interference contribution to bonding. Applications of IEA to systems ranging from simple diatomics to conjugated hydrocarbons (Fantuzzi et al., 2012) and aromatic systems such as benzene (Cardozo et al., 2021) reveal a unifying picture: chemical bonding originates from constructive quantum interference, manifested as kinetic-energy reduction arising from coherent superposition of one-electron states. Ultimately, the minimal condition for bond formation is not electron sharing or spin coupling, but one electron and two interfering states.

Keywords: Chemical Bond Theory; Valence Bond Theory; Quantum Interference.

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Computational Simulation of Vacuum-Ultraviolet Absorption Spectra of Astrochemical Ices

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Abstract: Ices play a central role in astrochemistry, both in the interstellar medium and throughout the Solar System (Cuppen et al. 2024). Laboratory studies of astrochemical ice analogues are therefore essential. Within this framework, vacuum-ultraviolet (VUV) spectroscopy provides key information (Zhang et al. 2024), resolving electronic excitations at cryogenic temperatures, quantifying band positions and intensities, and revealing phase-dependent signatures. However, solid-state VUV data remain scarce for many species. This work presents case studies (H_2O, CO, and O_2) from an ongoing experimental–computational programme encompassing ~30 astrochemically relevant molecules. We focus on the computational generation and characterisation of VUV spectra calculated at the DFT level using a molecular cluster approach, benchmarked against ~20 K spectra of laboratory ices. The calculated spectra reproduce experiments closely, with transition assignments largely agreeing with the literature. For H_2O, accuracy depends on cluster size. For CO, the elusive high-energy band (below 120 nm) is captured and is consistent with experiment-based assignments. The calculations also distinguish crystalline and amorphous phases. O_2 is an exemplary case, where α- and β-O_2 show features absent from the amorphous O_2 spectrum.

Keywords: Astrophysical Ices; VUV Spectroscopy; DFT; Computational Spectroscopy.

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Modulating electrostatic potential as a strategy to control mechanical sensitivity of high-energetiy materials

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Abstract:
Achieving the balance between mechanical sensitivity and detonation performance is the ultimate goal in the development of new high-energy materials (HEMs). Numerous studies in the area of material design have focused on developing HEMs with high performance and low sensitivity. Unfortunately, low sensitivity of HEMs is usually accompanied by poor detonation efficiency. One of the most reliable indicators of high sensitivity towards detonation of HEM molecules is the presence of areas of strongly positive electrostatic potential over the central regions of molecular surfaces. Adjusting the electrostatic potential values in these regions provides a path to control the mechanical sensitivity of HEMs.

In this work, we have studied the possible ways to fine-tune the electrostatic potential values and mechanical sensitivities of high-energy molecules using hydrogen bonds and other non-covalent interactions. Results of high-level ab initio calculations and analysis of crystallographic data showed that electrostatic interactions may significantly tune the electrostatic potential values and mechanical sensitivity of studied HEM compounds. Additionally, we have shown that tuning the electrostatic potential is particularly feasible in chelate coordination compounds, as the electrostatic properties of these molecules can be effectively modulated through careful selection of ligands and transition metals.

Keywords: High-energy Materials; Ab-initio Calculations; Electrostatic Potential.

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Tracing the molecular complexity of space through experimental–theoretical synergy in astrochemistry

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Abstract: Astrochemistry seeks to understand the formation and evolution of chemical species in extreme astrophysical environments. Our work focuses on the experimental study of molecules relevant to the interstellar medium through high-resolution spectroscopy and the analysis of radiation-induced fragmentation processes (Quitián-Lara et al. 2018, 2025, Gerlach et al. 2022). These studies enable us to explore stability, reactivity, and possible formation pathways of compounds with astrobiological significance. However, the experimental approach is complemented and reinforced by theoretical chemistry tools, which allow us to interpret astronomical observations and predict molecular behaviour under conditions that are difficult to replicate in the laboratory. Quantum chemical calculations provide key information on molecular geometries, fragmentation energies, spectroscopic modes, and reaction mechanisms (Santos, et al. 2022, Londoño-Restrepo et al, 2025). This synergy has enabled us to thoroughly explore the reactivity of species with prebiotic potential, as well as to propose viable routes for the formation of complex molecules even in the early stages of planetary evolution. The integration of theory and experiment is fundamental to advancing our understanding of the universe's chemistry and identifying new structures as candidates for future astronomical detections

