

4TH GENERAL MEETING OF COST ACTION CA21101 "COSY"



27-29 April 2026

CSIC CENTRAL CAMPUS, MADRID

Fourth General Meeting

COST Action CA21101 – COSY
Book of Abstracts

Editors

Manuel Mendoza Hurtado

University of Córdoba and University of Jaén, Spain

Katarzyna M. Krupka

Social Media Manager of COSY, AbinitSim Unit, ABINITFOT Group, IFF-CSIC, Madrid, Spain

María Pilar de Lara-Castells

Action Chair, AbinitSim Unit, ABINITFOT Group, IFF-CSIC, Madrid, Spain

Contents

Preface	1
Committees	3
Program	5
Invited Speakers	9
K. Aidas – Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling	11
L. Antonov – Make Tautomerism Great Again: New Challenges and New Possibilities	12
M. Bartolomei – Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ -Graphyne	13
M. Biczysko – QM- and AI-based Approaches to the Structure and Spectroscopy of Biological Macromolecules	15
A. G. Császár – Intriguing Manifestations of Noncovalent Interactions	16
B. Fernández – Efficient ML Barrier Height and Reaction Enthalpy Corrections	17
A. Fortunelli – Theoretical Models of Physi- and Chemi-Sorption on Supported Oxide Clusters	18
L. González – Molecules in Confinement: How Environment Shapes Reactivity	19
S. Grubišić – Molecular Motion in Confined Systems: WG2 Highlights	20
M. Hochlaf – Spectroscopy and Collisional Dynamics of Medium Sized Molecules . . .	22
D. Kedziera – Reliable PESs for Astrochemistry with autoPES	23
T. Kirova – Theoretical Study of Sensing Properties of KL 1421 Luminophore	24
M. J. López – Novel Single-Atom and Single-Cluster Metal Catalysts on Carbon Materials	25

J. M. C. Marques – Bio-Inspired Functionalization of Chitosan for Water Remediation	26
F. Martín – New Directions in Attosecond Chemistry	27
M. Meuwly – Machine Learning Interactions for Chemical Reactions: Validation and Applications	28
M. Mudrich – Tracking Microhydration of Salt Molecules by Penning Ionization	29
S. Perepelytsya – Metallized Ag-DNA: Computational Insights	31
C. Puzzarini – Modeling Reactivity under Interstellar Conditions	32
M. Quack – High Resolution Spectroscopy, Parity Violation and Quantum Tunneling .	33
F. G. Requejo – Understanding Catalytic Clusters under Operando Conditions by XANES	34
P. Scheier – Experimental Solution of the Thomson Problem	35
M. L. Senent – Ab Initio Calculations for Non-Rigid Molecules with Torsional Modes .	36
K. Sillar – Chemically Accurate Ab Initio Prediction of Adsorption in MOFs	37
I. Solá – Steering Complex Photodissociation Dynamics through Vibrational Coherences	38
V. Sreckovic – Modeling Astrochemical Reaction Rates in Confined Molecular Environments	39
M. Striccoli – Controlled Assembly of Luminescent Colloidal Nanocrystals	40
S. Vajda – From Single Atoms to Bimetallic Clusters: Dehydrogenation and H ₂ Production	41
Contributed Talks	43
J. Alonso de la Fuente – Photoionization of Phosphorous Hydrides	45
A. Berisha – How Oxide Nanocages Trap the Most Inert Greenhouse Gases	46
S. Bromley – Identifying Observable IR Signatures of Nanosilicate Dust Grains in the ISM	47
A. Cassidy – Self-Polarizing Molecular Films; Confined Electric Fields in Ices	48
M. Dimitrijevic – Molecular Data for Characterization of Confined Molecular Systems	49
L. Gahramanli – Plasmonic–Semiconductor–Metal Oxide Synergy in a 2D/1D Photocatalyst	50
E. García Arroyo – Selectivity of D ₂ /H ₂ Isotopologues by Adsorption on Na-Graphene	51
J. R. B. Gomes – Breaking the Oxygen Shield for Reactivity Control in Mo ₂ C-Based MXenes	52
J. Krupa – Matrix-Isolation Photochemistry: Insights for Astrochemical Complexity .	53
D. Lauvergnat – Quantum Dynamics with a Smolyak Scheme: Clathrate Hydrates . .	54
M. Lewandowski – Iron Nitrides Under Oxidizing Conditions	55
A. Malani – Thermodynamics of Confined Water in Swelling of Clays	56

M. Mendoza – Dual-Locality Learning Under Neighbourhood Coupling	57
K. Neyman – When Platinum Becomes Not Noble: Pt-Oxide Clusters on Ceria	58
N. Pop – Electron Scattering on H_2^+ , BeH^+ and Isotopologues	59
M. Saldyka – Photo-Transformations of Thiazole Carboxylic Acids in Low-T Matrices	60
A. S. Sarac – Confined Magnetic Ferrite NPs in PAN Nanofibers for Tissue Engineering	61
A. Savarese – Energetic and Spectroscopic Insights into $\text{C}_3\text{H}_6\text{O}_2$ Isomers	62
N. Uras-Aytemiz – First-Principles Study of Defects in s-I and s-II Gas Hydrates . . .	63
Poster Presentations	65
N. Abidi – Grand-Canonical DFT Investigation of TM Sulfide Nanoalloys for N_2 Reduction	67
C. Adjal – The role of Water in Physisorption and Chemisorption of Pollutants within Copper Squarate: A DFT cluster study	68
A. P. Aizpurua Leyva – Dynamics and Binding in Light-Responsive HDAC Inhibitors	69
F. M. Balci – Vacancy Bjerrum Defects in s-II Type Clathrate Hydrates	70
P. Čechová – Geometry and Phase Behaviour of Nonlamellar Lipids in Confined Environments	71
F. Colmenero – On the use of theoretical models as tools for the stability prediction of actinide extractants	72
I. Demiroglu – Gaussian Approximation Potentials for Pt–Cu Nanoparticles	73
A. de Donato – Emergent Stability of 2D Metal Oxides at the Nanoscale	74
H. Dihingia – Towards Accurate Description of Intermolecular Induction	75
J. Fabila – ML Modeling for Infrared Spectra of TiC Nanoparticles	76
S. Hajizada – Modeling Photo-Induced Interactions at the Ag NP–Bio Interface	77
A. Karimova – Confined Drug Organization in Fe_3O_4 @Dextran Nanostructures	80
A. Kyriazis – When Two Worlds Collide: Silicate and Carbonaceous Dust Grains . . .	81
J. Maljkovic – Elastic Electron Scattering on Halogenated Anaesthetics	82
L. Martín Encinar – ML Interatomic Potentials for H Adsorption on TM–C Platforms	83
E. A. Miranda Sáenz – Theoretical Study of ORR on Graphene and Pt-Supported Catalysts	84
L. M. Molina – Hydrogen adsorption at graphene layers doped with transition metals: Insight from DFT simulations	85

S. Nuriyeva – Size-Dependent Optical and Luminescence of ZnO Hybrid Nanostructures	86
J. Shi – From Methanol to C ₂ Products: Methane Conversion over Ce–LaO _x Catalysts	87
A. Tadjer – Na ⁺ /Cu ⁺ Rivalry in Organic Solvents and on an Inert Surface	89
V. Vujcic – Molecular Dissociative Recombination Data for Confined Molecular Systems	90
İ. Yazgan – Fluorescent Au NPs Using Dyes for Sensing Applications	92
Sponsors & Acknowledgements	93

Preface

March 17, 2026

Dear Participants,

We are delighted to introduce the event:

4th General Meeting of COST Action CA21101 "COSY" (FOURTHCOSY)

FOURTHCOSY is a 4th general meeting framed within the COST (European Cooperation in Science and Technology) Action CA21101: Confined Molecular Systems: From a New Generation of Materials to the Stars ("COSY"). It is directed at established researchers, post-doctoral researchers, and PhD and Master students, who are interested in science of confined molecular systems, from those relevant in new (bio)materials research, to those playing a key role in astrochemistry. The meeting leverages the strategic position of the "COSY" network addressing scientific fields of the five Working Groups (WGs).

This meeting has been conceived as an opportunity for active networking among Action members with complementary and diverse expertise, with the aim of developing collaborations aligned with the goals of the Fourth Grant Period of the COST Action. It emphasizes the importance of integrating advanced computational approaches with experimental synthesis and characterization (e.g., spectroscopic) techniques in order to strengthen the fundamental understanding of confined molecular systems and their relevance across a wide range of scientific and technological contexts. This perspective reflects the principle that only processes that are fundamentally well understood can be effectively controlled (see the Memorandum of Understanding of the COST Action "COSY"). In this way, the meeting addresses scientific challenges relevant to the different Working Groups (WGs) are:

- WG1. Fundamental studies of intermolecular interactions: new methods, benchmarks on confined systems. For instance, understanding the nature of cluster-support (cluster-cluster) interactions at the molecular-level is essential for optimizing (photo)catalyst performance and designing novel catalysts with improved properties. Ab initio methods that can be applied to, e.g., metal cluster-support interactions are necessary. Besides complementing state-of-the-art dispersion corrected DFT approaches, they serve to develop inter-atomic potential models that, enhanced with machine-learned potential models, can be applied to study the molecular dynamics of supported metal clusters (e.g., diffusion and aggregation processes) on the nanosecond scale. Moreover, generation of high-level ab initio potential energy surfaces (PES) for both ground and excited electronic states using symmetry-adapted perturbation theory (SAPT) and multireference electronic-structure approaches. This includes the treatment of non-adiabatic couplings, enabling the study of photodissociation processes involving molecules and radicals relevant to the Earth's atmosphere.
- WG2. Molecular motion in porous, biomolecular, and environmentally confined systems can be effectively explored using advanced simulation methods. In this context, ab initio molecular dynamics (AIMD) plays a crucial role in elucidating the dynamics and reactivity of molecules interacting with porous materials at the atomic scale. Particularly relevant systems include encapsulated cluster-oxide nanoparticles within metal-organic frameworks (MOFs) and zeolites, which are of interest in a number of fields such as (photo-)catalysis. Despite its accuracy, AIMD is computationally demanding, which limits the accessible time and length scales. To address these challenges, the integration of GPU-based computing and machine-learning (ML) accelerators has emerged as a powerful strategy to significantly enhance computational efficiency while reducing overall cost. Moreover, while studies have primarily focused on electronic ground-state properties, there remains a lack of theoretical investigations exploring the excited states and, in particular, the optical properties of these encapsulated systems. For this purpose, density functional theory (DFT) and a combined approach that integrates DFT with reduced density matrix theory, have been used to investigate the optical response of these system under solar irradiation.
- WG3. Advanced theoretical and experimental studies of confined metal/oxide clusters are essential for advancing catalytic and nanotechnology applications. In particular, the unique chemical and physical properties of subnanometric metal clusters remain largely unexplored and poorly understood.

Addressing this gap requires the development of integrated frameworks that combine complementary experimental, computational, and theoretical approaches for the characterization of surface-supported, atomically precise clusters at the subnanometer scale. Key techniques include infrared and X-ray absorption spectroscopy, alongside state-of-the-art scanning transmission electron microscopy. On the theoretical side, systematic benchmarking of selected density functional theory (DFT) methods against high-level ab initio approaches is needed to accurately predict infrared (IR) and Raman spectra of subnanometric metal clusters. These efforts should be extended to incorporate critical effects such as alloying, anharmonicity, support interactions, solvation, and temperature. Furthermore, a deeper understanding of the electronic-structure origins of fluxional behavior is required, with particular emphasis on its relationship to conical intersections and Jahn–Teller distortions. These advances also pave the way for a deeper understanding of metal–biomolecule (sub)nanocontacts through the study of well-defined model systems.

- WG4. Time-resolved and reactive dynamics, spectroscopy, and simulations of unimolecular processes and bimolecular reactions in He nanodroplets. The use of He nanodroplets as an ultra-cold, chemically inert confining environment, to synthesize and study metal and metal oxide clusters, including charged helium droplets and the interaction of these clusters with small molecules and polycyclic aromatic hydrocarbons (PAHs) of catalytic relevance. Size selection and trapping of charged He nanodroplets and He nanodroplets-mediated aggregation of nanostructures.
- WG5. Computational, theoretical, and experimental investigation of the formation of molecules and matter in the interstellar medium and in planetary and solar atmospheres. Generation of high-level ab-initio potential energy surfaces in ground and excited states, including non-adiabatic couplings, allowing the study of the photo-dissociation of molecules and radicals present in the Earth's atmosphere, with special focus on phenomena relevant for environmental remediation, such as ozone depletion. Identification of astro-Complex Organic Molecules (COMs) and molecule/cluster astro-chemical environments by their IR features. Experimental and theoretical support for astronomical detections of neutral and ionic astro-COMs; confinement (interstellar ices, planetary soils), protective and destructive effects on the astroCOM formation, stability and photoreactivity.

The scientific program comprises 10 sessions, with 7 overview lectures, 25 invited lectures, 21 contributed hot-topic presentations, and 23 flash poster presentations. A Management Committee Meeting will be celebrated at the end of the meeting.

We are thankful to the COST Association and our sponsors, the journal “Physical Chemistry Chemical Physics” from the Royal Society of Chemistry and the journal Small Structures from the Wiley Editorial, for having supported us in organizing this event. In particular, we extend our heartfelt thank to our COST Action CA21101 “COSY” for having provided the funding and to our Grant Holder Institution (The Universidad de Cádiz), specially our Scientific Grant Holder Representative, Juan Carlos Hernández-Garrido, for their administration. We are also thankful to our host institution (CSIC) and in particular the Protocol Department at Central CSIC, the “Centro de Física Miguel Antonio Catalán”, and the “Institute of Fundamental Physics” (IFF) at Madrid, for their human and logistic resources. The Fundación Española para la Ciencia y la Tecnología (FECYT), the Ministerio de Ciencia, Innovación y Universidades, and the COST National Coordinator, Noelia Romero López, are gratefully acknowledged for all the support provided to our “COSY” COST Action. We are also grateful to Leticia González, Elena de Lara-Castells, and Víctor Castells for their valuable support in organizing this event. And last but not least, we would like to express our gratitude to all of you, the participants of this meeting, for your invaluable contributions.

We welcome all of you to Madrid and wish a very pleasant stay and plenty of interesting scientific discussions.

The Organizers,

María Pilar de Lara-Castells (Action Chair, AbinitSim Unit, ABINITFOT Group, IFF-CSIC)
Katarzyna M. Krupka (AbinitSim Unit, ABINITFOT Group, IFF-CSIC)
Alberto García-Vela (ABINITFOT Group, IFF-CSIC)
Alexandre Zanchet (ASTROMOL Group, IFF-CSIC)
Manuel Mendoza Hurtado (University of Córdoba)

Committees

Scientific Committee

- **María Pilar de Lara-Castells** – Action Chair
- **Cristina Puzzarini** – Action Vice-Chair
- **Juan Carlos Hernández-Garrido** – Scientific Grant Holder Representative
- **Piotr Żuchowski** – Working Group 1 Leader
- **Sonja Grubišić** – Working Group 2 Leader
- **Alessandro Fortunelli** – Working Group 3 Leader
- **Marcel Mudrich** – Working Group 4 Leader
- **Lauri Halonen** – Working Group 5 Leader

Local Organizing Committee

- **María Pilar de Lara-Castells** – Action Chair, AbinitSim Unit, ABINITFOT Group, IFF-CSIC
- **Katarzyna M. Krupka** – AbinitSim Unit, ABINITFOT Group, IFF-CSIC
- **Alberto García-Vela** – ABINITFOT Group, IFF-CSIC
- **Alexandre Zanchet** – IFF-CSIC
- **Manuel Mendoza Hurtado** – University of Córdoba and University of Jaén

- Including support by: Leticia González, Elena de Lara-Castells, and Víctor Castells

Management Committee

Management Committee Members representing 22 Full COST Member Countries (in alphabetic order): Austria, Bosnia and Herzegovina, Bulgaria, Croatia, Czech Republic, Denmark, Estonia, Finland, France, Greece, Hungary, Italy, Latvia, Lithuania, Poland, Portugal, Serbia, Spain, Switzerland, Türkiye, United Kingdom.

Contact Information

General Inquiries (Meeting Organization):

cosy-gm@csic.es

Program

Monday 27th April – Session I

9:00–9:15	Opening	Noelia Romero López (National COST Coordinator) & Marta I. Hernández (Director of IFF-CSIC)	María Pilar de Lara-Castells (COST Action Chair) & Berta Fernández (Session Chair)
9:15–9:45	Overview I	Alessandro Fortunelli (CNR, Italy)	The COSY Working Group 3: “Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale”
9:45–10:10	Invited Lecture	Stefan Vajda (Czech Academy of Science, Czech Republic)	From Single Atoms to Bimetallic Clusters and Nanostructured Surfaces: Selective Dehydrogenation & Hydrogen Production
10:10–10:35	Invited Lecture	María J. López (University of Valladolid, Spain)	Novel single-atom and single-cluster metal catalysts supported on carbon based layered materials
10:35–10:50	Contributed Talk	Lala Gahramanli (Baku State University, Azerbaijan)	Plasmonic–Semiconductor–Metal Oxide Synergy in a 2D/1D Graphene/Ag–Ag₂S–Ag₂O Photocatalyst for photocatalysis
10:50–11:05	Contributed Talk	Konstantin Neyman (ICREA & University of Barcelona, Spain)	When Platinum Becomes Not Noble: Platinum-Oxide Clusters Supported on Ceria
11:05–11:45	Coffee Break	“Claustro” Serrano 123	

Monday 27th April – Session II. Session Chair: Stefan Vajda (Czech Academy of Science, Czech Republic)

11:45–12:15	Overview II	Avelino Corma (UPV-CSIC, Spain)	Molecular Sieves for Reactions in Confined Spaces that Mimic Enzymatic Catalysts
12:15–12:40	Invited Lecture	Félix G. Requejo (UNLP and CONICET, Argentina)	Understanding Catalytic Clusters under Operando Conditions by XANES
12:40–13:05	Invited Lecture	Marinella Striccoli (CNR, Italy)	Controlled assembly of luminescent colloidal nanocrystals into highly ordered 3D superstructures
13:05–13:20	Contributed Talk	José R. B. Gomes (University of Aveiro, Portugal)	Breaking the Oxygen Shield for Reactivity Control in Mo₂C-Based MXenes
13:20–15:00	Lunch		

Monday 27th April – Session III. Session Chair: Heribert Reis (National Hellenic Research Foundation, Greece)

15:00–15:30	Overview III	Sonja Grubisic (University of Belgrade, Serbia)	Molecular Motion in Confined Systems: Advances in Simulations, Methods, and Models – WG2 Highlights
15:30–15:55	Invited Lecture	Kaido Sillar (University of Tartu, Estonia)	Chemically Accurate Ab Initio Prediction of Adsorption Thermodynamics and Isotherms in Metal–Organic Frameworks
15:55–16:20	Invited Lecture	Sergiy Perepelytsya (National Academy of Science, Ukraine)	Metallized Ag-DNA: Computational insights into a novel biomolecular material
16:20–16:35	Contributed Talk	Mikolaj Lewandowski (University in Poznań, Poland)	Iron nitrides under oxidizing conditions: What we know from model studies on 2D Fe(x)N islands on copper?
16:35–16:50	Contributed Talk	Avni Berisha (University of Prishtina, Kosovo)	How Oxide Nanocages Trap the Most Inert Greenhouse Gases
16:50–17:30	Coffee Break	“Claustro” Serrano 123	

Monday 27th April – Session IV. Session Chair: Alexandre Zanchet (IFF-CSIC)

17:30–17:55	Invited Lecture	Jorge M. C. Marques (University of Coimbra, Portugal)	Bio-inspired functionalization of chitosan for water remediation: computational insights into neonicotinoid sequestration
17:55–18:20	Invited Lecture	Teodora Kirova (University of Latvia, Latvia)	Theoretical study of the sensing properties of KL 1421 luminophore interacting with carotenoids

	Contributed Talk	Ateeque Malani (IIT Bombay, India)	Thermodynamics of confined water in swelling of clays
18:20–18:35	Contributed Talk	Jorge Alonso de la Fuente (IFF-CSIC, Spain)	Photoionization of phosphorous hydrides: experimental and theoretical comparison
Tuesday 28th April – Session V. Session Chair: Maria Krikunova (ELI Beamlines Facility, Czechia)			
9:00–9:30	Overview IV	Marcel Mudrich (University of Kassel, Germany)	Tracking microhydration of salt molecules by Penning ionization electron spectroscopy in helium nanodroplets
9:30–9:55	Invited Lecture	Kestudis Aidas (Vilnius University, Lithuania)	Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling
	Invited Lecture	Francesca Mocci (Universita Degli Studi Di Cagliari, Italy)	Environmental Control of G-Quadruplex Stability: A Molecular Dynamics Perspective
9:55–10:10	Contributed Talk	David Lauvergnat (CNRS and Université Paris-Saclay, France)	Quantum Dynamics with a Smolyak scheme. Applications to clathrate hydrates
10:10–10:35	Contributed Talk	Nevin Uras-Aytemiz (Bandırma Onyedİ Eylöl University, Turkey)	First Principal Study of Defects in s-I and s-II Gas Hydrates
10:35–11:15	Coffee Break	“Calustro” Serrano 123	
Tuesday 28th April – Session VI. Session Chair: Alia Tadjer (University of Sofia “St. Kliment Ohridski”, Bulgaria)			
11:15–11:40	Invited Lecture	Paul Scheier (University of Innsbruck, Austria)	Experimental Solution of the Thomson Problem
11:40–12:05	Invited Lecture	Liudmil Antonov (Bulgarian Academy of Sciences, Bulgaria)	Make Tautomerism Great Again: New Challenges and New Possibilities
12:05–12:30	Invited Lecture	Massimiliano Bartolomei (IFF-CSIC, Spain)	Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ-Graphyne
12:30–12:55	Contributed Talk	Nicolina Pop (Politechnica University of Timisoara, Romania)	Electron scattering on H_2^+, BeH^+ and their isotopologues: Dissociative recombination and ro-vibrational transitions
12:55–13:10	Contributed Talk	Milan Dimitrijević (Astronomical Observatory, Belgrade, Serbia)	Molecular data for characterization of confined molecular systems and corresponding databases
13:10–14:45	Lunch		
Tuesday 28th April – Session VII Session Chair: Aggelos Avramopoulos (University of Thessaly, Greece)			
14:45–15:10	Invited Lecture	Leticia González (University of Vienna, Austria)	Molecules in Confinement: How Environmental Shapes Reactivity and Photochemistry
15:10–15:35	Invited Lecture	Majdi Hochlaf (Gustave Eiffel University, France)	Spectroscopy and collisional dynamics of medium sized molecules
15:35–16:00	Invited Lecture	Dariusz Kędziera (Nicolaus Copernicus University in Torun, Poland)	Reliable PESs for Astrochemistry with autoPES: Methodology, Pitfalls, and Case Studies
16:00–16:15	Contributed Talk	Esther García-Arroyo (IFF-CSIC, Spain)	Selectivity of D_2/H_2 isotopologues by means of adsorption on a sodium-decorated graphene prototype: a quantum-mechanical low-pressure study
16:15–16:30	Contributed Talk	Andrew Cassidy (Aarhus University, Denmark)	Self-polarizing molecular films; confined electric fields in ices
16:30–17:00	Coffee Break	“Claustro” Serrano 123	
Tuesday 28th April – Session VIII. Session Chair: Marina Sekutor (Ruder Boskovic Institute, Croatia)			
17:00–17:25	Invited Lecture	Attila G. Csaszar (ELTE, Hungary)	Intriguing Manifestations of Noncovalent Interactions

17:25–17:50	Invited Lecture	Markus Meuwly (University of Basel, Switzerland)	Machine Learning Interactions for Chemical Reactions: Validation and Applications
17:50–18:15	Invited Lecture	Berta Fernández-Rodríguez (University of Santiago de Compostela, Spain)	Efficient Machine Learning barrier height and reaction enthalpy corrections for low- and mid-level quantum mechanical calculations
18:15–19:00	Flash Poster Presentations	Session Chair	Ljiljana Suručić (University of Banja Luka, Bosnia & Herzegovina)
Wednesday 29th April – Session IX. Session Chair: Henrik Grum Kjærgaard (University of Copenhagen, Denmark)			
9:00–9:30	Overview VII	Cristina Puzzarini (University of Bologna, Italy)	Modeling Reactivity under Interstellar Conditions
9:30–9:55	Invited Lecture	María Luisa Senent-Díez (IEM-CSIC, Spain)	Ab initio calculations applied to the study of organic non-rigid molecules with (at least) three interacting torsional modes.
9:55–10:20	Invited Lecture	Malgorzata Biczysko (University of Wrocław, Poland)	QM- and AI-based Approaches to the Structure and Spectroscopy of Biological Macromolecules
10:20–10:35	Contributed Talk	Magdalena Saldyka (University of Wrocław, Poland)	Photo-transformations of thiazole carboxylic acids in low temperature matrices
10:35–10:45	Contributed Talk	Justyna Krupa (University of Wrocław, Poland)	Matrix-Isolation Photochemistry: Experimental–Theoretical Insights for Astrochemical Complexity
10:45–11:00	Contributed Talk	Alessandra Savarese (University of Bologna, Italy)	Energetic and Spectroscopic Insights into the C₃H₆O₂ Isomer Family for Astrochemical Purposes
11:00–11:30	Coffee Break	“Claustro” Serrano 123	
Wednesday 29th April – Session X. Session Chair: Alberto García Vela (IFF-CSIC)			
11:30–11:55	Invited Lecture	Fernando Martín (Universidad Autónoma de Madrid, Spain)	New directions in Attosecond Chemistry
11:55–12:20	Invited Lecture	Ignacio Solá (Universidad Complutense de Madrid, Spain)	Steering Complex Photodissociation Dynamics through Initial Vibrational Coherences
12:20–12:45	Invited Lecture	Martin Quack (ETH Zurich, Switzerland)	High resolution spectroscopy, parity violation and quantum tunneling dynamics in chiral molecules of astrophysical and general interest
12:45–13:10	Invited Lecture	Vladimir Sreckovic (Institute of Physics Belgrade, Serbia)	Modeling Astrochemical Reaction Rates in Confined Molecular Environments
13:10–13:25	Contributed Talk	Stefan Bromley (University of Barcelona, Spain)	Identifying Observable Infrared Signatures of Nanosilicate Dust Grains in the Interstellar Medium
13:25–13:40	Contributed Talk	Manuel Mendoza-Hurtado (University of Córdoba, Spain)	Dual-locality learning under neighbourhood coupling: interpretable and transferable models for structured trace data
13:40–13:55	Contributed Talk	Abdulkadir Sezai Sarac (Istanbul Technical University, Turkey)	Confined Magnetic Ferrite Nanoparticles in Polyacrylonitrile Nanofibers: Tunable Nanostructures for Tissue Engineering
13:55–14:55	Lunch		
14:55–15:20	Best Contributed Talk and Poster Awards	Katarzyna M. Krupka (IFF-CSIC) & Manuel Mendoza Hurtado (University of Cordoba). Poster Awards, SPONSOR: RSC PCCP	María J. López (University of Valladolid) & Alessandro Fortunelli (CNR, Italy). Contributed Talk Awards, SPONSOR: Wiley Small Structures
15:20–15:50	Coffee Break	“Claustro” Serrano 123	
15:50–19:15	MC Meeting		
19:30–21:00	Get-together Event	“Claustro” Serrano 123	

Invited Speakers

Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling

Kęstutis Aidas¹, Žyginta Murnikova¹, Einaras Sipavičius¹, Dovilė Lengvinaitė¹

¹*Institute of Chemical Physics, Faculty of Physics, Vilnius University, Saulėtekio ave. 3,
LT-10257 Vilnius, Lithuania
kestutis.aidas@ff.vu.lt*

Molecular dynamics (MD) simulations combined with the quantum mechanics/molecular mechanics (QM/MM) models have proven to be a powerful computational technique for accurate predictions of electronic properties of extensive molecular systems. In this presentation we will discuss our recent successes in describing the structural and nuclear magnetic resonance (NMR) properties of ionic liquid (IL) systems using the integrated MD-QM/MM scheme based on classical MD simulations and density functional theory.

Relative ¹H NMR spectra of the [C₄mim][BF₄] IL and its aqueous mixtures were recently computed with the overall root-mean-square deviation of 0.2 ppm.^a Even the previously troublesome chemical shift of the proton at position 2 in the imidazolium ring was also predicted very accurately.

Scrutinizing intermolecular organization in aqueous mixtures of [Cho][Lys] IL, the analysis of MD trajectories revealed the formation of highly polar and less polar domains in IL-rich mixtures.^b Isolated water pockets were found to be situated at the interface of the polar and nonpolar ionic domains. The experimentally observed upfield shift of the NMR signal of protons in fast exchange with the rising content of the IL was successfully rationalized.

We have used the MD-QM/MM computational scheme to study the molecular mechanism behind the increased solubility of antidiabetic drug molecule glibenclamide in aqueous solution of [Cho][Trp] IL.^c Classical MD simulations indicate prolific interactions between the constituent ions of the IL and glibenclamide, and thus these ions are screening the hydrophobic drug molecule from the polar water molecules.

Very recent computational results regarding the structural and NMR properties of a model tetrapeptide Ala-Glu-Pro-Phe in aqueous mixtures of [C₂mim][TFA] IL will be presented as well.

References:

^a Sipavičius, E.; Majauskaitė, G.; Lengvinaitė, D.; Bielskutė, S.; Klimavicius, V.; Mocci, F.; Laaksonen, A.; Aidas, K. Towards accurate modelling of ¹H NMR spectra of ionic liquids: The case of [C₄mim][BF₄] and its aqueous mixtures. *Chem. Phys. Lett.*, 2025, 877, 142295. <https://doi.org/10.1016/j.cplett.2025.142295>

^b Sipavičius, E.; Mikalauskas, L.; Klimavicius, V.; Aidas, K. Intermolecular organization in aqueous mixtures of choline lysinate studied via NMR and molecular dynamics/quantum mechanics. *Phys. Chem. Phys. Chem. Phys.*, 2025, 27, 14790-14803. <https://doi.org/10.1039/D5CP00861A>

^c Murnikova, Ž.; Klimavicius, V.; Mocci, F.; Laaksonen, A.; Aidas, K. On the mechanism behind the enhanced solubility of glibenclamide in aqueous ionic liquid solution. *J. Mol. Liq.*, 2025, 422, 127153. <https://doi.org/10.1016/j.molliq.2025.127153>

Make Tautomerism Great Again: New Challenges and New Possibilities

Liudmil Antonov

*University Centre on Tautomeric Research and Education in Science and Technology,
University of Plovdiv, Plovdiv 4000, Bulgaria
Institute of Electronics, Bulgarian Academy of Sciences, Sofia 1782, Bulgaria
E-mail address: lantonov@tautomer.eu*

Prototropic tautomerism is one of the most important phenomena in organic chemistry despite the relatively small proportion of molecules in which it can occur. Tautomers are the chameleons of chemistry, capable of changing by a simple change of environment from an apparently established structure to another not perhaps till then suspected, then back again when the original conditions are restored, and of doing this in an instant: intriguing, disconcerting, perhaps at times exasperating¹. It therefore becomes vital to know and/or to predict which tautomer is the major one, since not only structure but chemical properties are bound up with this.

Although currently this field of research is considered mainly as fundamental one, it gives a lot of opportunities for useful applications.

In the present lecture a historical overview of the concept of the tautomerism and methods for investigations of tautomeric systems will be given. Fundamental processes, both structural and environmental, affecting the tautomerism will be discussed. Several tautomeric systems will be considered from the viewpoint of the applicability of the tautomerism and proton transfer: excited state proton transfer, tautomerism in the drug design (curcumin solubility case), tautomeric metal binding ligands (red shift upon complexation), tautomeric vs zwitterionic proton cranes as prototypes of molecular switches and motors.

References:

¹ Taylor, P.J.; van der Zwan, G.; L. Antonov, L. Tautomerism: Introduction, History, and Recent Developments in Experimental and Theoretical Methods. Tautomerism Methods and Theories. (Ed.: L. Antonov), Wiley-VCH, Weinheim, Germany, 2013, pp. 1–24

Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ -Graphyne

Massimiliano Bartolomei¹, Giacomo Giorgi² and Fernando Pirani³

¹Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Madrid (Spain) presenting author (maxbart@iff.csic.es)

²Department of Civil & Environmental Engineering, The University of Perugia, Perugia (Italy)

³Department of Chemistry, Biology & Biotechnology, The University of Perugia, Perugia (Italy)

Addressing carbon dioxide (CO₂) emissions represents a major challenge for modern society and the development of innovative and efficient technologies for CO₂ capture and conversion is paramount. Carbon materials are promising candidates for this purpose due to their versatility and sustainability and the recently synthesized^{1,2} γ -graphyne 2D carbon layers are here theoretically investigated to assess their CO₂ adsorption capacity. The motivation comes from a previous validation³ of γ -graphyne as an optimal substrate for sodium (Na) decoration with single alkali atoms hosted by each of its subnanometric pores and providing the 2D carbon layer with strongly adsorbed and positively charged metal species.

By means of a combination of finite-cluster models and periodic boundary condition DFT calculations (at the B3LYP-D3 and PBE-D3(BJ) levels, respectively) we demonstrate that Na decorated γ -graphyne layers show a significant and selective adsorption of CO₂ with respect to other representative post-combustion gas species. In particular, this occurs for a high density of Na decoration and in such cases CO₂ is adsorbed as an activated anionic species. Importantly, in this activated form CO₂ becomes very reactive and can be easily converted into sodium formate in presence of water via a highly exothermic process.

The obtained results suggest that Na-decorated γ -graphynes represent very promising adsorbing platforms based on earth-abundant elements to be used for the efficient CO₂ capture and *in-situ* conversion into added-value products.

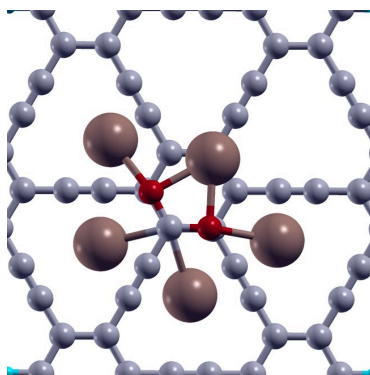


Fig. 1 CO₂ strongly adsorbed ($E_{int} \cong -1.9$ eV) on γ -graphyne featuring a high density of sodium decoration. The molecular species is adsorbed as an anionic and activated form which can be easily converted into sodium formate.

References:

1. V.G. Desyatkin et al., *J. Am. Chem. Soc.* **144**, 17999–18008 (2022)
2. S. He et al., *Nanoscale Adv.* **5**, 2487–2492 (2023)
3. M. Bartolomei et al. *ACS Materials Letters*, **6**, 4682–4689 (2024)

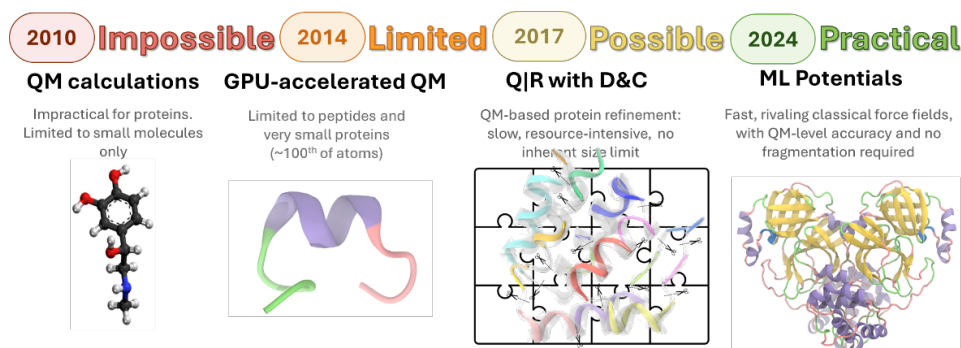
QM- and AI-based Approaches to the Structure and Spectroscopy of Biological Macromolecules

Malgorzata Biczysko

University of Wroclaw, Wroclaw, 50-384, Poland

Protein structures and their physicochemical properties are essential for understanding biological function and improving drug–protein interactions. Most structures in the Protein Data Bank (PDB) [1] have been determined by X-ray crystallography and cryo-electron microscopy, while recent advances in structure prediction [2] support but do not replace experimental studies [3].

Spectroscopic techniques provide complementary insight into protein dynamics and environmental effects, yet structural and spectroscopic data are often analyzed separately. Quantum chemistry (QM) computations establish a physically grounded link between molecular structure and spectroscopic observables, enabling direct comparison with experiment. This is particularly important for proteins and protein–ligand systems, where local interactions and spatial confinement can significantly affect structural and spectral properties. In this talk, I will present a project developing integrated computational tools that use QM and AI-based approaches to improve structural consistency and advance understanding of protein properties through systematic integration of experimental data [4–10].



References:

- [1] H.M. Berman et al., Nucleic Acids Research 28 (2000) 235, <http://www.rcsb.org>
- [2] J. Abramson, et al., Nature 630 (2024) 493.
- [3] T. C. Terwilliger et al. Nature Methods 21 (2024) 110.
- [4] M. Zheng, J. R. Reimers, M. P. Waller, P. V. Afonine, Acta Cryst. D 73 (2017) 45.
- [5] M. Zheng, N. W. Moriarty, Y. Xu, J. R. Reimers, P. V. Afonine, M. P. Waller, Acta Cryst. D 73 (2017) 1020.
- [6] M. Zheng, M. Biczysko, Y. Xu, N. W. Moriarty, H. Kruse, A. Urzhumtsev, M. P. Waller, P. V. Afonine, Acta Cryst. D 76 (2020) 41.
- [7] L. Wang, H. Kruse, O. V. Sobolev, N. W. Moriarty, M. P. Waller, P. V. Afonine, M. Biczysko, Acta Cryst. D 76 (2020) 1184.
- [8] Y. Wang, H. Kruse, N. W. Moriarty, M. P. Waller, P. V. Afonine, M. Biczysko, Theor. Chem. Acc. 142 (2023) 100.
- [9] Y. Liu, M. Biczysko, N. W. Moriarty, Acta Cryst. D 78 (2022) 43.
- [10] R. Zubatyuk, M. Biczysko, K. Ranasinghe, N. W. Moriarty, H. Gokcan, H. Kruse, B. K. Poon, P. D. Adams, M. P. Waller, A. E. Roitberg, O. Isayev, P. V. Afonine, Nat. Commun. 16 (2025) 9224.