Keywords: Interstellar Chemistry; Radiation-Induced Fragmentation; Quantum Chemical Modelling; Prebiotic Molecules; Spectroscopy.

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Non-covalent sulfur interactions through the lens of quantum chemistry

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Abstract: Among the chalcogens, sulfur stands out for the remarkable diversity of its chemical bonding and physical forms, from covalent chains and rings to polymeric structures and non-covalent interactions in molecular and crystalline systems. On the occasion of the centenary of quantum chemistry, this work highlights how modern quantum-chemical approaches, such as DFT calculations, electrostatic potential maps, NBO analysis, and potential energy surface investigation, enable a deeper understanding of sulfur-based interactions. Particular attention is given to S···S contacts that determine molecular geometry, crystal packing, and the stability of sulfur-containing systems.

Examples from our studies, including quantum-chemical investigations of S···S interactions in the α-allotrope of elemental sulfur *(Kretić, Medaković & Veljković, 2023)*, illustrate (i) preferred geometries and energetic characteristics of these contacts, (ii) their influence on molecular arrangement and crystal packing, and (iii) how theoretical analysis provides predictive insights into structures once rationalized only empirically. This work also demonstrates how quantum-chemical knowledge of sulfur interactions can be extended to the design of new materials and supramolecular assemblies.

Keywords: Sulfur–Sulfur Interactions; Non-covalent bonding; Qantum-chemical Calculations.

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A theoretical study of electronic and geometric properties of biologically relevant [4Fe-4S] clusters

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Abstract: Iron-sulfur clusters bound to proteins are polynuclear combinations of iron and sulfur found in all domains of life. These clusters are among the most functionally diverse cofactors found in nature, most importantly serving as catalytic centers for electron transfer reactions in processes such as photosynthesis and cellular respiration. In this work, we have investigated the electronic and geometric properties of two types of iron-sulfur clusters: [4Fe-4S] and [4Fe-4S](SCH_3)$_4$. Both models are derived from ferredoxin crystal structures (PDB: 1IQZ and PDB: 1CKU). All calculations are based on the DFT Broken Symmetry (BS) method using BP86, OPBE, and B3LYP* exchange-correlation functionals and TZP basis set. The results indicate that the BS states are always more stable than the "high spin" states, have shorter bonds, and are antiferromagnetically coupled. This is because weak bridging ligands in polynuclear complexes, such as thiolates and sulfides, facilitate long-range, rapid electron exchange. The results all agree with experimental data obtained from various structural methods [1, 2].

Keywords: Iron-Sulfur Clusters; Density Functional Theory; Broken Symmetry.

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Electronic Structure and Stability of Rhodium(III)–EDTA Complexes

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Abstract: Rhodium(III) complexes with EDTA-type ligands provide a versatile platform for exploring how chelate denticity and geometry govern structure, stability, and electronic properties. Density functional theory (DFT) calculations, combined with Energy Decomposition Analysis (EDA) and density-functional-based Ligand Field Theory (LF-DFT), were applied to a series of pentadentate and hexadentate Rhodium(III) complexes. Benchmarking against crystallographic data identified the most reliable density functional approximations for reproducing Rh–donor distances and coordination-sphere geometries, which are critical for accurate ligand-field splitting. LF-DFT reveals systematic correlations between chelate-ring arrangements and d–d excitation energies, while EDA disentangles electrostatic and covalent contributions to isomer stability. The comparison of pentadentate versus hexadentate coordination highlights how subtle variations in denticity and ring size modulate excited-state patterns and bonding interactions. These results establish quantitative links between structure and spectroscopy in Rh(III)–EDTA systems, offering a framework for interpreting experimental spectra and guiding the rational design of aminopolycarboxylate ligands and metal complexes.