Intriguing Manifestations of Noncovalent Interactions

Attila G. Császár¹

¹*Institute of Chemistry, ELTE Eötvös Loránd University
Pázmány Péter sétány 1/A, Budapest, Hungary, H-1117*

Interest in noncovalent interactions has grown substantially in recent years, leading to numerous experimental and computational investigations of weakly bound dimers. Studies of their structures, dynamics, and vibrational fingerprints have revealed several intriguing—and in some cases puzzling—phenomena. This contribution focuses on such observations arising from high-level computational studies.

For weakly bound oligomers, constrained geometry optimizations are often performed, followed by harmonic vibrational analyses at geometries that are not true stationary points. A typical example is a counterpoise-corrected geometry optimization followed by a harmonic analysis that neglects the counterpoise correction. We observed^a that extreme care is required in handling the resulting nonzero forces (this is the nonzero force dilemma^b), as even the Hessian index can depend on the choice of coordinates in which these forces are neglected.

We have developed^c full-dimensional potential energy surfaces for a wide range of systems involving linear triatomic molecules—neutral species such as CO₂, CS₂, N₂O, and OCS, as well as charged species including HHe⁺, HNe⁺, HAr⁺, HHeNe⁺, HHeAr⁺, and HNeAr⁺—solvated by a single rare-gas atom (He, Ne, or Ar). A particularly intriguing structural finding^d is the pronounced quantum delocalization of the solvating atom.

Finally, dynamical and spectroscopic studies based on newly developed full-dimensional potential energy surfaces for the N₂^e and CO^f homodimers reveal additional unexpected behavior. In particular, the calculated rovibrational spectra of the N₂ dimer exhibit clear signatures of quasistructural^g behavior.

References:

^aTóbiás, R.; Árendás, P.; Császár, A. G. Normal-Mode Vibrational Analysis of Weakly Bound Oligomers at Constrained Stationary Points of Arbitrary Order. *J. Chem. Theory Comput.*, 2022, 18, 1788-1798. <https://doi.org/10.1021/acs.jctc.1c01148>

^bAllen, W. D.; Császár, A. G. On the Ab Initio Determination of Higher-Order Force Constants at Nonstationary Reference Geometries. *J. Chem. Phys.* 1993, 98, 2983-2015. <https://doi.org/10.1063/1.464127>

^cSimkó, I.; Tóbiás, R.; Császár, A. G. Unusual Dynamics and Spectroscopic Fingerprints of van der Waals Dimers Formed by Linear Molecules and Rare-Gas Atoms, *J. Chem. Theory Comput.* 2023, 19, 8767-8781. <https://doi.org/10.1021/acs.jctc.3c00914>

^dSimkó, I.; Schran, C.; Briec, F.; Fábri, C.; Asvany, O.; Schlemmer, S.; Marx, D.; Császár, A. G. Quantum Nuclear Delocalization and its Rovibrational Fingerprints, *Angew. Chem. Int. Ed.* 2023, 62, e202306744. <https://doi.org/10.1002/anie.202306744>

^eTóbiás, R.; Fábri, C.; Bosquez, M.; Kodrycka, M.; Patkowski, K.; Császár, A. G. Rovibrational Dynamics of the Quasistructural N₂ dimer. *Commun. Chem.* 2025, 8, 339. <https://doi.org/10.1038/s42004-025-01716-7>

^fBosquez, M.; Zuchowski, P. S.; Császár, A. G. Surveying the ground electronic state potential energy surface of the “mysterious” CO dimer. *Mol. Phys.* 2026, submitted for publication.

^gCsászár, A. G.; Fábri, C.; Sarka, J. Quasistructural Molecules. *WIREs Comput. Mol. Sci.*, 2020, 10, e1432. <https://doi.org/10.1002/wcms.1432>

Efficient Machine Learning barrier height and reaction enthalpy corrections for low- and mid-level quantum mechanical calculations

Omar Rodríguez-López, Emilio Martínez-Núñez, Saulo A. Vázquez, and
Berta Fernández Rodríguez

*University of Santiago de Compostela, Department of Physical Chemistry, Santiago de
Compostela, Spain*

Automated methods for the prediction of reaction mechanisms are a key tool for the study of complex chemical reactions. Many of these methodologies involve a first step based on extensive exploration of the configurational space using a low-level electronic structure method, followed by a further refinement by high-level calculations, which results in a considerable computational effort when a complex reaction involves a very large number of elementary steps. Therefore, the availability of efficient, low- or mid-cost yet accurate approaches for thorough exploration of complex reactive potential energy surfaces is of great interest. In this work, efficient machine learning (ML) corrections were developed to improve the accuracy of a few low- and mid-level electronic structure methods for the calculation of barrier heights and reaction enthalpies. We followed the Δ -ML strategy, training the model on the energies of stationary points in the RDB7 dataset.^a The baseline methods utilized in this work were PM6, HF/3-21G, and r²SCAN-3c. The results show that the r²SCAN-3c method, together with our corrections, provides very good accuracy, similar to or even surpassing that of other ML potentials published recently. The use of energies only, without including gradients or Hessians, makes it easier to extend the approach to large chemical spaces.

References:

^a Spiekermann, K.; Pattanaik, L.; Green, W.H. High accuracy barrier heights, enthalpies, and rate coefficients for chemical reactions. *Sci. Data* 2022, 9 (417), 1-12. <https://doi.org/10.1038/s41597-022-01529-6>.

The COSY Working Group 3: “Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale”

Alessandro Fortunelli¹, Lyudmila Moskaleva²

¹CNR-ICCOM, Consiglio Nazionale delle Ricerche, Pisa, Italy

²University of the Free State, South Africa

email: alessandro.fortunelli@cnr.it

We will present a report on the achievements of WG3 in the last Grant Period. WG3 has delivered a coordinated and high-impact research program advancing the fundamental understanding, predictive modeling, and application of atomically precise clusters and nanostructured materials across catalysis, energy conversion, optoelectronics, and biomedicine. Through tight integration of first-principles theory, machine learning, synthesis, and operando spectroscopy, WG3 has established robust structure-property-function relationships spanning subnanometer clusters to mesoscale assemblies.

A central focus has been the mechanistic role of size, support, and ligand effects in cluster catalysis. Size-selected Pt clusters on TiO₂ and SnO₂ revealed how metal-support interactions and size govern CO oxidation activity/stability (Valtera *et al.*, *Small Struct.*, 2025). MD simulations of Au nanoparticles demonstrated orientation- and support-dependent melting (Pavloudis *et al.*, *Small Struct.*, 2025). Ligand-protected Au nanoclusters exhibited support- and pretreatment-dependent selectivity in alkyne hydrogenation (Banu *et al.*, *Nanoscale*, 2025), while Cu-doped Au clusters showed how staple flexibility and partial deligation govern electrochemical CO₂ reduction (Ibáñez-Alé *et al.*, *Small*, 2024). Methane-to-methanol conversion over CeO₂ identified the cooperative role of water and oxygen in sustaining reactive hydroxyl species (Li *et al.*, *ACS Catal.*, 2025). SrFe_{0.9}Mo_{0.1}O_{3-δ} perovskite was demonstrated as a robust catalyst for nonredox water splitting (Anemone *et al.*, *Small Struct.*, 2025). At the atomic scale, DFT studies identified graphdiyne and boron-graphdiyne as platforms for single-atom/cluster catalysis (Sandoval Menjívar *et al.*, *Small Struct.*, 2026). High-level *ab initio* benchmarking clarified the electronic origins of fluxionality, linking Jahn-Teller distortions, conical intersections, and stability (Krupka *et al.*, *Small Struct.*, 2026), while systematic DFT studies of transition-metal tetramers and hexamers revealed cross-scale correlations between structural motifs, energetics, and “magic” patterns (Garcia-Alfonso *et al.*, *Small Struct.*, 2026). A defining contribution of WG3 lies in methodological innovation. Conformal sampling of catalytic processes achieved subchemical accuracy with high-throughput capability (Roongcharoen *et al.*, *J. Chem. Theory Comput.*, 2025; Melani *et al.*, *J. Phys. Chem. C*, 2025), enabling transferable MLIPs for alloy screening. Dispersion-corrected MLIPs accurately reproduced structural, thermodynamic, and dynamical properties of water and aqueous MgCl₂ (Ferretti *et al.*, *J. Chem. Inf. Model.*, 2025). Beyond catalysis, WG3 explored functional nanomaterials, e.g., Mn-doped perovskite supercrystals with spatially resolved emission (Dibenedetto *et al.*, *Small Struct.*, 2025); defect-engineered hybrid perovskites for enhanced electromagnetic wave absorption (Cai *et al.*, *Small Struct.*, 2025); tunable nonlinear optical response in perylene diimides (Skentzos *et al.*, *Mater. Adv.*, 2026); and iron oxide nanoclusters enhanced phosphate transport under dialysis conditions (Lucante *et al.*, *Small Struct.*, 2026).

These results establish predictive, mechanistically grounded design principles for confined metal and metal-oxide nanostructures, bridging atomic-scale insight with functional performance in catalysis, materials science, and biomedicine.

Molecules in Confinement: How Environmental Shapes Reactivity and Photochemistry

Leticia González¹

¹*Institute of Theoretical Chemistry, Faculty of Chemistry, University of Vienna,
Währingerstrasse 17, 1090 Vienna, Austria
leticia.gonzalez@univie.ac.at*

Chemical function does not emerge from molecules alone, but from molecules embedded in complex environments. For this reason, understanding how microsolvation influences reactivity and stability of molecules remains a central challenge in catalysis and beyond. In this talk, I will present a theoretical perspective on how local surroundings modulate reactivity, photochemistry, and energy flow in several systems. One example is a manganese-vanadium cubane water oxidation catalyst, $[\text{Mn}_4\text{V}_4\text{O}_{17}(\text{OAc})_3]^{3-}$, which we have characterized in different environments, comparing its properties in dry acetonitrile, acetonitrile-water mixtures and when embedded in a block copolymer membrane based on poly[2(dimethylamino)ethyl methacrylate] (pDMAEMA), here modelled as a polymer brush. Second, we explore a photosensitizer–bridge–catalyst dyad, where the bridge is protected by a mechanically interlocked ring reminiscent of a rotaxane architecture. Confining within this heterodinuclear rotaxane photocatalyst preserves both, structural integrity and activity of its components, leading to enhanced long-term photocatalytic performance, under enzyme-like H-bond-driven substrate preorganization. Finally, we examine the ultrafast photodynamics of a ruthenium complex in water, following excited-state relaxation and the associated energy flow from the solute into the solvent. These results highlight the active role of the environment in mediating dissipation pathways and determining excited-state lifetimes.

Molecular Motion in Confined Systems: Advances in Simulations, Methods, and Models - WG2 Highlights

Sonja Grubišić

sonja.grubisic@ihtm.bg.ac.rs

*University of Belgrade, Institute of Chemistry, Technology, and Metallurgy, National
Institute of Republic of Serbia, Njegoševa 12, Belgrade, 11000 Serbia,*

Working Group 2 (WG2), Molecular Motion in Confined Systems, brings together nearly 200 experts focused on developing efficient computational approaches, from coarse-grained to atomistic and mesoscopic molecular dynamics, in order to elucidate molecular behavior in confined environments such as molecular cages, interfaces, and systems exposed to strong electromagnetic or optical fields. Through extensive international collaboration, WG2 members have delivered significant advances in both methodology and application.

In particular, collaborative teams have developed multiscale first-principles frameworks combined with Grand Canonical Monte Carlo simulations to accurately predict gas adsorption in novel metal–organic frameworks (MOFs), achieving improved performance for carbon dioxide and sulfur compound capture. Complementary studies on porous Mg-MOF-74 materials have optimized gas separation strategies, contributing to enhanced energy efficiency in carbon capture and biogas upgrading.

WG2 activities also extend to biological confinement, where computational investigations have clarified how crowding and nanoscale restriction modulate DNA–polyamine interactions, providing insights into molecular organization relevant for biotechnology. On the theoretical side, advances in semiclassical methodologies have helped bridge the gap between accuracy and computational cost in quantum molecular dynamics, enabling improved modeling of catalytically relevant systems such as copper clusters. Understanding hydrogen bonding at the quantum level is one of science’s fundamental challenges. Continued work on hydrogen-bond quantum effects and light-driven molecular processes further strengthens the connection between quantum molecular dynamics and emerging applications, such as artificial photosynthesis and renewable energy.



Figure 1. Chemically Accurate Prediction of CO₂ Adsorption Thermodynamics in Metal-Organic Framework CALF-20 (left); Conformational flexibility of spermidine³⁺ interacting with DNA double helix (middle); WG2 participants during the COST COSY Training School, 19-22 September 2023, Belgrade (right)

Together, these achievements demonstrate WG2’s strong commitment to integrate state-of-the-art computational methods with collaborative research to address key challenges in confined molecular systems, with impact across environmental sustainability, biomedicine, and

energy technologies. This overview talk will highlight several important scientific results and collaborative outcomes of WG2 of COSY COST Action [1-14].

Beyond research outputs, WG2 has actively supported community building and knowledge transfer through several very successful training schools (Belgrade, Iași, Kyiv, Ostrava, and Coimbra), an online WG2 workshop, and an upcoming in-person WG2 meeting planned for May 2026 in Lausanne, Switzerland. Further details are available on the meeting websites and the COSY Action website, where a complete list of WG2 publications can also be found.

Acknowledgements: I thank all COSY WG2 members for their continuous efforts and numerous contributions, and for the opportunity to represent this very productive community. WG2 activities have been made possible through strong commitment and collaborative work of their members.

References:

1. Sillar, K.; Grubišić, S.; Đorđević, I. S.; Hochlaf, M. Chemically Accurate Prediction of CO₂ Adsorption Thermodynamics in Metal–Organic Framework CALF-20: Complementary Ab Initio Modeling and Grand Canonical Monte Carlo Simulations. *Small Structures*, 2026, 7(2). <https://doi.org/10.1002/ssstr.202500781>
2. Jovanovic, M.; Bernhard, N.; Baldofski, M.; Rybicki, M.; Stankovic, I. Linking Density and Nanoscale Crystallinity to Hydration in Nafion PEMFC Membranes: Insights From Experiment and Molecular Dynamics Simulations. *Small Structures*, 2026, 7(2). <https://doi.org/10.1002/ssstr.202500573>
3. Perepelytsya, S.; Vasiliu, T.; Laaksonen, A.; Engelbrecht, L. D. V.; Brancato, G.; Mocci, F. Conformational Flexibility of Spermidine³⁺ Interacting with DNA Double Helix. *Journal of Molecular Liquids*, 2023, 389, 122828. <https://doi.org/10.1016/j.molliq.2023.122828>
4. Sillar, K.; Kundu, A.; Sauer, J. Ab Initio Prediction of Adsorption Selectivities for Binary Gas Mixtures on a Heterogeneous Metal–Organic Framework Surface. *The Journal of Physical Chemistry C*, 2023, 127(27), 13317–13326. <https://doi.org/10.1021/acs.jpcc.3c02494>
5. Grubisic, S.; Dahmani, R.; Djordjevic, I.; Sentic, M.; Hochlaf, M. Selective Adsorption of Sulphur Dioxide and Hydrogen Sulphide by Metal–Organic Frameworks. *Physical Chemistry Chemical Physics*, 2023, 25, 954–965. <https://doi.org/10.1039/D2CP04295A>
6. Garrido-Aldea, J.; de Lara-Castells, M. P. Aggregation and Support Effects in the Oxidation of Fluxional Atomic Metal Clusters: The Paradigmatic Cus Case. *Physical Chemistry Chemical Physics*, 2022, 24, 24810–24822. <https://doi.org/10.1039/D2CP02169B>
7. Vaniček, J. Family of Gaussian Wavepacket Dynamics Methods from the Perspective of a Nonlinear Schrödinger Equation. *The Journal of Chemical Physics*, 2023, 159. <https://doi.org/10.1063/5.0146680>
8. Murnikova, Z.; Klimavicius, V.; Mocci, F.; Laaksonen, A.; Aidas, K. On the Mechanism Behind the Enhanced Solubility of Glibenclamide in Aqueous Ionic Liquid Solution. *Journal of Molecular Liquids*, 2025, 422, 127153. <https://doi.org/10.1016/j.molliq.2025.127153>
9. Hippler, M.; Oeltjen, L.; Quack, M. Mode-Selective Vibrational-Tunneling Dynamics in the N = 2 Triad of the Hydrogen-Bonded (HF)₂ Cluster. *Israel Journal of Chemistry*, 2023, 63, e202300092. <https://doi.org/10.1002/ijch.202300092>
10. Paloncýová, M.; Valério, M.; Dos Santos, R. N.; Kührová, P.; Šrejber, M.; Čechová, P.; Dobchev, D. A.; Balasubramani, A.; Banáš, P.; Agarwal, V.; et al. Computational Methods for Modeling Lipid-Mediated Active Pharmaceutical Ingredient Delivery. *Molecular Pharmaceutics*, 2025, 22(3), 1110–1141. <https://doi.org/10.1021/acs.molpharmaceut.4c00744>
11. Nedělníková, A.; Stadlbauer, P.; Otyepka, M.; Kührová, P.; Paloncýová, M. Atomistic Insights Into Interaction of Doxorubicin With DNA: From Duplex to Nucleosome. *Journal of Computational Chemistry*, 2025, 46(3). <https://doi.org/10.1002/jcc.70035>
12. Tippner, S.; Hernández-Castillo, D.; Schacher, H. F.; González, L. All-Atom Molecular Dynamics Simulations of Grafted Poly(N-dimethylaminoethyl methacrylate) Brushes. *The Journal of Physical Chemistry B*, 2025, 129(7), 2105–2114. <https://doi.org/10.1021/acs.jpcc.4c07928>
13. Li, X.; Yin, X.; Bai, Y. L.; Biczysko, M. Interpretation and Prediction of Optical Properties: Novel Fluorescent Dyes as a Test Case. *Frontiers in Physics*, 2023, 11. <https://doi.org/10.3389/fphy.2023.1236987>
14. Martín Santa Daría, A.; Hernández-Rodríguez, J.; Ibele, L. M.; Gómez, S. Photofragmentation of Cyclobutanone at 200 nm: TDDFT vs CASSCF Electron Diffraction. *The Journal of Chemical Physics*, 2024, 160, 114303. <https://doi.org/10.1063/5.0197895>

Spectroscopy and collisional dynamics of medium sized molecules

Majdi Hochlaf¹

¹ *Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes, 77454 Champs sur Marne, France.*

I will present several examples of the use of high-level theoretical characterization of low-energy isomers of molecular species (MS) relevant in interstellar media (ISM) and the subsequent collision treatment to deduce their abundances in these media. First, we explore their ground state potential energy surface using coupled cluster (CC) theory. Next, precise equilibrium structures and relative energies are determined using composite schemes based on CC theory and taking into account extrapolation to the complete basis set limit and core correlation effects. For all stable forms, rotational spectroscopy parameters as well as fundamental vibrational frequencies and infrared intensities are also determined. Furthermore, to support astrophysical modeling and improve abundance estimates of these MSs in the ISM, we conduct extensive theoretical investigations on the collisional excitation and de-excitation of these molecules by the most abundant species in the ISM (i.e., X = H₂, H, and He). Our strategy is as follows: first, we generate an accurate multidimensional potential energy surface for the weakly bound MS–X complex at the CCSD(T)-F12/aug-cc-pVTZ level, where we also take into account basis set superposition error corrections. Next, an analytical form of this potential is derived, which is then incorporated into close-coupling quantum scattering calculations for MS colliding with X, yielding state-to-state cross sections and temperature-dependent rate coefficients under conditions relevant to the ISM (5–100 K).

Our work should contribute to the identification of MS in laboratory and astrophysical environments. In particular, it should enable a more accurate interpretation of current and future astronomical observations dealing with MS relevant to astrophysics

Several examples will be presented, including the spectroscopic characterization of protonated HNCO species (in collaboration with Prof. C. Puzzarini group, U. Bologna, Italy),^a the rotational (de-)excitation of cis-/trans-HONO colliding with He (in collaboration with Prof. D. Ben Abdallah group, U. Tunis, Tunisia)^b and the rotational (de-)excitation of cis-HNSO colliding with He (in collaboration with Dr. B. Mehnen and Prof. P. Zuchowski group, U. Torun, Poland)^c.

References:

^aHochlaf, M.; Linguerr, R.; Kandi, N. C.; Alessandrini, S.; Puzzarini, C. Ab Initio Characterization of the [H₂C,N,O]⁺ Isomeric System: Structures, Spectroscopy, and Electronic States. *J. Phys. Chem. A*, 2026. Submitted.

^bBen Abdallah, D.; Mogren Al Mogren, M.; Dhaif Allah Al Harbi, S.; Al Salhi, M. S.; Hochlaf, M. Collision excitation of nitrous acid (HONO) by helium: isomerization effect. *MNRAS*, 2023, 521, 4162–4172. <https://doi.org/10.1093/mnras/stad797>

^cMehnen, B.; Hendaoui, H.; Ben Abdallah, D.; Zuchowski, P.; Jaidane, N. J.; Hochlaf, M. Rotational excitation and de-excitation of interstellar thionylimide (cis-HNSO) by helium collisions. *MNRAS*, 2026, 545, 1–10. <https://doi.org/10.1093/mnras/staf2142>

Reliable PESs for Astrochemistry with autoPES: Methodology, Pitfalls, and Case Studies

Dariusz Kędziera¹

¹*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, ul. Gagarina 7, Toruń, Poland*

Reliable potential energy surfaces (PESs) are a prerequisite for astrochemical applications that rely on an accurate description of intermolecular interactions. In practice, the main bottlenecks are often not only computational cost, but also methodological and workflow issues: how to sample efficiently, choose a robust representation, and detect when an apparently smooth fit is physically wrong. In this lecture, I present a user's perspective on building reliable PESs with the autoPES^a framework, focusing on common pitfalls, practical diagnostics, and lessons learned from case studies. Depending on the system size and the target accuracy, the reference electronic-structure data are generated using SAPT(DFT) and, when necessary, CCSD(T). Although autoPES provides powerful automation, it is not a black-box tool: reliable surfaces still require active user control. I therefore discuss practical safeguards: (i) consistent stitching between the long-range and intermediate-range regions, and (ii) protecting short-range behaviour through energy regularization and elimination of spurious holes (unphysical low-energy pockets) in the fitted PES.

To illustrate how these issues evolve with increasing complexity of the collision partner, I start from an atom collider (He), using CH₃CHO–He and benzonitrile–He as benchmarks that expose dispersion- and anisotropy-related fitting challenges.^b I then move to a linear molecular collider (H₂), highlighting the methodological difficulties encountered for ion–molecule interactions on H₂Cl⁺–H₂^c and discussing ongoing PES development for benzonitrile–H₂. Finally, I consider a nonlinear polyatomic collider (H₂O), illustrated by CS–H₂O, HCN–H₂O, and CH₃OH–H₂O, with H₂O–HCN as a recent reference case.^{d, e}

References:

^a Metz, M. P.; Piszczatowski, K.; Szalewicz, K. Automatic Generation of Intermolecular Potential Energy Surfaces. *J. Chem. Theory Comput.*, 2016, **12**(12), 5895–5919. <https://doi.org/10.1021/acs.jctc.6b00913>

^b Derbali, E.; Ajili, Y.; Mehnen, B.; Żuchowski, P. S.; Kędziera, D.; Al-Mogren, M. M.; Jaidane, N.-E.; Hochlaf, M. Towards the generation of potential energy surfaces of weakly bound medium-sized molecular systems: the case of benzonitrile–He complex. *Phys. Chem. Chem. Phys.*, 2023, **25**(44), 30198–30210. <https://doi.org/10.1039/D3CP02720A>

^c Demes, S.; Kędziera, D.; Faure, A.; Lique, F. Rotational excitation cross sections for chloronium based on a new 5D interaction potential with molecular hydrogen. *J. Phys. Chem. A*, 2025, **129**(1), 253–261. <https://doi.org/10.1021/acs.jpca.4c07467>

^d Vindel-Zandbergen, P.; Kędziera, D.; Żółtowski, M.; Kłos, J.; Żuchowski, P.; Felker, P. M.; Lique, F.; Bačić, Z. H₂O–HCN complex: a new potential energy surface and intermolecular rovibrational states from rigorous quantum calculations. *J. Chem. Phys.*, 2023, **159**(17), 174302. <https://doi.org/10.1063/5.0173751>

^e Żółtowski, M.; Lique, F.; Żuchowski, P.; Kłos, J.; Loreau, J.; Kędziera, D. Collisional excitation of HCN by H₂O. *MNRAS*, 2025, **540**(1), 626–632. <https://doi.org/10.1093/mnras/staf477>

Theoretical study of the sensing properties of KL 1421 luminophore interacting with carotenoids

J. Tamuliene¹, T. Kirova², I. Tepliakova², V. Zabolotnii², A. Kinens³ and R. Viter²

¹*Institute of Theoretical Physics and Astronomy, Vilnius University, Sauletekio av. 3, Vilnius, 10222 Lithuania*

²*Institute of Atomic Physics and Spectroscopy, Faculty of Exact Sciences and Technologies, University of Latvia, Jelgavas street 3, Riga, LV-1004, Latvia*

³*Latvian Institute of Organic Synthesis, Aizkraukles street 21, Riga, LV-1006, Latvia*
Presenter's email address: teo@lu.lv

Applications of sensors vary from measuring temperature to detecting the presence of harmful materials, the variety of sensors occurring due to their advantages in certain situations (for example, non-contact high-precision measurements in harsh environments are performed mostly by optical sensors). In a recent work¹ we demonstrated that the KL 1421 luminophore exhibits selective sensing behavior toward acetic acid vapors, and no significant photoluminescence response was observed for other tested substances.

We further investigated the incorporation of carotenoids in KL 1421 and their effect on its absorption efficiency and sensitivity of the optical sensor². The geometry, its change, and the charge redistribution in KL 1421 when the molecule interacts with carotenoids and/or sensed molecules such as NH₃ and acetic acid, were studied by the B3LYP/cc-pVTZ approach. The increase in molar absorptivity is observed in compounds with carotenoids, leading to higher absorbance of KL 1421. The conjugated double-bond number influences charge redistribution in KL 1421 & carotenoid & sensed molecule compounds. Results of our investigation prove that NH₃ could not be sensed by KL 1421, although this could be possible by KL 1421 & carotenoid, due to the energy level variations and shifts of peaks corresponding to the excitations due to charge transfer from the sensed molecule. Additionally, the singlet-triplet transfer in the compounds with carotenoids is faster than that in KL 1421 & sensed molecule, while the transfer from triple to ground state is longer and more efficient. The molar absorptivity indicates higher absorbance of the compound under study with carotenoids than without them.

In conclusion, carotenoids are good candidates to enhance the sensory properties of KL 1421 novel organic luminophores, opening possibilities for improved sensor applications in biotechnology, nanomaterials and environmental science.

References:

¹Zabolotnii, V.; Tamuliene, J.; Drava, M. M.; Kirova, T.; Tepliakova, I.; Lukinsone, V.; Kinens, A.; Viter, R. Investigation of structure, optical properties and chemical stability of the pyridinium luminophore with high quantum yield. *Applied Materials Today*, 2025, 46, 102890-1-102890-11. <https://doi.org/10.1016/j.apmt.2025.102890>

²Tepliakova, I.; Zabolotnii, V.; Kinens, A.; Tamuliene, J.; Kirova, T.; Viter, R. Could carotenoids advance the sensing properties of KL 1421 luminophore? *Theoretical Study*. *Lithuanian Journal of Physics*, 2026, accepted

Novel single-atom and single-cluster metal catalysts supported on carbon based layered materials

María J. López, Johanna Sandoval-Menjívar, Estefanía Germán, Sahar Mahnaee, Irene Belloso, Julio A. Alonso

Departamento de Física Teórica, Atómica y Óptica, University of Valladolid, Valladolid, Spain
mariajlopez@uva.es

Developing novel catalysts tailored to specific chemical reactions and processes is of great relevance, since 90% of the chemical products are synthesized through catalytic processes. Transition metals (TM) are effective catalysts due to their unfilled d-shells, different oxidation states, and good selectivity and activity. The concepts of single-atom catalysts (SAC) and single-cluster catalysts (SCC) have emerged in recent years as a new paradigm in nanocatalysis. These approaches minimize the use of TMs by dispersing isolated atoms and clusters on a support, thus increasing the concentration of active sites and maintaining the activity and selectivity of the catalysts. With the aim of contributing to the rational design of SACs and SCCs we have investigated, using the density functional formalism (DFT), a variety of transition metals (V, Co, Pd) supported on two carbon based layers, namely graphdiyne GDY and boron-graphdiyne BGDY^a. GDY (BGDY) layers have a structure of uniformly distributed triangular (hexagonal) nanopores whose boundaries are formed by diacetylenic chains. Our study shows that TM atoms and clusters bind strongly to the substrate pores, while moderate to high diffusion barriers inhibit metal agglomeration and promote the stability of these catalytic platforms. Adsorption of TM atoms and clusters induce distortions of the BGDY lattice, whereas GDY is more robust. BGDY bilayers^b with different stacking configurations have been also investigated and characterized. The bilayers offer the opportunity to tailor the size of the nanopores and provide suitable supports for SACs and SCCs with higher stability than the corresponding monolayer. This work gives support to the development of highly stable SACs and SCCs that can be built through deposition of TM atoms and clusters on GDY and BGDY monolayers and bilayers.

References:

- ^a Sandoval Menjívar, J.; Germán, E.; Alonso, J.A.; López, M.J. Building single-atom and single-cluster metal catalysts supported on graphdiyne and boron-graphdiyne. *Small Structures*, 2026; 7:e202500508. <https://doi.org/10.1002/sstr.202500508>
- ^b Mahnaee, S.; López, M.J.; Germán, E.; Alonso, J.A. Structure and electronic properties of bilayers of boron-graphdiyne, *Solid State Communications*, 2025; 406, 116189. <https://doi.org/10.1016/j.ssc.2025.116189>

This work was supported by MCIN/AEI/10.13039/501100011033 and FSE+ (PID2022-138340OB-I00); Junta de Castilla y León - Apoyo a GIR (VA029G24); University of Valladolid; RES: BSC in MareNostrum 5 (FI-2024-2-0031); RES: CSUC in Pirineus III (FI-2025-1-0029, FI-2025-2-0004); Schlumberger Foundation.

Bio-inspired functionalization of chitosan for water remediation: computational insights into neonicotinoid sequestration

Jorge M. C. Marques¹, Joana R. C. Santos¹, Paulo E. Abreu¹

¹CQC-IMS, Department of Chemistry, University of Coimbra, Portugal
qtmarque@ci.uc.pt

Computational techniques can significantly enhance the design of materials with high adsorption affinity for target molecules, a capability crucial for the sequestration of pesticides in water remediation. This work employs a multi-stage computational protocol^a to guide the design of bio-inspired, chitosan-based materials for the efficient adsorption of neonicotinoids, including imidacloprid, thiacloprid, acetamiprid, clothianidin, and dinotefuran (considering both *R*- and *S*-enantiomers). By employing molecular dynamics (MD) simulations, we investigated the interactions between these pesticides and the *Aplysia californica* acetylcholine-binding protein (*Ac*-AChBP) to identify key amino acids responsible for stabilizing the protein-pesticide complexes within the binding pocket. High-level electronic-structure calculations were subsequently performed on isolated residues, identifying tryptophan (Trp) and tyrosine (Tyr) as the most promising candidates for functionalizing chitosan. The adsorption efficiency of these functionalized models was evaluated against non-functionalized chitosan through comparative MD simulations in aqueous media. Our results demonstrate that the incorporation of aromatic amino acids significantly enhances the adsorption properties of chitosan, especially for imidacloprid, acetamiprid, and thiacloprid. This integrated computational strategy provides a robust framework for selecting molecular targets to improve the performance of biodegradable natural resources in environmental applications.

References:

^aSantos, J. R. C.; Abreu, P. E.; Marques, J. M. C. Towards nature-inspired materials for adsorbing pesticides: a multi-stage computational approach. *Phys. Chem. Chem. Phys.*, 2025, 27, 18665-18680. <https://doi.org/10.1039/D5CP01445J>

New directions in Attosecond Chemistry

Fernando Martín^{1,2}

¹*Departamento de Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain*

²*Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nano), Cantoblanco, 28049 Madrid, Spain*

Presenter's email address: fernando.martin@uam.es

With the advent of attosecond light pulses at the dawn of the twenty first century, access to the time scale of electronic motion, i.e., the ultimate time scale responsible for chemical transformations, was finally at our reach. Since the first attosecond pump-probe experiments performed in molecules^{1,2}, the field has grown exponentially, leading to a discipline that we call attochemistry³. As a result, it is nowadays possible to follow in real time the motion of the “fast” electronic motion in molecules, mostly in the gas phase, and understand how this motion affects the “slower” motion of atomic nuclei and vice versa. There are, however, new scenarios⁴ that will allow one to extend the range of applications, including more complex molecular systems and the condensed phase, and to overcome some of the limitations of current attosecond technologies⁵⁻¹¹ such as the low intensity of attosecond pulses produced by high harmonic generation, the impossibility to generate such pulses in the visible and UV spectral regions to avoid molecular ionization, or the difficulties to combine them with truly imaging methods for direct time-resolved observations of the electron density without the need for reconstruction from measured photoelectron, photoion or transient absorption spectra. In this talk, I will describe current experimental and theoretical efforts aiming at overcoming the above-mentioned limitations, thus giving attochemistry the necessary push to investigate problems of real chemical interest.

- [1] G. Sansone, F. Kelkensberg, J. F. Pérez-Torres, F. Morales, M. F. Kling, W. Siu, O. Ghafur, P. Johnsson, M. Swoboda, E. Benedetti, F. Ferrari, F. Lépine, J. L. Sanz-Vicario, S. Zherebtsov, I. Znakovskaya, A. L'Huillier, M. Yu. Ivanov, M. Nisoli, F. Martín, and M. J. J. Vrakking, *Nature* **465** 763 (2010).
- [2] F. Calegari, D. Ayuso, A. Trabattoni, L. Belshaw, S. De Camillis, S. Anumula, F. Frassetto, L. Poletto, A. Palacios, P. Decleva, J. B. Greenwood, F. Martín, and M. Nisoli, *Science* **346**, 336 (2014).
- [3] M. Nisoli, P. Decleva, F. Calegari, A. Palacios, and F. Martín, *Chem. Rev.* **117**, 10760 (2017).
- [4] F. Calegari and F. Martín, *Commun. Chem.* **6**, 184 (2023).
- [5] A. Palacios and F. Martín, *WIREs Comput. Mol. Sci.* e1430 (2020).
- [6] G. Grell, Z. Guo, T. Driver, P. Decleva, E. Plésiat, A. Picón, J. González-Vázquez, P. Walter, J. P. Marangos, J. P. Cryan, A. Marinelli, A. Palacios, and F. Martín, *Phys. Rev. Res.* **5**, 023092 (2023).
- [7] M. Galli et al, *Optics Letters* **44**, 1308 (2019).
- [8] M. Reduzzi et al, *Optics Express* **31**, 26854 (2023).
- [9] M. Garg, A. Martín-Jiménez, M. Pisarra, Y. Luo, F. Martín and K. Kern, *Nature Photonics* **16**, 196 (2022).
- [10] F. Vismarra, F. Fernández-Villoria, D. Mocci, J. González-Vázquez, Y. Wu, L. Colaizzi, F. Holzmeier, J. Delgado, J. Santos, L. Bañares, L. Carlini, M. Castrovilli, P. Bolognesi, R. Richter, L. Avaldi, A. Palacios, M. Lucchini, M. Reduzzi, R. Borrego-Varillas, N. Martín, F. Martín and M. Nisoli, *Nature Chemistry* **16**, 2017 (2024).
- [11] L.-M. Koll, A. J. Suñer-Rubio, T. Witting, R. Bello, A. Palacios, F. Martín and M.J.J. Vrakking, *Nature* (in press)

Machine Learning Interactions for Chemical Reactions: Validation and Applications

Markus Meuwly¹

*¹Department of Chemistry, University of Basel, Klingelbergstrasse 80, 4056 Basel,
Switzerland.
m.meuwly@unibas.ch*

In this talk I will describe neural network and kernel-based methods suitable to construct full-dimensional, reactive potential energy surfaces for molecular dynamics studies. The focus will be on validating the PESs and using them for computing observables to compare with experiments. An additional aspect concerns the role of numerical accuracy and uncertainty quantification which emerge as an important technical aspect. Illustrative examples ranging from triatomics to molecules relevant to atmospheric chemistry will be discussed.

Tracking microhydration of salt molecules by Penning ionization electron spectroscopy in helium nanodroplets

L. Ben Ltaief¹, N. Scheel¹, M. Mortensen¹, K. Sishodia², R. Rajni³, F. Calvo⁴, M. Mudrich³

¹Department of Physics and Astronomy, Aarhus University, Denmark

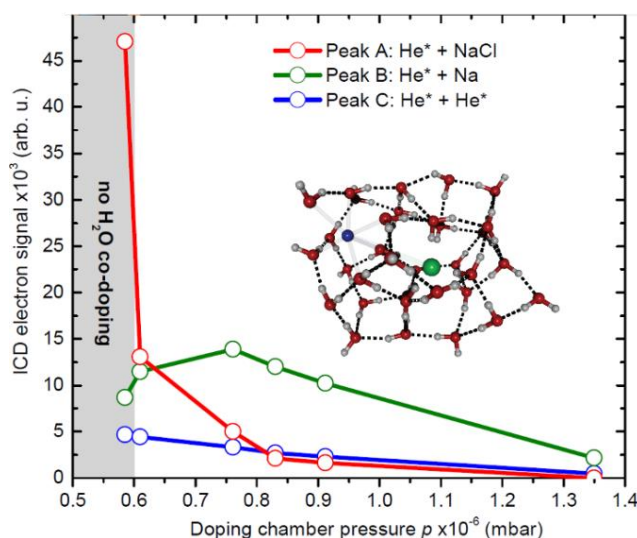
²Department of Physics, Indian Institute of Technology Madras, Chennai, India

³Institute of Physics, University of Kassel, Germany

⁴Université Grenoble Alpes, CNRS, LIPhy, Grenoble, France
mudrich@uni-kassel.de

The microhydration of salt molecules (NaCl, NaBr, KBr) is investigated by Penning ionization electron spectroscopy (PIES) in helium nanodroplets ^a. Although model calculations predict that NaCl molecules are fully submerged inside the droplets, PIES of NaCl are highly resolved, similar to surface-bound alkali-metal atoms. PIES of salt molecules reveal efficient simultaneous ionization and excitation into high-lying charge-transfer states; benchmark measurements on alkaline-earth metals (Mg) show that only simultaneous ionization and excitation leads to the ejection of atomic ions from the helium droplets, whereas ground-state Mg⁺ ions remain bound to the droplets.