Keywords: Rhodium(III) Complexes; DFT; LF-DFT; Electronic Structure; Chelate Ligands.

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THE APPLICATION OF QUANTUM SCIENCE TO OUR WIDER UNDERSTANDING OF PHENOMENA, INCLUDING RADIATION SCIENCES

Quantum diffraction and interference phenomena in atomic processes

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Abstract: Diffraction of matter particles on various targets, such as lattices, slit shields, other particles, etc., and study of the resulting interference patterns were key experiments that established the quantum-wave nature of matter. Beginning with the Davison-Germer experiment in 1927, which confirmed the wave properties of electrons, experiments of this type have been performed throughout the century-long history of Quantum Mechanics. To demonstrate the universality of quantum principles, of particular importance were the experiments that confirmed the wave nature of very massive particles, such as the fullerene molecule C_{60}, and more recently, molecules consisting of several thousand atoms [1]. On the other hand, the structure of large particles like C_{60} have been investigated using electron scattering on these molecules as spherical diffraction lattices [2]. In this lecture we will present the results of experimental and theoretical research on several problems on this topic, in which the Laboratory for Atomic Collision Processes of the Institute of Physics Belgrade was involved in recent years. Among them will be presented the results of research on the diffraction of a beam of atoms on a crystal lattice at grazing incident angles [3], diffraction of electrons on atomic particles [4], as well as specific cases of superposition of electron wave packets known as dynamic and exchange interference [5,6].

Keywords: Quantum Mechanics; Diffraction; Interference; Atomic Processes.

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The Enduring Mystery of Wigner’s Friend

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Abstract: The enormous success of quantum theory over the past century often makes us forget that Feynman’s famous remark, “nobody understands quantum mechanics”, is probably as valid today as ever. While experimental violations of Bell’s inequalities have forced us to abandon the hope of ever recovering a (local) mechanistic picture of the universe, the Wigner’s friend conundrum highlights what is perhaps the deepest yet unresolved problem at the foundations of quantum science. Exemplifying the seeming inconsistency at the very heart of its mathematical formulation, this quantum thought experiment is one of the rare cases where even a consensus about the outcome is lacking among experts. We will revisit this thought experiment and some of its recent developments, discussing both the known possible resolutions and advocating some novel ones.

Keywords: Wigner’s Friend Paradox; Measurement Problem; Interpretations of Quantum Mechanics.

Comparative analysis of machine learning algorithm results in predicting the probability of rectal tumor presence

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Abstract: This study examines the application possibilities of machine learning (ML) algorithms in the analysis of computed tomography (CT) scans aimed at diagnosing tumor changes in specific organs. The focus of this study is on detecting tumor tissue in the rectal area. The plan is to train a model that will recognize and identify the tumor location using exclusively CT scans, without relying on magnetic resonance imaging. The long-term goal is the development and validation of algorithms that could be integrated into medical devices for automatic identification of tumor tissue, where the device would display the probability that the tissue is affected by a tumor. The study included data from 140 patients. Only those slices depicting the rectal region were selected, resulting in approximately 3,600 images suitable for analysis. A set of the most relevant features was extracted from the images, and a table was created for training and testing multiple ML algorithms. In addition to classical ML algorithms, neural networks were trained to compare performance and explore the potential of deep learning in tumor detection. Models were trained on the same feature set with a training and testing split. Evaluation focused particularly on sensitivity and specificity parameters, which are critical in medical diagnostics. The best result on the available dataset was achieved using the support vector machines algorithm, which reached over 80\% accuracy in tumor area detection. Neural networks demonstrated potential for higher sensitivity, with a need for further model architecture tuning to improve specificity. This approach can contribute to more efficient diagnostics, resource and time savings for physicians, as well as enabling more precise therapy planning and a personalized patient approach.