Adding to the NaCl-doped helium droplets a controlled number of $n = 1$ -10 water molecules leads to efficient quenching of NaCl Penning ionization and to its full suppression for $n > 30$, see the red line in the figure below. Accompanying density-functional theory (DFT) and force field (FF) calculations reveal a transition from contact ion pair structures to solvent-separated ion pairs at $n = 12$ -15. However, it takes $n \approx 17$ water molecules to form a complete solvation shell around the Cl⁻ anion and as many as $n \approx 34$ to fully hydrate the Na⁺ cation, thus the entire NaCl molecule, which rationalizes the experimental findings. In addition to presenting these recent results, I will report on the progress of research activities in WG4.



Electron signals measured for Penning ionization of NaCl, Na and excited He* embedded in helium nanodroplets as a function of the vapor pressure of water co-doped into the droplets. The inset shows the structure of NaCl solvated by a cluster of 34 water molecules obtained from force field (FF) exploration.

References:

^a Ben Ltaief, L., Sishodia, K., Richter, R., Pi, M., Barranco, M., Eloranta, J., Krishnan, S.R., Calvo, F., Mudrich, M., Tracking Microhydration of the NaCl Rocksalt Molecule in Helium Nanodroplets by Penning Ionization Electron Spectroscopy, submitted to Small Structures, 2026; <https://doi.org/10.XXXarXiv:2510.22000>.

Metallized Ag-DNA: Computational insights into a novel biomolecular material

Yevhen Osokin¹, Sergiy Perepelytsya¹

¹*Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine. 14-B Metrolohichna str., Kyiv, 03143, Ukraine
perepelytsya@bitp.kyiv.ua*

Metallized DNA, in which Ag^+ ions form complexes with the nucleotide bases and arrange inside the double helix as a chain of atoms, is of great practical importance due to the potential use of such systems as nanowires in various technological applications. In the present work, the quantum-chemical DFT study of Ag^+ complexes with DNA nucleotide bases has been carried out^a. The B3LYP and M06-2X functionals in combination with the PCM and SMD solvation models have been used. The results have shown that electrically neutral complexes of silver ions with thymine (Ag^+ at N3) and guanine (Ag^+ at N1) possess the highest thermodynamic stability, whereas the positively charged adenine complexes (Ag^+ at N1) are the least stable (Figure 1). The obtained results are in agreement with experimental X-ray data indicating that silver ions in metallized Ag-DNA displace adenine bases from the double helix^b. Comparison of computational methods indicates that the B3LYP functional combined with the SMD solvation model provides the most reliable description. These findings contribute to understanding the structural characteristics of metallized Ag-DNA and its potential applications as a nanomaterial.

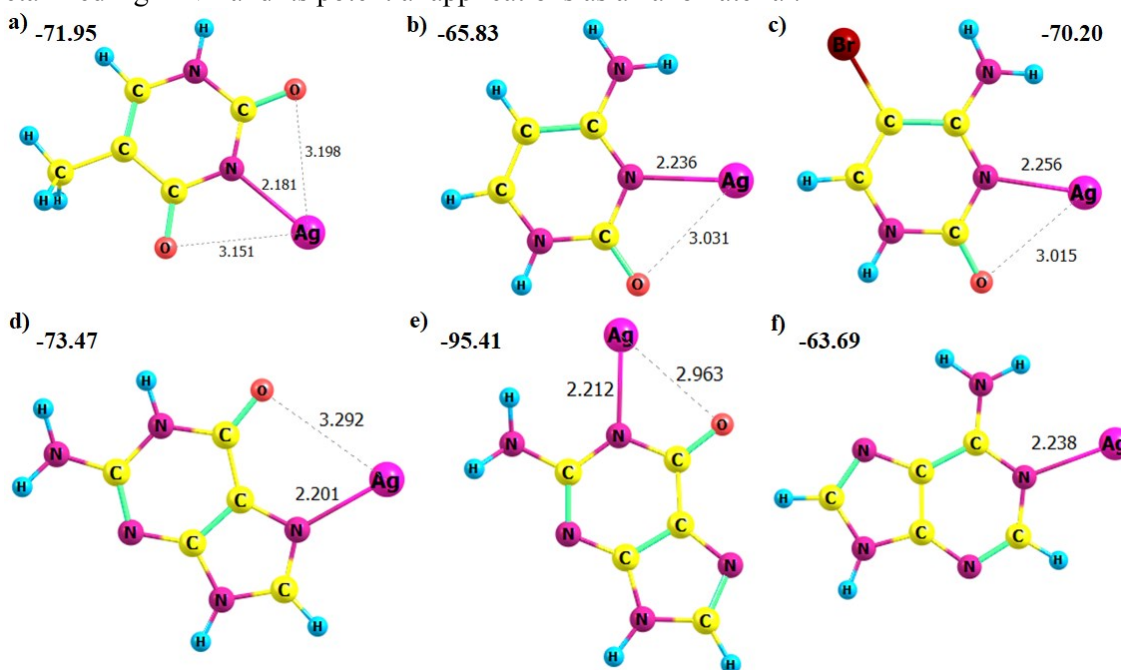


Figure 1. Ag^+ -nucleobase complexes: thymine (a), cytosine (b), 5-bromocytosine (c), guanine (d,e), adenine (f). Distances in Å; energies in kJ/mol.

References:

^aOsokin, Ye.; Perepelytsya, S. Low Temperature Physics, 2026, Volume 52 (accepted)

^bKondo, J., et al., Nature Chemistry, 2017, Volume 9, 956–960. <https://doi.org/10.1038/nchem.2808>

Modeling Reactivity under Interstellar Conditions

Cristina Puzzarini¹

¹*Department of Chemistry "Giacomo Ciamician", University of Bologna,
Via P. Gobetti 85, I-40129 Bologna, Italy
cristina.puzzarini@unibo.it*

The detection of complex organic molecules in the interstellar medium raises fundamental questions about how chemistry can proceed under the extreme conditions of very low temperatures, low densities, and intense radiation.¹ In this environment, conventional chemical intuition breaks down, and a molecular-level description becomes essential. Computational chemistry has therefore become a key tool for identifying viable reaction pathways and providing the kinetic data required for astrochemical models.¹⁻⁴

This overview talk will present recent progress in the quantum-chemical exploration of reactive potential energy surfaces relevant to interstellar chemistry.²⁻⁵ Modern electronic-structure methods, combined with automated reaction-discovery workflows,⁵ allow the systematic identification of barrierless or low-barrier processes consistent with interstellar conditions. The resulting energetic information can be coupled with kinetic simulations to derive temperature-dependent rate coefficients and branching ratios, revealing how small energetic differences can strongly affect reaction rates at cryogenic temperatures.¹ Finally, we will discuss advances in modeling chemistry on interstellar grain analogues, where surface and ice chemistry plays a crucial role in the formation of complex and prebiotic molecules.⁶

Together, these developments highlight how the integration of quantum chemistry, automated reaction discovery, and kinetic modeling is making astrochemistry an increasingly predictive and quantitatively grounded field.

References:

- ¹Puzzarini, C.; Alessandrini, S. Chemistry in Extreme Environments: The Mystery of Molecular Complexity in Space. *ACS Cent. Sci.*, 2026, ASAP article. DOI: 10.1021/acscentsci.5c02122
- ²Ye, H.; Alessandrini, S.; Puzzarini, C. Gas-phase formation route for *trans* -HC(O)SH and its isomers under interstellar conditions: a state-of-the-art quantum-chemical study. *MNRAS*, 2023, 525, 1158. <https://doi.org/10.1093/mnras/stad2253>
- ³Ye, H.; Alessandrini, S.; Puzzarini, C. On the General Mechanism for the Gas-phase Reaction of Methanimine with a Radical Species in the Interstellar Medium: Some Failures and an Important Success. *Astrophys. J.*, 2024, 962, 32. <https://doi.org/10.3847/1538-4357/ad11dd>
- ⁴Alessandrini, S.; Ye, H.; Puzzarini, C. Gas-Phase Reactions of H₂CS and H₂CO with CN: Similarities and Differences from a Computational Study *ACS Earth Space Chem.*, 2025, 9, 1217. <https://doi.org/10.1021/acsearthspacechem.5c00034>
- ⁵Bensberg, M.; Alessandrini, S.; Melosso, M.; Puzzarini, C.; Reiher, M. Automated Exploration of Radical-molecule Chemistry: The Case of Oxirane + CH in the Interstellar Medium. *Astrophys. J.*, 2026, 998, 104. <https://doi.org/10.3847/1538-4357/ae2d0a>
- ⁶Perrero, J.; Alessandrini, S.; Ye, H.; Puzzarini, C.; Rimola, A. Formation of the glycine isomer glycolamide (NH₂C(O)CH₂OH) on the surfaces of interstellar ice grains: Insights from atomistic simulations *Astron. Astrophys.* 2025, 698, A51. <https://doi.org/10.1051/0004-6361/202554330>

High resolution spectroscopy, parity violation and quantum tunneling dynamics in chiral molecules of astrophysical and general interest

Martin Quack¹

¹*Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir Prelog Weg 2
CH-8093 Zurich, Switzerland, Martin@Quack.CH, www.ir.ETHz.CH*

The quantum dynamics of chiral molecules were central to the discovery of tunneling shortly after the development of quantum mechanics in the form of the Heisenberg equations of motion and the Schrödinger equation^{a,b,c}. Later in the 20th century they were again crucial in understanding the fundamental role of parity violation for stereochemistry and in introducing electroweak quantum chemistry^{d,e,f}. In the 21st century chiral molecules may become the key to the discovery of extraterrestrial life by using small chiral molecules as tracers for homochirality in astrophysical spectroscopy. In the lecture we shall start with a short historical and conceptual introduction and then report about recent work of our group in Zurich including in particular work supported in the recent years by COST COSY. After an effort of 40 years we are close to finally measuring the parity violating energy difference between the enantiomers of chiral molecules, which has been well studied by theory but so far not yet observed in any experiment^{d,e,f}. Major current efforts concern the understanding of the complex high resolution spectroscopy and quantum dynamics of chiral molecules and isotopic chirality as governed by the interplay of rotation, vibration, tunneling, and parity violation which is important both for the design of the experiment for detecting molecular parity violation and also for astrophysical spectroscopy (See^{f,g,h,i} www.ir.ETHz.CH and references therein)

References:

- ^aHeisenberg, W. ; Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. Z. Physik , 1925, 33, 879-893.
- ^bSchrödinger, E ; Quantisierung als Eigenwertproblem . Ann. d. Physik. 1926, 79, 361-376, 489-527, 734-756, 80, 437-450, 81, 109-139
- ^cHund, F.; Zur Deutung von Molekülspektren. Z.Physik., 1927, 43, 742-764, 788-804, 805-826
- ^dQuack, M. ; On the measurement of the parity violating energy difference between enantiomers. Chem. Phys. Lett., 1986, 132, 147-153.
- ^eBakasov, A., Ha, T. K., Quack, M. ; Ab initio calculations of molecular energies including parity violating interactions. J.Chem Phys. , 1998, 109, 7263-7285.
- ^fQuack, M. , Seyfang, G., Wichmann, G., Perspectives on parity violation in chiral molecules. Chem. Science., 2022, 13, 10598-10643. (see also M. Quack COST-COSYmeeting Madrid 2026)
- ^gAlbert, S., Chen, Z., Keppler, K. Wichmann, G., Quack, M., Stohner, J., Schurig V., Trapp, O; High resolution infrared spectroscopy of monodeutero-oxirane (c-C₂H₃DO) and analysis of two fundamentals between 820 and 850 cm⁻¹, Phys. Chem. Chem. Phys. (PCCP)2025, **27**, 14240 – 14253 (2025)
- ^hWichmann, G., Albert, S., Lerch, P., Keppler, K., Quack, M., High-resolution GHz and THz (FTIR) spectroscopy and quantum dynamics of tunneling in aniline Mol. Phys. **000**, e2593929 (2025) DOI: 10.1080/00268976.2025.2593929
- ⁱChen, Z., Albert, S., Keppler, K. Wichmann, G., Quack, M., Schurig V., Trapp, O; Isotopic chirality and high-resolution gigahertz and terahertz spectroscopy of trans-2,3-dideuterooxirane (tcCHDCHDO) Phys. Chem. Chem. Phys. (PCCP)2026, **28**, 751- 763 (2026), DOI: 10.1039/d5cp03143e

Understanding Catalytic Clusters under Operando Conditions by XANES.

Félix G. Requejo¹

*¹Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA, CONICET and FCE, UNLP).
1900 La Plata, ARGENTINA
requejo@inifta.unlp.edu.ar*

Subnanometer metal clusters composed of only a few atoms exhibit unique properties that make them highly attractive for catalytic applications. In this presentation, we discuss recent advances in the study of five-atom copper and silver clusters (Cu_5 and Ag_5), with an emphasis on their catalytic performance as revealed by operando X-ray absorption near-edge structure (XANES) spectroscopy. Ag_5 clusters have demonstrated remarkable activity in the complete oxidation of sulfur-containing compounds, including dibenzothiophene and other highly refractory thiophenes, under ambient conditions, offering a simple and environmentally benign route for fuel desulfurization. Additionally, Cu_5 clusters supported on TiO_2 display exceptional selectivity and efficiency in CO_2 methanation, achieving 100% selectivity toward CH_4 at temperatures as low as 300 °C and exhibiting low activation energy. Their performance has been rationalized through a combined operando XANES and density functional theory (DFT) approach. In both systems, XANES spectroscopy provides crucial insights into oxidation-state dynamics and reaction pathways, revealing the reversible redox behavior of Cu_5 during CO_2 hydrogenation and the oxidation routes promoted by Ag_5 in sulfur removal. Together, these results highlight the potential of subnanometer clusters as efficient, stable, and environmentally relevant catalysts, while underscoring the power of operando XANES to elucidate structure–activity relationships under working conditions.

Experimental Solution of the Thomson Problem

Thomas Pohl¹, Jan Mayerhofer¹, Shengfu Yang², Andrew M. Ellis², Paul Scheier¹

¹*Institut für Ionenphysik und Angewandte Physik, University of Innsbruck, Technikerstr. 25,
A-6020 Innsbruck, Austria*

²*School of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, UK
paul.scheier@uibk.ac.at*

In multiply charged helium droplets like-charge Coulomb repulsion pushes the charge centers to the surface of the superfluid droplet where they adopt a minimum energy configuration in the form of the famous Thomson problem¹. Coherent diffraction imaging of large multiply charged helium droplets doped with xenon confirms that most for the dopants are found in the form of clusters close to the surface of the droplet², however, the quality of the images does not allow a comparison with the solution of the Thomson problem for any specific number of charges.

By doping multiply charged helium droplets with gold vapor, monodisperse nanoparticles containing typically a few thousand atoms are formed. Upon soft-landing onto a transmission electron microscope (TEM) grid, each droplet prints its gold particles onto the substrate. The orthographic projection of the numerical solution of the Thomson problem³ can be fitted to the experimental TEM images of individual droplets by appropriate rotation and scaling. For droplets with a final radius smaller than 200 nm we obtain perfect agreement between the experimental results and the numerical solution of the Thomson problem. This indicates minimal displacement of the several 100 kDa gold particles upon surface collision of the doped helium droplets. The regular patterns observed in imprints of helium droplets with a radius larger than 400 nm can only be explained when particles located on the back hemisphere are splashed sideways and backwards⁴.

References:

- ¹ Thomson, J. J. On the structure of the atom. *Philosophical Magazine*, 1904, 7, 237–265. <https://doi.org/10.1080/14786440409463107>
- ² Feinberg, A. J.; et al. X-ray diffractive imaging of highly ionized helium nanodroplets. *Physical Review Research*, 2022, 4, L022063. <https://doi.org/10.1103/PhysRevResearch.4.L022063>
- ³ Wales, D. J.; Ulker, S. Structure and Dynamics of Spherical Crystals Characterised for the Thomson Problem. *Physical Review B*, 2006, 74, 212101. <https://doi.org/10.1103/PhysRevB.74.212101>
- ⁴ Martini, P.; et al. Splashing of Large Helium Nanodroplets upon Surface Collisions. *Physical Review Letters*, 2021, 127, 263401. <https://doi.org/10.1103/PhysRevLett.127.263401>

AB initio calculations applied to the study of organic non-rigid molecules with (at least) three interacting torsional modes.

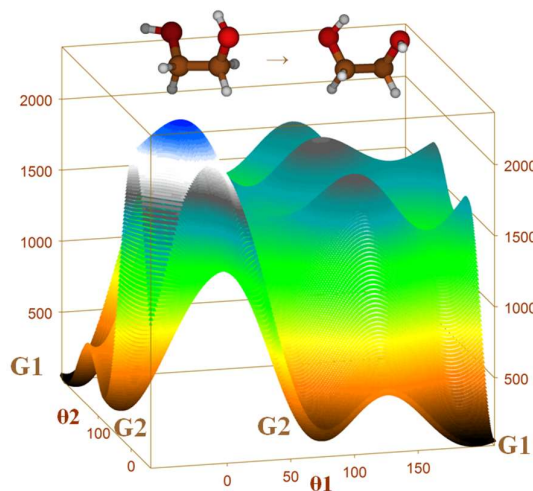
María Luisa Senent¹

¹ *Departamento de Química y Física Teóricas, Instituto de Estructura de la Materia, IEM-CSIC, Serrano 121, Madrid 28006; Unidad Asociada GIFMAN, CSIC-UHU, Spain.*

Presenter's email address: ml.senent@csic.es

Methods applicable to the spectroscopic study of non-rigid organic molecular species with various large amplitude motions (torsional or inversion modes), are presented. Recent studies of species containing C, H, O, and N are presented as examples^{a,b,c}.

Many organic molecules display non-rigidity. Vibrational modes of inversion and torsion interconvert different conformers separated by relatively low barriers. Some conformers can be stabilized by the presence of hydrogen intermolecular bonds that can determine their geometry, symmetry and internal dynamics. When a species displays three or more large amplitude motions, which cannot be separated because they interact strongly, the variational calculation of vibrational levels is complex and requires to search how to reduce the computational consuming. Especially tricky is the classification of the vibrational levels and their splittings.



Paths connecting the G1 and G2 conformers of ethylene glycol

References:

^a Weak intramolecular interaction effects on the low temperature spectra of ethylene glycol, an astrophysical species, Boussasi, R.; Senent, M.L.; Jaïdane, N.; J.Chem.Phys., 2016, 144, 164110.

<http://dx.doi.org/10.1063/1.4947088>

^b Ab initio study of the large amplitude motions of methoxy-methanol (CH₃-O-CH₂OH), Missaoui, D.; Brahem, S.; Najar, F.; Yazidi, O.; Senent, M.L.; ACS Earth and Space Chemistry, 2024, 8, 1236.

<https://doi.org/10.1021/acsearthspacechem.4c00053>

^c Theoretical spectroscopic study of isopropyl alcohol (CH₃-CHOH-CH₃), Salah, M.; Marachi, K.; Komiha, N.; Senent, M.L. Astrophys. J., 2024, 963, 143 -154. <https://doi.org/10.3847/1538-4357/ad1fef>

Chemically Accurate *Ab Initio* Prediction of Adsorption Thermodynamics and Isotherms in Metal–Organic Frameworks

Kaido Sillar

Institute of Chemistry, University of Tartu, Ravila 14a, 50411, Tartu, Estonia
kaido.sillar@ut.ee

Current environmental and energy challenges necessitate the development of advanced nanoporous adsorbents, making predictive atomistic modeling essential for both materials design and process integration. The key descriptor is the gas-surface interaction strength, expressed most fundamentally as the adsorption Gibbs free energy, which determines the adsorption isotherm, i.e., the equilibrium uptake as a function of gas pressure at fixed temperature. To be meaningful, predictions must achieve chemical accuracy ($\pm 4 \text{ kJ mol}^{-1}$),^a requiring both a reliable potential-energy surface and rigorous statistical-mechanical sampling of the relevant configurational space.

Here we focus on two MOFs proposed for CO₂ capture – Mg₂(dobdc) (CPO-27-Mg/MOF-74) and CALF-20 – and show how chemical accuracy can be achieved by going beyond standard periodic DFT+D workflows. We first compute periodic DFT+D adsorption energetics and then add high-level correlation corrections using periodic MP2 together with CCSD(T) corrections evaluated on adsorption-site cluster models, yielding chemically accurate adsorption energies at equilibrium structures.^{a–e} Adsorption entropies and Gibbs free energies are then obtained by local sampling of this surface via vibrational partition functions that include quantum nuclear effects and anharmonicity. To capture coverage-dependent nonlocal effects, we account for lateral adsorbate-adsorbate interactions either through a mean-field (Bragg-Williams) isotherm model or via a nonisolated-site treatment in which additional intermolecular modes augment the adsorbed-state partition function, thereby substantially improving adsorption entropies and Gibbs free energies. For CALF-20, the resulting *ab initio* isotherms and heats of adsorption reproduce experiment within chemical accuracy and agree with independent GCMC simulations based on a newly parametrized force field, providing a triple cross-validation across *ab initio* thermodynamics, GCMC simulations, and experiment.^e

References:

- ^aKundu, A.; Piccini, G. M.; Sillar, K.; Sauer, J. *Ab Initio* Prediction of Adsorption Isotherms for Small Molecules in Metal–Organic Frameworks. *J. Am. Chem. Soc.*, 2016, 138(42), 14047–14056. <https://doi.org/10.1021/jacs.6b08646>
- ^bSillar, K.; Hofmann, A.; Sauer, J. *Ab Initio* Study of Hydrogen Adsorption in MOF-5. *J. Am. Chem. Soc.*, 2009, 131(11), 4143–4150. <https://doi.org/10.1021/ja8099079>
- ^cSillar, K.; Sauer, J. *Ab Initio* Prediction of Adsorption Isotherms for Small Molecules in Metal–Organic Frameworks: The Effect of Lateral Interactions for Methane/CPO-27-Mg. *J. Am. Chem. Soc.*, 2012, 134(44), 18354–18365. <https://doi.org/10.1021/ja307076t>
- ^dSillar, K.; Koppel, I. *Ab Initio* Calculation of Thermodynamic Functions for CO₂ Adsorption in Metal–Organic Frameworks: Entropic Effects of Lateral Interactions. *J. Phys. Chem. C*, 2023, 127(24), 11712–11719. <https://doi.org/10.1021/acs.jpcc.3c02234>
- ^eSillar, K.; Grubišić, S.; Đorđević, I. S.; Hochlaf, M. Chemically Accurate Prediction of CO₂ Adsorption Thermodynamics in Metal–Organic Framework CALF-20: Complementary *Ab Initio* Modeling and Grand Canonical Monte Carlo Simulations. *Small Structures*, 2026, 7, e202500781. <https://doi.org/10.1002/sstr.202500781>

Steering Complex Photodissociation Dynamics through Initial Vibrational Coherences

Ignacio R Sola¹, Alberto García-Vela²

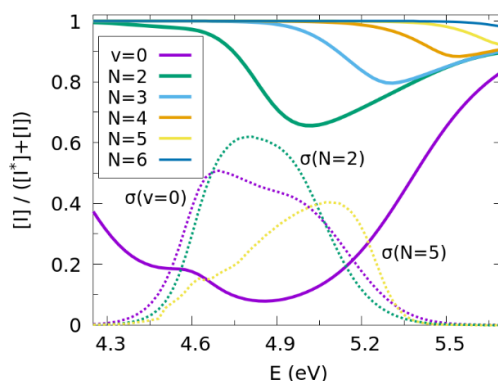
¹Departamento de Química Física, Universidad Complutense de Madrid, Madrid (Spain)

²IFF, Consejo Superior de Investigaciones Científicas, Madrid (Spain)

isolarei@ucm.es

The control of quantum interference is a central concept in coherent control and underpins a wide range of applications in chemistry, from quantum-state preparation to photochemical reaction dynamics and quantum information processing¹. In chemical physics, a primary objective of quantum control is the manipulation of chemical reactions to enhance yields and, in particular, to improve product selectivity among competing reaction or fragmentation channels. The conventional control scheme involves a two-step process in which a pump pulse initiates the dynamics by preparing a vibronic wave packet in excited electronic states, followed by a control pulse that directs nuclear motion along specific reaction coordinates by modifying phase relationships or inducing transitions between electronic states. In many experimental realizations, the pump and control fields are combined into a single shaped laser pulse, whose complex temporal and spectral structure is optimized using pulse shapers and adaptive learning algorithms².

Here we introduce an alternative control strategy, referred to as geometrical optimization³, in which reaction control is achieved by tailoring the initial molecular wave function. Operationally, this corresponds to reversing the conventional sequence by applying a control pulse prior to photoexcitation. We demonstrate that the coherences imprinted in the initial state are sufficient to determine the reaction outcome even in polyatomic molecules subject to strong nonadiabatic couplings, as illustrated for the A band of CH₃I.



Quantum yield of the I channel in the A band of CH₃I, as a function of the number N of vibrational states participating in the initial optimized superposition state

References:

- ¹Sola, I. R.; Chang, B.; Malinovskaya, S.; Malinovsky, V. Adv. At. Mol. Opt. Phys. 2018, 67, 151-256.
- ²Judson, R. S.; Rabitz, H. Phys. Rev. Lett. 1992, 68, 1500.
- ³Sola, I. R.; García-Vela, A. Chem. Sci. 2024, 15, 15255.

Modeling Astrochemical Reaction Rates in Confined Molecular Environments

Srećković Vladimir¹

*¹Institute of Physics Belgrade, National Institute of the Republic of Serbia,
Pregrevica 118, 11080 Zemun,
Belgrade, Serbia*

Astrochemistry aims to explain the formation and evolution of interstellar molecules within structured and partially confined environments such as molecular clouds. In these shielded regions, reduced photodestruction enhances molecular survival, making radiative and collisional processes essential for accurate modeling. Reliable atomic and molecular data are therefore critical for diagnostics and simulations across scales ranging from dense cloud edges to giant molecular clouds. We present rate coefficients for collisional and radiative processes involving e.g. hydrogen, helium, and silicon systems, analyzed using the dipole resonant mechanism and compared with MQDT calculations to evaluate methodological reliability. We also explore machine-learning approaches for predicting reaction rates using computed and literature data. Moreover, we convert new molecular datasets into a standardized format, ready for integration into the databases (interoperable, reusable, and FAIR-compliant datasets).

Controlled assembly of luminescent colloidal nanocrystals into highly ordered 3D superstructures

C.N. Dibenedetto¹, R. Grisorio², D. Conelli², I. Manet³, A. Panniello¹, D. Altamura⁴, F. Scattarella⁴, G. Suranna², C. Giannini⁴, E. Fanizza^{5,1}, M.L. Curri^{5,1}, M. Striccoli^{1*}

¹ CNR-IPCF, Via Orabona 4 - Bari (Italy)

²DICATECh Department, Polytechnic of Bari -Via Orabona 4 Bari (Italy)

³CNR-ISOF, Via Piero Gobetti n.101 – Bologna (Italy).

⁴Chemistry Department, University of Bari “Aldo Moro”, Via Orabona 4- Bari (Italy)

⁵ CNR-IC, Via Amendola 122/O - Bari (Italy)

*marinella.striccoli@cnr.it

Recent progress in colloidal synthesis has profoundly advanced the synthesis of metallic, semiconductor, and magnetic nanoparticles, opening new perspectives for technological innovation. Among them, quantum dots and halide perovskite nanocrystals have attracted considerable interest due to their tuneable electronic structures and distinctive emission properties, making them promising candidates for optoelectronic applications and quantum information technologies¹. The controlled organization of nanocrystals into microscale architectures represents a powerful approach for the design of novel materials with enhanced and emergent functionalities, while preserving the intrinsic properties of the individual nanoscale building blocks². Within this context, supercrystals consist of large-scale, self-assembled arrays of nanocrystals forming highly ordered three-dimensional crystalline lattices³. Their final architecture is governed by interparticle ligand–ligand interactions and by the shape and size of the constituent nanocrystals, potentially giving rise to collective electronic and optical phenomena⁴. In this work, a slow destabilization strategy based on capillary-driven self-assembly in an antisolvent vapor atmosphere is investigated for the direct growth of superstructures on solid substrates. Undoped and manganese-doped CsPbCl₃Br_{3-x} perovskite nanocrystals, CdSe quantum dots and gold nanoparticles, are employed as model building blocks⁵. The resulting superstructures, optically, morphologically and structurally investigated reveal remarkable differences in terms of assembly behaviour, morphology, and optical properties. These findings provide crucial insights into how the nanoparticle structures and their optical properties influences the assembly processes and the collective optical behaviour in supercrystals, allowing to design functional nanomaterial-based architectures with tailored properties for next-generation optoelectronic applications.

Acknowledgements: the Project “Network 4 Energy Sustainable Transition - NEST” (code PE0000021), funded under NRRP by the European Union - Next Generation EU, the PRIN 2022 project "SUPERNANO" (code 2022C7Z2RA) funded by the MUR, and the COST Action CA21101 COSY are gratefully acknowledged.

¹ Ahmed, T., et al., *Advanced Photonics Research* 2024, 5, 2300216.

² Lapkin, D., et al., *Nature Communication* 2022, 13, 892.

³ Boles, M. A., et al., *Chemical Reviews* 2016, 116, 11220-11289.

⁴ Reichhelm, A., et al., *Advanced Functional Material* 2017, 27, 1700361.

⁵ Dibenedetto, C. N. et al., *Small Structures* 2025, e202500373

From Single Atoms to Bimetallic Clusters and Nanostructured Surfaces: Selective Dehydrogenation & Hydrogen Production

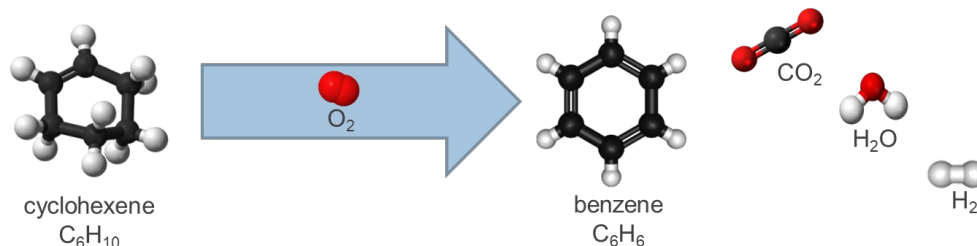
Stefan Vajda

*Department of Nanocatalysis,
J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences,
Dolejskova 2155/3, 18200 Prague, Czech Republic*

The presentation will, on the example of cyclohexene as model compound, provide an overview of tunability of catalyst performance in function of the size and composition of the catalytic active site and support materials.

The primary focus of the studies is on achieving high selectivity in the oxidative dehydrogenation of cyclohexene to benzene on mono- and bimetallic atomic CuPd clusters of well-defined size and composition^{a,b} and single Cu and Pd atoms.^{a,b}

In the second part of the presentation, emerging results on the use of atomic clusters towards efficient hydrogen production^c will be shown, along with the expansion of the materials search place to nanostructured bimetallic films.^c



From oxidative dehydrogenation to hydrogen production

References:

- a) Jašík, J.; Valtera, S.; Vaidulych, M.; Bunian, M.; Lei, Y.; Halder, A.; Tarábková, H.; Jindra, M.; Kavan, L.; Frank, O.; Bartling, S.; Vajda, Š. Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu_{4-n}Pd_n (0 ≤ n ≤ 4) tetramer clusters: The effect of cluster composition and support on performance. *Faraday Discuss.* **2023**, 242, 70-93. DOI: 10.1039/D2FD00108J, [link](#)
- b) Valtera, S.; Jašík, J.; Vaidulych, M.; Olszówka, J.E.; Zlámalová, M.; Tarábková, H.; Kavan, L.; Vajda, Š. Atom by Atom Built Subnanometer Copper Cluster Catalyst for the Highly Selective Oxidative Dehydrogenation of Cyclohexene. *J. Chem. Phys.* **2022**, 156, 114302-114310. DOI: 10.1063/5.0065350, [link](#)
- c) *in preparation*

Contributed Talks

Photoionization of phosphorous hydrides: experimental and theoretical comparison

P. Recio¹, J. Alonso de la Fuente², M. Drissi³, N. Bulut⁴, J.-C. Loison⁵, G. A. Garcia³, S. Gomez-Carrasco⁶, C. Sanz-Sanz⁷, L. Bañares⁸, S. Marggi Poullain¹, A. Zanchet²

¹Dept. de Química Física, Facultad de Ciencias Químicas, UCM, 28040, Madrid, Spain; ²Instituto de Física Fundamental, CSIC, Serrano 123, 28006, Madrid, Spain; ³Synchrotron SOLEIL, L'Orme des Merisiers, St. Aubin BP 48, 91192 Gif Sur Yvette, France; ⁴Dept. of Physics, Firat University, 23169, Elazig, Turkey; ⁵Institut des Sciences Moléculaires (ISM), CNRS, Univ. Bordeaux, 351 Cours de la Libération, 33400, Talence, France; ⁶Dept. de Química Física Aplicada, Facultad de Ciencias, UAM, 28049, Madrid, Spain; ⁷Dept. de Química Física Aplicada, Facultad de Ciencias, UAM, 28049, Madrid, Spain; ⁸Dept. de Química Física, Facultad de Ciencias Químicas, UCM, 28040, Madrid, Spain and IMDEA Nanociencia, Faraday 9, 28049, Madrid, Spain.

Presenter's email address: Jorge.alonso@iff.csic.es

Phosphorous-bearing molecules have attracted increasing attention in astrochemistry due to their potential role in prebiotic chemistry and the growing number of detections in diverse astrophysical environments. However, the chemistry of phosphorous remains comparatively poorly understood.^a In this contribution, we present a combined theoretical and experimental study of the photoionization of the phosphorous hydrides PH, PH₂ and PH₃.

The photoionization of several phosphorous, sulphur and oxygen-bearing molecules experiments were carried out at SOLEIL synchrotron. These data serve as a benchmark for theoretical simulations and allow us to assess the reliability of the underlying electronic structure description.

The theoretical calculations include high-level multireference Potential Energy Curves (PEC) and Surfaces (PES) for the relevant neutral and cationic species, explicitly accounting for spin-orbit coupling (SOC), effects. Photoionization spectra are simulated using the SHARC software and is use to interpret the experimental results, allowing us to gain further insight into which electronic states of the cationic species get populated. For PH, we been able to simulate rovibrationally resolved photoionization spectrum using the DUO software.^b

This approach enables consistent treatment of the electronic states, spin-orbit interactions and the nuclear geometries of the system. Overall, this work provides a unified description of the photoionization behavior of phosphorous hydrides and delivers new data of relevance for astrochemical models of P-bearing species in irradiated environments.

Acknowledgements: We would like to acknowledge the support by Ministerio de Ciencia e Innovación (Spain) (Ref. PID2021-122549NB-C21 and Ref. PRE2022-102568). As well as the COST Action COSY for the support during the STSM to make this work possible.

References:

^a Maciá, E., *et al.*, *Astrobiology*, **2021**, 21, 1277-1304.

^b S. N. Yurchenko, *et al.*, *Comput. Phys. Commun.* **2016**, 202, 262-275.

How Oxide Nanocages Trap the Most Inert Greenhouse Gases

Avni Berisha¹

¹ *Department of Chemistry, Faculty of Mathematics and Natural Sciences, University of Prishtina, Prishtina, Kosovo*

Ultra-inert fluorinated greenhouse gases such as CF₄, C₂F₆, C₃F₈, and SF₆ pose a major challenge for adsorption-based capture and sensing technologies due to their extreme chemical stability, low polarity, and weak polarizability. We present a comprehensive theoretical investigation of the interaction of these molecules on oxide nanocages Be₁₂O₁₂^a and Mg₁₂O₁₂^b, which act as zero-dimensional electrostatic confinement environments. Density functional theory calculations, combined with DLPNO-CCSD(T) local energy decomposition (LED) and QTAIM topological analysis, are employed to elucidate the physical mechanisms governing interactions.

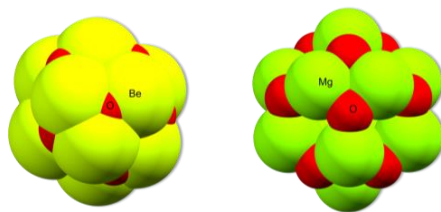


Figure 1. Optimized geometries of the Be₁₂O₁₂ and Mg₁₂O₁₂ nanocage clusters obtained via DFT

Despite their similar geometries, the two nanocages exhibit fundamentally different interaction regimes. Mg₁₂O₁₂ displays an electrostatic-induction-dominated confinement mechanism arising from the highly ionic nature of Mg-O bonds, leading to strong polarization of the adsorbed molecules and significantly enhanced interaction energies. In contrast, Be₁₂O₁₂ operates in a mixed induction-dispersion regime, reflecting its more covalent bonding topology and weaker surface electric field. Energy-decomposition analysis reveals that electrostatics accounts for up to $\approx 90\%$ of the total interaction energy in Mg₁₂O₁₂ complexes, whereas dispersion and correlation contributions play a comparatively larger role in Be₁₂O₁₂.

Acknowledgment

The author acknowledges COST (European Cooperation in Science and Technology) for financial support for scientific networking and dissemination activities through COST Action CA21101 (COSY).

References:

- ^a Rahali, S.; Zaiter, A.; Said, R. B.; Kenouche, S.; Belhocine, Y.; Alhudhaibi, A. M.; et al. DFT insights into the Be₁₂O₁₂ nanocage as a promising nanomaterial for amino acid detection. *Journal of Cluster Science*, 2025, 36(4), 1–16.
- ^b Fallahi, P.; Jouypazadeh, H.; Farrokhpour, H. Theoretical studies on the potentials of some nanocages (Al₁₂N₁₂, Al₁₂P₁₂, B₁₂N₁₂, Be₁₂O₁₂, C₁₂Si₁₂, Mg₁₂O₁₂ and C₂₄) on the detection and adsorption of Tabun molecule: DFT and TD-DFT study. *Journal of Molecular Liquids*, 2018, 260, 138–148.