Keywords: Computed Tomography; Machine Learning; Rectal Carcinoma.

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Transport and spatial relaxation of electrons in atomic and molecular gases: Revisiting the Franck-Hertz experiment and beyond

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Abstract: The Franck-Hertz experiment stands as a cornerstone of quantum and atomic physics, providing the first direct evidence of quantized energy states in atoms (Franck and Hertz 1914). In this contribution, we revisit its classical interpretation through the lens of modern kinetic theory, offering new insights into electron transport and spatial relaxation phenomena in atomic and molecular gases.

Using a multi-term solution of Boltzmann's equation and Monte Carlo simulations (Dujko *et al.* 2010, 2011), we investigate the spatial relaxation of electrons in mercury vapor. The periodic features observed in the spatial profiles of transport properties in our simulations reflect the same underlying physics as the periodic structure in the current-voltage characteristics of the original Franck-Hertz experiment, where the 4.9 V spacing between peaks revealed an electronic excitation energy of 4.9 eV.

A direct link exists between the Franck-Hertz and steady-state Townsend experiments, as both probe transport and spatial relaxation of electrons through elastic and inelastic collisions with neutral atoms and molecules (Dujko *et al.* 2008). In this work, we investigate the spatial relaxation of electrons under steady-state Townsend conditions in noble gases, enabling a comparative analysis of transport phenomena across atomic species. As a representative molecular system, we also examine the spatial relaxation of electrons in carbon monoxide (CO). Emphasis is placed on the impact of anisotropic scattering for rotational excitations on the spatial relaxation behavior.

Special attention is given to electron transport in mercury vapor, where the influence of mercury dimers on transport properties is examined in detail (Mirić *et al.* 2016). In addition, we present results on electron transport in indium vapor. Periodic oscillatory profiles of transport properties are obtained under steady-state Townsend conditions, revealing distinctive relaxation behavior (Dujko *et al.* 2021). Additionally, we investigate the inception and propagation of streamers in indium vapor, analyzing their evolution across varying temperatures and highlighting the role of metastable indium atoms in shaping streamer dynamics.

This comprehensive study not only deepens our understanding of electron transport and relaxation in atomic and molecular gases but also reinforces the enduring relevance of the Franck-Hertz experiment in contemporary plasma science.

Keywords: Franck-Hertz Experiment; Steady-state Townsend Experiment; Boltzmann Equation; Monte Carlo; Electrons; Spatial Relaxation; Mercury Vapor; Indium Vapor.

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Molecular nanorotators in the foundations of quantum mechanics

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Abstract: For decades after its inception, quantum mechanics has been regarded merely for application purposes. Return to the foundational issues of quantum mechanics led to the new quantum sciences (quantum information and computation, open quantum systems, quantum metrology, quantum thermodynamics etc.). In this paper, we place a focus on the topic of quantum control of molecular nanorotators (Jeknic-Dugic *et al.*, 2018, Petrovic *et al.*, 2020, Jeknic-Dugic *et al.*, 2025) as a foundational quantum-mechanical topic.

Keywords: Quantum Foundations; Transition from Quantum to Classical; Molecular nanorotators; Open Quantum Systems; Quantum Brownian motion.