Identifying Observable Infrared Signatures of Nanosilicate Dust Grains in the Interstellar Medium

Stefan T. Bromley^{1,2}, Joan Mariñoso Guiu¹, Antoni Macià Escatllar¹

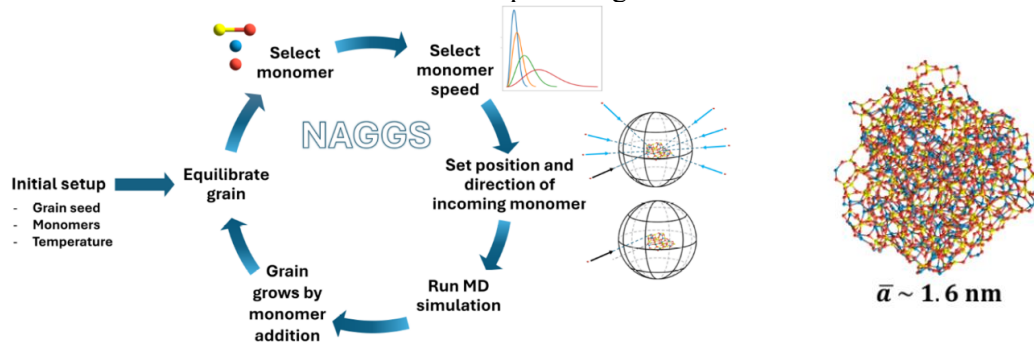
¹*Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/Martí i Franquès 1-11, 08028 Barcelona, Spain*

²*Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, 08010 Barcelona, Spain*

Presenter's email address: s.bromley@ub.edu

Collisional processing of dust in the interstellar medium (ISM) massively favours higher populations of smaller grains. Even if such species account for a relatively small fraction of the total silicate dust grain mass in the ISM, nano-sized grains could potentially dominate dust populations by number. Indirect evidence for a large population of nanosilicate grains comes from their potential as carriers of the anomalous microwave emission.¹ However, more direct spectroscopic evidence is lacking.

Employing our new NAGGS (Nucleated Atomistic Grain Growth Simulator)² approach we have prepared a large set of atomistically detailed nanosilicates with sizes up to 4-5 nm diameter. Previously, we showed that ultrasmall nanosilicates with diameters less than 1 nm have specific infrared (IR) features that should be discernible with the James Webb Space Telescope (JWST)³. By analysing the accurately calculated IR spectra of different populations of nanosilicates we show how these molecular IR features evolve with increasing size. We find that nanosilicates have a signature IR spectrum which is consistent with recent JWST observations of silicates in the diffuse ISM providing.⁴



Left: Workflow of the NAGGS code. Right: an example NAGGS-prepared nanosilicate grain.

References:

- ¹ Macià Escatllar, A.; Bromley, S. T. Assessing the viability of silicate nanoclusters as carriers of the anomalous microwave emission: a quantum mechanical study, *A&A* 2020, 634, A77.
- ² Mariñoso Guiu, J.; Macià Escatllar, A.; Bromley, S. T. The Nucleated Atomistic Grain Growth Simulator (NAGGS): application to the size-dependent structural and physical properties of nanosilicate dust *A&A* 2025 (doi.org/10.1051/0004-6361/202557664)
- ³ Zeegers, S. T.; Mariñoso Guiu, J.; Kemper, F.; J. Marshall, J. P.; Bromley, S. T. Predicting observable infrared signatures of nanosilicates in the diffuse interstellar medium, *Faraday Discuss.* 2023, 245, 609.
- ⁴ Zeegers, S. T.; *et al* Investigating Silicate, Carbon, and Water in the Diffuse Interstellar Medium: The First Shots from WISCI ApJ, 2025, 987, 25.

Self-polarizing molecular films; confined electric fields in ices

Andrew Cassidy¹, Rachel James², Frank Pijpers², Lars Borchert¹, David Field¹.

¹Center for Interstellar Catalysis, Dep. Physics & Astronomy, Aarhus University, Denmark

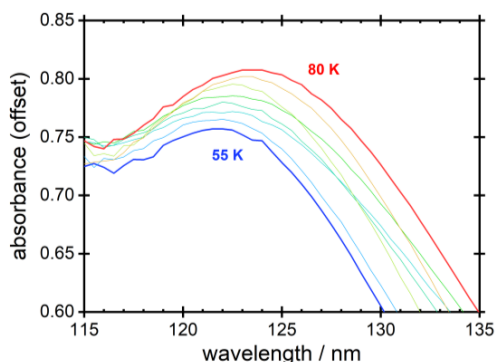
²The University of Manchester, Manchester, UK

³University of Amsterdam, Amsterdam, Netherlands

Presenter's email address: amc@phys.au.dk

Spontaneous electric fields develop in condensing films of dipolar molecules.^a The electric fields arise from the concerted orientation of molecular dipoles throughout the film. The 2D geometry of the film orients the electric fields, such that they lie parallel to the substrate normal. There are no macroscopic electric fields in the plane of the film. These electric fields manifest as a polarization charge at the film-vacuum interface and can be detected, as will be shown here, via a Stark effect in the spectroscopic signature of the film in the vacuum ultraviolet range. Data were collected at the AUUVices end station attached to the ASTRID2 synchrotron at Aarhus.

Research in our laboratory has focused on condensed films of small dipolar molecules including ammonia, methanol, carbon monoxide and water ice. All these species produce nanoscale molecular films that can harbour electric fields up to 10^8 V m^{-1} . This contribution will focus on recent results for water ice, in the context of the role of water ice as the reservoir from which chemical complexity is derived in the interstellar medium,^b and expand to demonstrate how measurements of electric field strength can be used to follow the dynamics of molecular rotation in condensed molecular solids.



The vacuum ultra-violet spectrum of solid ammonia is Stark-shifted to the red as the film is condensed at increasingly higher temperatures, indicating a temperature dependent electric field.

References:

^aCassidy, A.; McCoustra, M. R. S.; Field, D. A Spontaneously Electrical State of Matter. Acc. Chem. Res, 2023, 56, 1909-1919. <https://doi.org/10.1021/acs.accounts.3c00094>

^bJames, R. L.; Pijpers, F. P.; Borchert, L.; Field, D.; Cassidy, A. Spontaneously polarised crystalline water ice. Nanoscale, *accepted*.

Molecular data for characterization of confined molecular systems and corresponding databases

Milan S. Dimitrijević¹

¹Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia

Reliable molecular data are of great interest for investigation, characterization and convenient description and understanding of confined molecular systems and phenomena of astrochemical and astrophysical relevance. For example line cross sections for different collisional processes, rate coefficients, energies and other data. In this contribution we will present some databases of interest, as for example databases of Belgrade Astronomical observatory as MolD containing photodissociation cross-sections of molecular ions from individual ro-vibrational states and cross-sections and rate coefficients for radiative ion-atom collisional processes, BEAMBD (Belgrade electron/atom(molecule) database) with electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering and ACol database with data for collisional processes of excitation/deexcitation and ionization/recombination in hydrogen, helium, and alkali plasmas, which all are and nodes of European Virtual Atomic and Molecular Data Center, containing 39 different databases which can be searched simultaneously. We will also discuss some of them which are of interest for COSY COST action.

Plasmonic–Semiconductor–Metal Oxide Synergy in a 2D/1D Graphene/Ag–Ag₂S–Ag₂O Photocatalyst for photocatalysis

Lala Gahramanli

Nano Research Laboratory, Center of Excellence, Baku, AZ1148, Azerbaijan

In this study, novel 2D/1D graphene/silver–silver sulfide–silver oxide (Ag–Ag₂S–Ag₂O) hybrid nanocomposites were synthesized and systematically characterized in terms of their structural and physical properties. Furthermore, their potential catalytic activity for the degradation of methylene blue under different pH conditions was investigated. To confirm the crystal structure, XRD analysis is presented in Fig. 1(a). After evaluating the structural features, the photocatalytic performance was investigated using pure Ag, Ag₂S–Ag₂O, and graphene–Ag₂S–Ag₂O samples. Photocatalytic degradation experiments were carried out over a range of pH values, and the degradation efficiencies for all samples were determined. The corresponding degradation efficiencies, along with their standard deviations, are presented in Fig. 1(b).

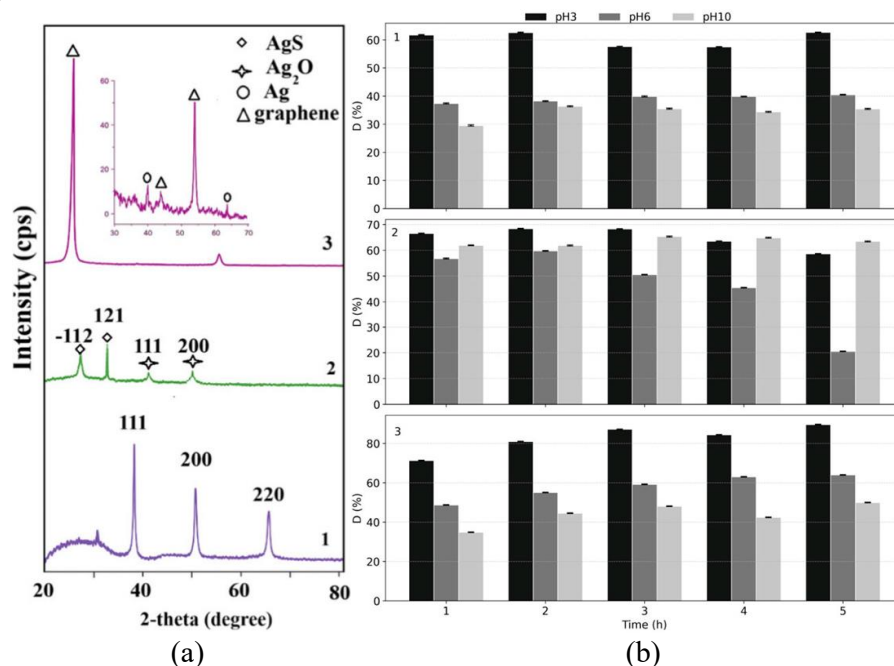


Figure 1. XRD patterns of Ag, Ag₂S–Ag₂O, and graphene–Ag₂S–Ag₂O nanocomposites(a), photocatalytic degradation efficiency of methylene blue at different pH values (error bars indicate standard deviation) (b).

XRD confirmed Ag, Ag₂S, and Ag₂O phases, and FTIR verified Ag–S/Ag–O bonds with graphene signatures. As a result, the hybrid achieved the fastest MB degradation in acidic media (pH 3: $k_{\text{obs}} = 0.5349 \text{ h}^{-1}$; 89.55% in 5 h), surpassing both Ag–Ag₂S and Ag. Performance was moderated at neutral pH with the same activity order, while alkaline conditions favored Ag–Ag₂S (pH 6: $k_{\text{obs}} = 0.2779 \text{ h}^{-1}$) as surface chemistry and site competition reduced graphene's advantage. The characterization confirms successful hybrid formation and explains its pH-responsive, high-efficiency dye removal, positioning graphene/Ag–Ag₂S as a tunable platform in the catalysis, with Ag–Ag₂S alone recommended for alkaline conditions.

Selectivity of D₂/H₂ isotopologues by means of adsorption on a sodium-decorated graphene prototype: a quantum-mechanical low-pressure study

E. García-Arroyo^{1*}, M. I. Hernández¹, M. Bartolomei¹, J. Campos-Martínez¹ and M. Mella²

¹*Instituto de Física Fundamental (IFF-CSIC), C/ Serrano 123, Madrid 28006, Spain*

²*Dipartimento di Scienza ed Alta Tecnologia, Università degli Studi dell'Insubria, Como, 22100, Italy*

**esther.garcia@iff.csic.es*

Molecular deuterium (D₂) is essential for many applications, but it is scarcer than hydrogen (H₂), making it a great challenge to separate them using standard techniques that rely on their very similar physicochemical properties. An alternative for an efficient D₂/H₂ separation is exploiting mass-dependent quantum effects. Here, we have performed a quantum-mechanical study of H₂/D₂ adsorption on circumcircumcoronene (CCCor) decorated with a sodium atom (proved to enhance molecular adsorption¹), as we have also analyzed in previous studies of hydrogen adsorption on metal-decorated carbon-based substrates^{2,3}. An analytical interaction potential for H₂-[Na-CCCor] was built³ (left panel of Fig.1) and employed to calculate the energy levels and partition functions of H₂/D₂ adsorbed on Na-CCCor (central panel of Fig.1). At low temperatures and pressures, we have determined the adsorption isotherms and D₂/H₂ separation selectivity (right panel of Fig.1). The H₂/D₂ molecules have been treated within pseudoatom and rigid rotor models, the latter allowing us to analyze *ortho* and *para* spin isomers. It has been found that Na-CCCor provides quite promising D₂/H₂ separation factors (several tens or more in the 20-30 K range). However, although the pseudoatom model proved to be accurate for other studies, it fails at determining the D₂/H₂ selectivity order of magnitude.

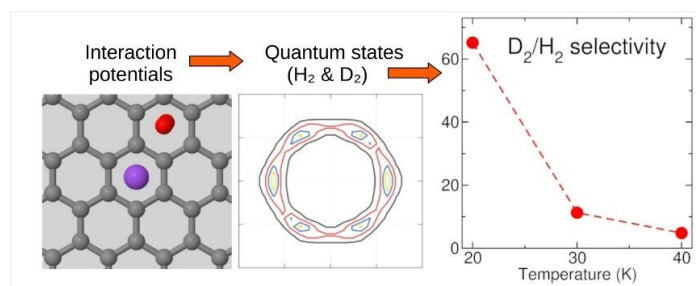


Figure 1: Interaction potentials, probability density of the quantum states and D₂/H₂ selectivity by means of adsorption on Na-decorated circumcircumcoronene.

References:

- ¹Mella, M.; García-Arroyo, E.; Hernández, M.I.; Bartolomei, M.; Campos-Martínez, J. (to be published, 2026).
- ²García-Arroyo, E.; Reider, A. M.; Kollotzek, S.; Foitzik, F.; Campos-Martínez, J.; Bartolomei, M.; Pirani, F.; Hernández, M. I.; Mella, M.; Scheier, P. The role of Na decoration on the hydrogen adsorption on coronene: A combined experimental and computational study. *Int. J. Hydrog. Energy*, 2024, 83, 387. <https://doi.org/10.1016/j.ijhydene.2024.07.425>
- ³García-Arroyo, E.; Bartolomei, M.; Hernández, M. I.; González-Lezana, T.; Mella, M.; Campos-Martínez, J. Adsorption of molecular hydrogen on extended graphene prototypes decorated with sodium: a quantum-mechanical study. *Phys. Scr.*, 2025, 100, 015411. <https://doi.org/10.1088/1402-4896/ad9e4b>

Breaking the Oxygen Shield for Reactivity Control in Mo₂C-Based MXenes

José D. Gouveia¹, José R. B. Gomes²

¹*CICECO-Aveiro Institute of Materials, Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*

²*CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*

Presenter's email address: jrgomes@ua.pt

MXenes are a class of promising two-dimensional catalysts whose reactivity can be tuned through surface termination chemistry, with molybdenum carbide MXenes serving as a particularly compelling example. While bare Mo₂C MXenes bind reaction intermediates too strongly, leading to limited catalytic turnover, oxygen functionalization provides a controlled strategy to attenuate surface reactivity without compromising structural stability. In this context, first-principles and machine-learning approaches have emerged as powerful and reliable tools for interpreting and predicting the structure–property and structure–reactivity relationships of MXenes^a.

Here, density functional theory combined with reaction energy profiling and transition-state searches is used to investigate the forward and reverse water–gas shift (WGS) reaction on Mo₂C-based MXenes with different surface terminations. Fully O-terminated Mo₂CO₂ is found to be catalytically inactive^b: the oxygen overlayer passivates surface Mo sites, suppressing metal–adsorbate interactions, weakening molecular adsorption, and imposing prohibitively high dissociation barriers. In contrast, breaking this “oxygen shield” by reducing the O coverage, either through the creation of termination vacancies^c or by introducing mixed O/F terminations^b, fundamentally reshapes the reaction landscape. Partial oxygen termination restores direct Mo participation in adsorption and bond activation, leading to moderate adsorption energies, lower dissociation barriers, and reaction energetics approaching the Sabatier optimum.

The obtained mechanistic picture explains why experimentally relevant Mo₂CT_x catalysts, which inevitably contain mixed terminations or vacancies, exhibit high forward or reverse WGS activity, respectively, despite the apparent inactivity predicted for fully terminated surfaces. More broadly, our findings establish oxygen coverage as a decisive reactivity control parameter in molybdenum carbide MXenes, providing clear mechanistic insight and practical design rules for optimizing O-functionalized MXene catalysts.

References:

^aGouveia, J. D.; Galvão, T. L. P.; Nassar, K. I.; Gomes, J. R. B. First-principles and machine-learning approaches for interpreting and predicting the properties of MXenes. *npj 2D Materials and Applications*, 2025, 9, 8. <https://doi.org/10.1038/s41699-025-00529-5>.

^bGouveia, J. D.; Gomes, J. R. B. The determining role of T_x species in the catalytic potential of MXenes: water adsorption and dissociation on Mo₂CT_x. *Catalysis Today*, 2023, 424, 113848. <https://doi.org/10.1016/j.cattod.2022.07.016>.

^cMorales-García, Á.; Gouveia, J. D.; López, A. V.; Comas-Vives, A.; Viñes, F.; Gomes, J. R. B.; Illas, F. MXene Termination and Stacking Bias on the Reverse Water Gas Shift Reaction Catalysis. *Materials Today Catalysis*, 2024, 7, 100076. <https://doi.org/10.1016/j.mtcata.2024.100076>.

Matrix-Isolation Photochemistry: Experimental–Theoretical Insights for Astrochemical Complexity

Justyna Krupa¹

¹ Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław Poland
justyna.krupa@uwr.edu.pl

Photochemical processes occurring under cryogenic and confined conditions play an important role in the development of molecular complexity in astrochemical environments. Matrix-isolation photochemistry provides a controlled laboratory framework to investigate such processes by stabilizing reactive species and transient intermediates at low temperatures. In this study, we present a combined experimental and theoretical investigation of light-induced molecular transformations in cryogenic matrices.

Photochemical experiments were performed using FTIR matrix-isolation spectroscopy, enabling direct detection of photoproducts, weakly bound complexes, and short-lived intermediates formed upon irradiation^{a–e}. Experimental observations were supported by quantum-chemical calculations, allowing reliable vibrational assignments, structural characterization, and identification of feasible photochemical pathways. The strong integration of experiment and theory provides reference spectroscopic data and mechanistic insight relevant to laboratory astrochemistry and astrochemical modelling.

References:

- ^a Krupa, J.; Kosendiak, I.; Wierzejewska, M.; Lundell, J. Experimental and theoretical investigation of hydrogen bonded complexes between glycolic acid and water, *Spectrochimica Acta Part A-Molecular and Biomolecular Spectroscopy*, 2025, 325, 125081. <https://doi.org/10.1016/j.saa.2024.125081>
- ^b Krupa, J.; Kosendiak, I.; Wierzejewska, M.; Ahokas, J.; Lundell, J. UV laser induced photolysis of glycolic acid isolated in argon matrices. *Journal of Photochemistry and Photobiology A-Chemistry*, 2021, 412, 113236. <https://doi.org/10.1016/j.jphotochem.2021.113236>
- ^c Krupa, J.; Biczysko, M.; Kosendiak, I.; Lundell, J. UV Photoreactivity of Hydrogen-Bonded Glycolic Acid–Water Complexes in Cryogenic Matrices, *in preparation*
- ^d Krupa, J.; Wierzejewska, M.; Lundell J. Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates, *Molecules*, 2023, 28, 1430. <https://doi.org/10.3390/molecules28031430>
- ^e Krupa, J.; Biczysko, M. UV Photochemistry of HNCO–H₂O₂ in Astrochemical Ice Analogues, *in preparation*

Acknowledgements:

This research was supported by the National Science Centre (Poland) and by the Academy of Finland. Computational resources were provided by the Wrocław Centre for Networking and Supercomputing (Poland). The support of the COST Action CA21101 (COSY) is gratefully acknowledged.