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From Molecules to Magnetic Materials: Structural Tuning of Organic Radicals for Quantum Technologies and Sustainable Nanomagnetism

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Abstract:

Integrating nanostructures in devices has acquired growing importance, pushing new advances in research and technology.(Yuan et al., 2024, Sun et al., 2014) Many emerging spin-based technologies require control of the position and the dimensions of the assemblies, such as in sensor and quantum technologies.(Wasielewski et al., 2020)

These new technologies need new visions and materials and, specifically, sustainable materials. In this context, molecules are a less researched resource for spin-based and nanomagnetism phenomena with huge potential.(Gubbiotti et al., 2024)

We investigate X-ray magnetic circular dichroism (XMCD) at the carbon and nitrogen K-edges in purely organic radical thin films.[2] Purely organic radicals are composed only of light elements, and they carry at least one unpaired electron that gives rise to a permanent magnetic moment; therefore, they are materials with magnetic properties.(Epifanov, 1979, Gatteschi et al., 2006, Getzlaff, 2008, Rajca, 1994, Rajca et al., 2001).

Our results reveal that the magnetic behaviour of the films differs from that of single crystals, depending on the preparation conditions. Theoretical simulations suggest that this difference arises from variations in molecular arrangement within the films compared to the single crystal. The ability to tune magnetic properties by controlling molecular arrangement is a powerful tool for uncovering new phenomena and designing novel applications.

Furthermore, the production and investigation of three-dimensional (3D) magnetic nanostructures represent a significant advancement in both fundamental research and practical applications, with immense potential for next-generation technologies, as also explicitly discussed in the “2025 Roadmap on 3D Nano-magnetism” by Gubbiotti et al.(Gubbiotti et al., 2024) However, the critical situation created by climate change, with 2024 being the hottest year to date and the first year with global warming exceeding 1.5 °C,(Tollefson, 2025)poses severe challenges. We addressed the production of new purely organic radical 3D nanostructures and its sustainability in terms of circular economy.

Keywords: Organic Radicals; 3D Nanostructures; Soft X-ray Spectroscopies.

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THE USE OF ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR ATOMIC AND MOLECULAR DATA ANALYSIS AND GENERATION

AI-Generated Framework for Machine Learning in Plasma Diagnostics: A Meta-Demonstration of Artificial Intelligence in Atomic Spectroscopy

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Abstract: In this work, we have presented some of the excellent possibilities of using AI/ML in the physical sciences, with special reference to atomic and molecular spectroscopy. This paper is a meta-demonstration of sorts: At our request and under our supervision, AI (Claude, Anthropic) generated a complete research framework that analyzes the current state of AI/ML applications in spectroscopy and implements a fully functional example - from physical simulations to the use of machine learning.

For a demonstration, we chose plasma diagnostics - an area that is very important for collisional physics and atmospheric sciences. Using AI, we developed: (i) a physics-based argon plasma emission spectrum simulator incorporating collisional-radiative models, NIST atomic data, and electron impact excitation kinetics, generating 2,000 synthetic spectra across electron temperature ranges of 1-5 eV and densities of 10^{16}-10^{18} m^{-3} (Srikar, 2024); and (ii) deep neural networks, random forests, multi-layer perceptrons and XGBoost trained to perform inverse diagnostics—predicting plasma parameters from optical emission spectra.

The work demonstrates AI's transformative potential in spectroscopy through a recursive approach: AI analyzing AI applications, AI generating physical simulations, and AI building diagnostic tools.

Keywords: Artificial Intelligence; Machine Learning; Plasma Diagnostics; Optical Emission Spectroscopy; Collisional-radiative Model.

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The Role of Small Molecules in Astrophysics: From Collisions to Radiation

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Abstract: Atomic and molecular collisions, together with radiative processes, play a fundamental role in shaping the diverse environments of our universe. These interactions govern molecular energy transfer, excitation, and de-excitation, thereby influencing the spectra of numerous astrophysical sources such as planetary atmospheres, interstellar clouds, and circumstellar envelopes (see, e.g., Sreckovic et al. 2022). Reliable data and comprehensive databases on atomic and molecular processes have become increasingly vital for the development of models and simulations of complex physical and chemical systems, as well as for interpreting observational and experimental results across multiple scientific domains (Vujcic et al. 2023). Such data are also essential for a range of applications, including modeling the non-local thermal equilibrium chemistry of the early universe, the solar atmosphere, and white dwarf environments. Advancing this field requires the development of new methodologies and the refinement of existing models to incorporate a broader range of processes and utilize more precise datasets compatible with modern computational tools. For environments such as laboratory plasmas, planetary atmospheres, and the ionosphere, the primary objective is to determine accurate cross sections and rate coefficients for key collisional and radiative processes (Albert et al. 2020). In this work, we present and discuss such data, contributing to the ongoing effort to enhance the accuracy and applicability of atomic and molecular databases for astrophysical and plasma research.

Keywords: Atomic and Molecular Collisions; Radiative Processes; Cross Sections and Rate Coefficients; Astrophysical Modeling and Plasma environments.

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Development and applications of Machine learning and Artificial Intelligence in High energy physics and Nuclear physics

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Abstract: I'm presenting a view on reach and development of Machine learning and Artificial Intelligence in High energy physics and Nuclear physics, with my 20 years of experience in the field. The most important research and development milestones and most important applications, both for widely popular use, and for most interesting physics experiments are discussed. AI tools used by beginners, and tools for advanced users are presented and discussed. Furthermore, most important elements in using, and development of your own AI application are presented and explained in sufficient details. Lastly, I'm presenting several examples from elementary particle physics and nuclear physics which I was developing or working on.

Keywords: Machine learning, Artificial Intelligence , AI applications

Understanding Artificial Intelligence: Navigating Through Physical and Virtual Worlds

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Abstract: The present moment in human history is marked by the rapid and far-reaching advancements of artificial intelligence (AI) and related technologies. Applications of AI-based research now extend across nearly every domain of science, industry, and daily life. From predictive modeling to image recognition, from large language models to robotics, from game AI to real-time industrial applications – AI research is covering an extensive array of topics. Looking at the past, one could notice that in the very foundations of AI research lies the desire to emulate human intellectual capabilities, therefore making the pursuit of intelligent and autonomous agent behavior a central topic of the entire field. This desire to replicate human capabilities can be traced back in history, even before AI was established as a scientific field. As a result, it is not surprising that both general and academic non-expert audiences sometimes misinterpret the capabilities of advanced AI systems, attributing to them a human-level intelligence. Additionally, especially bearing in mind the present moment, a non-expert audience sometimes perceives and uses AI systems as black-box solutions, often without a clear understanding of their underlying principles and mechanisms. In this invited talk, we will critically examine these issues by navigating through physical and virtual world challenges, thereby elucidating the origins and present capacities of machine intelligence. This will be achieved through a multidisciplinary approach, dealing not only with AI algorithms but also with human evolution, physical and virtual embodiment, and other topics of interest. Ultimately, we will examine the current boundaries of AI development and discuss the implications for achieving human-like AI. This will include exploring both the real world and immersive virtual environments as AI research platforms.

Keywords: Artificial Intelligence; Machine Learning; Human-Level AI; Embodiment; Virtual Worlds.

Reproducibility as a Foundation for Reliable Computational Quantum Chemistry Data

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Abstract: Artificial intelligence (AI) and machine learning (ML) are transforming spectroscopy and chemical physics, yet their success depends on the availability of reliable and reproducible data. Computational quantum chemistry provides a powerful source of such data when workflows are transparent, systematically benchmarked, and rigorously documented. Reproducible protocols ensure that calculated spectra and molecular properties can be trusted, reused, and integrated into AI/ML models without hidden biases and inconsistencies. By embedding reproducibility into computational practice, quantum chemical results become trustworthy resources that can be directly reused, compared, and expanded within machine learning frameworks.

Beyond technical rigor, reproducibility is framed as a driver of equity and participation: by lowering barriers to entry, reproducible workflows empower broader engagement in global science. Reproducibility is not only a methodological necessity but also a cultural transformation, aligning with open science principles and the UN Sustainable Development Goals.

Keywords: Reproducibility; Computational Quantum Chemistry; Reliable Data; AI/ML.

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