Quantum Dynamics with a Smolyak scheme. Applications to clathrate hydrates.

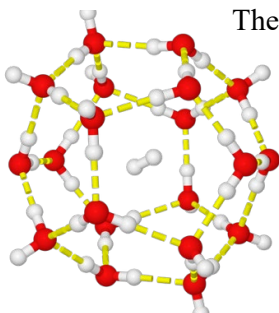
D. Lauvergnat¹, M. Segaud^{1,2}, Y. Scribano²

¹ *Institut de Chimie Physique, CNRS and Université Paris-Saclay, France*

² *Laboratoire Univers et Particules de Montpellier, Université de Montpellier, France*

David.Lauvergnat@université-Paris-Saclay.fr

The use of Smolyak scheme in quantum dynamics is an approach that pushes the limits of the current calculations based on a multidimensional basis set and grid. More precisely, the Smolyak scheme^{a-c} can be viewed as an approach involving a selection of basis functions and a sparse grid adapted to that basis set. The parameter, L , controls the selection and thus the size of the basis set and grid. With this scheme, the numerical complexity grows as a polynomial of degree L with respect to the number of degrees of freedom d . Systems with up to 12 degrees of freedom can be studied,^{d-f} although larger systems ($d=21$) are possible if few states are needed.^g This limit can be pushed away using a system-bath separation, and in our Smolyak scheme.^h



The spectroscopy studies (neutron, Raman ...) of encapsulated molecules in cages such as clathrates hydrates (see figure on the left), fullerenes, enable precise characterization of these systems.^{i-l} In particular, vibrational shifts and/or translation/rotation motions of the encapsulated molecule provide information about the interactions between the encapsulated molecule and the cage. Results for H₂ or CO encapsulated in rigid or flexible cages will show the efficiency of this sparse grid technique.^{m,h}

References:

- ^a Smolyak, S. A. Soviet Mathematics Doklady 1963, 4, 240. <https://www.mathnet.ru/eng/dan27586>
- ^b Avila, G.; Carrington, T. JCP 2009, 131, 174103. <https://doi.org/10.1063/1.3246593>
- ^c Lauvergnat, D.; Nauts, A. PCCP 2010, 12, 8405–12. <https://doi.org/10.1039/C001944E>
- ^d Lauvergnat, D.; Nauts, A.; Spectrochimica Acta Part A: 2014, 119, 18–25. <https://doi.org/10.1016/j.saa.2013.05.068>
- ^e Avila, G.; Carrington, T. JCP 2017, 147, 064103. <https://doi.org/10.1063/1.4994920>
- ^f Avila, G.; Mátyus, E. JCP 2019, 150, 174107. <https://doi.org/10.1063/1.5090846>
- ^g Lauvergnat, D.; Nauts, A.; ChemPhysChem, 2023, 24, 202300501. <https://doi.org/10.1002/cphc.202300501>
- ^h Chen, A.; Benoit, D. M.; Scribano, Y.; Nauts, A.; Lauvergnat, D. JCTC 2022, 18, 4366–4372. <https://doi.org/10.1021/acs.jctc.2c00108>
- ⁱ Ulivi, L. et al., Phys. Rev. B 2007, 76, 161401. <https://doi.org/10.1103/PhysRevB.76.161401>
- ^j Strobel, T. A. et al. CPL 2009, 478, 97–109. <https://doi.org/10.1016/j.cplett.2009.07.030>
- ^k Xu, M.; Sebastianelli, F.; Bačić, Z. JCP 2008, 128, 244715. <https://doi.org/10.1063/1.2945895>
- ^l Valdés, Á.; Prosimiti, R. JCP, 2024, 160, 184304. <https://doi.org/10.1063/5.0210866>
- ^m Lauvergnat, D.; Felker, P.; Scribano, Y.; Benoit, D. M.; Bačić, Z. JCP 2019, 150, 154303. <https://doi.org/10.1063/1.5090573>

Iron nitrides under oxidizing conditions: What we know from model studies on 2D Fe_xN islands on copper?

Mikołaj Lewandowski

*NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3,
61-614 Poznań, Poland*

Presenter's email address: lewandowski@amu.edu.pl

Iron nitrides constitute an interesting group of synthetic materials with a very rich phase diagram^a. These materials exhibit superior mechanical and magnetic properties, being also catalytically-active in several industrially-relevant reactions, such as ammonia (NH₃) synthesis and decomposition. The catalytic activity of iron nitrides under oxidizing conditions is often related to iron nitride/iron oxide interconversion, the mechanism of which is, to a wide extent, unknown. My group focuses on the structural evolution of iron nitrides under oxidizing conditions. The experiments are performed on model systems consisting of ultrathin iron nitride islands epitaxially grown on a copper single-crystal substrates^b. The results obtained on Cu(001) provided atomic-level insight into the reduction of N-terminated Fe_{1.33}N islands to the Fe₂N phase under mild oxidizing conditions, as well as further oxidation of Fe₂N to iron oxides: FeO and Fe₃O₄^c. The process was found to lead to the formation of nitrogen oxides (NO, NO₂). With the theoretical support from our collaborators, we were able to propose the possible reaction mechanism, which involves dissociation of O₂ on both iron nitride and copper regions, followed by reaction of oxygen atoms with nitrogen in iron nitride. As the surface structure of 2D iron nitride species is virtually-identical to that observed for the corresponding bulk crystals, the obtained findings constitute an important step towards the understanding of the catalytic activity of iron nitride surfaces and structural stability of different Fe–N phases under oxidizing conditions.

References:

^aWojciechowski, P.; Lewandowski, M. Iron Nitride Thin Films: Growth, Structure, and Properties, *Cryst. Growth Des.*, 2022, 22, 4618–4639. <https://doi.org/10.1021/acs.cgd.1c01528>

^bWojciechowski, P.; Andrzejewska, W.; Dobrotvorska, M. V.; Wang, Y.; Miłosz, Z.; Ossowski, T.; Lewandowski, M. Structure of monolayer iron nitride islands on Cu(001) revisited, *Vacuum*, 2024, 220, 112716. <https://doi.org/10.1016/j.vacuum.2023.112716>

^cAndrzejewska, W.; Wojciechowski, P.; Wang, Y.; Dobrotvorska, M. V.; Ossowski, T.; Fishman, E.; Benezova, T.; Heard, C. J.; Synoradzki, K.; Miłosz, Z.; Florczak, P.; Lewandowski, M. Understanding the chemistry of iron nitride surfaces: Iron nitrides-to-oxides transformation on copper under mild oxidizing conditions. *Small Structures*, 2026, submitted.

Acknowledgements:

The studies were financially supported by the Foundation for Polish Science through the First TEAM/2016-2/14 project No. POIR.04.04.00-00-28CE/16-00 (2017–2021). Part of the research was based upon the work of the COST Action CA21101 “Confined molecular systems: from a new generation of materials to the stars” (COSY) supported by COST (European Cooperation in Science and Technology).

Thermodynamics of Confined Water in Swelling of Clays: Role of Competitive Cation Hydration

Sai Adapa and Ateeque Malani*

Department of Chemical Eng, Indian Institute of Technology (IIT) Bombay, Mumbai, India)

The swelling capacity and stability of clay play a crucial role in various areas ranging from cosmetics to oil extraction; hence change in their swelling behaviour is important for their efficient utilization. Here we focus on understanding the role of different hydration properties of cation on the thermodynamics of clay swelling by water adsorption. We have used mica as the reference clay, Na^+ , Li^+ , and H^+ ions as the interstitial cations, and performed grand canonical Monte Carlo simulations of water adsorption in mica pores (of widths $d = 4 - 40 \text{ \AA}$). The disjoining pressure, swelling free energy, and several structural properties of confined water and ions were calculated. We expected higher water density in H-mica pores (ρ_{H}) due to the smaller size of H^+ ions having higher hydration energy. However, the counter-intuitive trend of $\rho_{\text{Li}} > \rho_{\text{Na}} > \rho_{\text{b}}$ (bulk density) $> \rho_{\text{H}}$ was observed. The swelling free energy for Na-mica is characterized by global minima at $d = 6 \text{ \AA}$ corresponding to crystalline swelling with significant and multiple barriers for crystalline swelling to osmotic swelling ($d > 12 \text{ \AA}$). A shift in the location of global minima of swelling free energy as well as it becoming more repulsive is observed in the increasing order of Na^+ , Li^+ , and H^+ ions. We found that the competition between surface atoms and water molecules to hydrate the Na^+ ions favour the non-swelling nature, whereas, it changes significantly in the Li^+ ions and H^+ ions case thus favouring clay swelling.

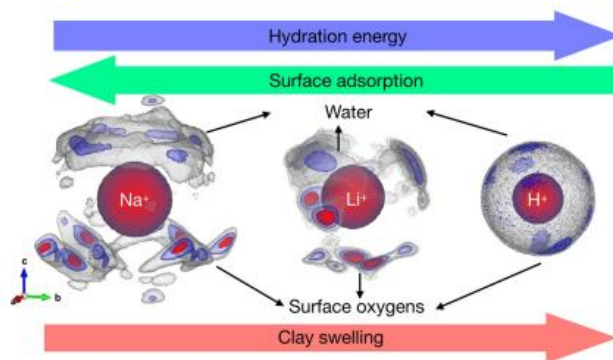


Figure 1: Three-dimensional pair-correlation function illustrating cation (central atom) hydration by oxygen of water molecules (top-side) and surface (bottom side) for various cations.

References:

- ^aS Adapa and A Malani, Sci. Rep., 2022, 12, 17810.
- ^bS Adapa and A Malani, chemrxiv, 2021.
- ^cS Adapa and A Malani, J. Colloids Interface Sci., 2021, 599, 694.
- ^dS Adapa and A Malani, chemrxiv, 2020.
- ^eS Adapa, D R Swamy, S Kancharla, S Pradhan and A Malani, Langmuir, 2018, 34, 14472.

Dual-locality learning under neighbourhood coupling: interpretable and transferable models for structured trace data

Manuel Mendoza-Hurtado^{1,2}, Domingo Ortiz-Boyer¹

¹ *Department of Computer Science and Numerical Analysis, University of Córdoba, Campus de Rabanales, 14071 Córdoba, Spain*

² *Department of Computer Science, University of Jaén, 23071 Jaén, Spain*

mmendoza@uco.es

Local interactions, confinement and neighbourhood coupling often generate heterogeneous regimes in structured systems. Analogous effects arise in large-scale spatiotemporal trace data, where a single global hyperparameter can underfit dense regions and overfit sparse ones, and naive splits can leak spatial dependence^a.

A dual-locality, interpretable machine-learning framework is presented for functional-pattern identification from structured spatiotemporal traces. Feature-space locality is captured through prototype-specific local-k optimisation for multi-label kNN, improving over fixed-k baselines without increasing inference cost^b. Neighbourhood locality is incorporated via Moore-adjacency influence sets for gridded activity fields (ML-proxkNN), explicitly modelling local context while preserving feature-space similarity.

On CDR-derived benchmarks in Milan and Trento, the dual-locality classifier reaches high precision and retains its advantage under spatial block cross-validation that controls for spatial autocorrelation^c. Complementary experiments on trajectory-derived mobility features from geolocated social traces detect cross-border home-work commuting with high accuracy and reproduce official flow directionality through zero-shot transfer across multiple European border regions^d. Overall, the contribution emphasises relevant design principles: encode neighbourhood structure, adapt model complexity locally, validate under non-leaky splits, and use explanations to assess descriptor portability across domains.

References:

^a Mendoza-Hurtado, M., Romero-del-Castillo, J. A., & Ortiz-Boyer, D. MAPLID: a new multi-label approach for place identification using data supplied by mobile network operators. *International Journal of Geographical Information Science*, 2026, 1–24. <https://doi.org/10.1080/13658816.2026.2617932>

^b Romero-del-Castillo, J. A.; Mendoza-Hurtado, M.; Ortiz-Boyer, D.; García-Pedrajas, N. Local-based k values for multi-label k-nearest neighbors rule. *Engineering Applications of Artificial Intelligence*, 2022, 116, 105487. <https://doi.org/10.1016/j.engappai.2022.105487>

^c Mendoza-Hurtado, M.; Romero-del-Castillo, J. A.; García-Pedrajas, N.; Ortiz-Boyer, D. A new local proximity-based k-nearest neighbors method for multi-label land use identification using mobile phone data. Manuscript under review, 2026.

^d Mendoza-Hurtado, M.; Järv, O.; Malekzadeh, M.; Karasov, O.; Ortiz-Boyer, D. Sensing labour mobility flows of cross-border urban regions using machine learning and geolocated social network data. Manuscript under review, 2026.

When Platinum Becomes Not Noble: Platinum-Oxide Clusters Supported on Ceria

Konstantin M. Neyman^{1,2}, Pablo Castro-Latorre², Albert Bruix²

¹ICREA (Catalan Institution for Research and Advanced Studies), 08010 Barcelona, Spain

²Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTUB), Universitat de Barcelona, 08028 Barcelona, Spain
konstantin.neyman@icrea.cat

Platinum is a noble metal extremely resistant to oxidation. Nevertheless, platinum in the sub-nanoscale state may lose this prominent resistivity. Indeed, experiments indicated a formation of small ceria-supported platinum-oxide clusters in Pt/CeO₂ catalytic materials even at very low oxygen pressure.^a Such clusters were proposed to expose active sites that enable efficient CO oxidation already at temperatures below 0°C.

We explored oxidation of small free-standing and supported on CeO₂(111) platinum clusters using a DFT global structure optimization in combination with *ab initio* thermodynamics.^b These studies revealed thermodynamically stable at temperatures up to several hundred °C substantially oxidized supported Pt clusters at O₂ pressure below 0.01 atm. So high stability indicates that the clusters with Pt-O-Pt bonds are abundantly present on the CeO₂(111) support. Calculated by us Pt_nO_m clusters exhibit peculiar O-Pt-O and Pt-O-Pt motifs typical for the coordination compounds formed by Pt cations. Modelling of CO adsorption on the supported Pt_nO_m clusters and subsequent CO₂ desorption suggested that such surface structures can trigger the observed CO oxidation at extraordinary low temperature.^c Our recent DFT calculations of the full catalytic cycles for the low-temperature CO oxidation confirmed that.^d The obtained new mechanistic insights pave the way for designing very low-temperature oxidation catalysts based on stable supported metal-oxide clusters.

We will discuss data of the above mentioned DFT studies of the Pt_nO_m/CeO₂ systems in relation with the experimental data on their structure and oxidative catalytic activity. A general conclusion is that studies of small Pt clusters have to include oxidized states even at quite low oxygen pressures: ignoring that may hinder obtaining a complete understanding.

References:

^aBoronin, A.I.; Slavinskaya, E.M.; Figueroba, A.; Stadnichenko, A.I.; Kardash, T.Yu.; Stonkus, O.A.; Fedorova, E.A.; Muravev, V.V.; Svetlichnyi, V.A.; Bruix, A.; Neyman, K.M. CO oxidation activity of Pt/CeO₂ catalysts below 0°C: Platinum loading effects. *Appl. Catal. B: Environ.* 286 (2021) 119931. doi: 10.1016/j.apcatb.2021.119931

^bQuinlivan Domínguez, J.E.; Neyman, K.M.; Bruix, A. Stability of oxidized states of free-standing and ceria-supported PtO_x particles. *J. Chem. Phys.* 157 (2022) 094709. doi: 10.1063/5.0099927

^cSlavinskaya, E.M.; Stadnichenko, A.I.; Quinlivan Domínguez, J.E.; Stonkus, O.A.; Vorokhta, M.; Šmíd, B.; Castro-Latorre, P.; Bruix, A.; Neyman, K.M.; Boronin, A.I. States of Pt/CeO₂ catalysts for CO oxidation below room temperature. *J. Catal.* 421 (2023) 285. doi: 10.1016/j.jcat.2023.03.004

^dCastro-Latorre, P.; Bruix, A.; Grönbeck, H.; Neyman, K.M. How PtO_x/CeO₂ nanostructures catalyze CO oxidation at very low temperature, submitted.

Electron scattering on H_2^+ , BeH^+ and their isotopologues: Dissociative recombination and ro-vibrational transitions

N. Pop¹, R. Hassaine², E. Djuissi², J. Zs Mezei³, M. D. Epée Epée⁴, O. Motapon⁵,
K. Chakrabarti⁶, I. F. Schneider^{2,7}

¹Department of Fundamentals of Physics for Engineers, Politehnica University Timisoara, Romania

²Laboratoire Ondes et Milieux Complexes, CNRS, Univ. du Havre, France

³Inst. of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, Hungary

⁴Department of Physics, Faculty of Sciences, University of Douala, Cameroon

⁵Faculty of Science, University of Maroua, Maroua, Cameroon

⁶Dept of Mathematics, Scottish Church College, Calcutta, India

⁷Laboratoire Aimé Cotton, CNRS, ENS Cachan and Univ. Paris-Sud, Orsay, France

nicolina.pop@upt.ro

A new series of computations has been performed to obtain cross sections and rate coefficients for state-to-state ro-vibrational transitions in the H_2^+ and HD^+ ion, induced in collisions with low-energy electrons¹. We describe the major low-energy electron-impact processes involving H_2^+ and its isotopologues relevant for the early universe astrochemistry^{2,3,4}. Dissociative recombination (DR), vibrational excitation (VE), vibrational de-excitation (VdE), based on the multichannel quantum defect theory (MQDT) is extended to higher collision energies and fully accounts the dissociative excitation (DE) in the case of the BeH^+ ion⁵. Three electronic symmetries of BeH^+ - 2Π , $2\Sigma^+$, and 2Δ - have been included in the calculations cross sections and rate coefficients. At low energies the DR is dominated by capture into states of 2Π symmetry. The results are an extension of our results^{6,7,8} and are suitable for the modeling of beryllium transport in the plasma and the determination of influxes of beryllium hydrides into the plasma.

References:

- ¹R. Hassaine, et al., Electron impact ro-vibrational transitions and dissociative recombination of H_2^+ and HD^+ . Rate coefficients and astrophysical implications, A&A, 2025, 703, A220
- ²MD Epée Epée., et al., Dissociative recombination and rotational transitions of D^+ in collisions with slow electrons, MNRAS, 2022, 512, 424–429.
- ³E. Djuissi, N. Pop et al, Electron driven reactive processes involving H_2^+ and HD^+ molecular cations in the Early Universe, Romanian Astronomical Journal, 2020, 30(2), 10.
- ⁴O. Motapon, N. Pop, et al., Rotational transitions induced by collisions of HD^+ ions with low-energy electrons, Phys. Rev. A, 2014, 90, 012706.
- ⁵E. Djuissi, N. Pop, et al., Reactive collisions between electrons and BeH^+ above dissociation threshold, Phys. Chem. Chem. Phys., 2024, 26, 18311.
- ⁶N. Pop, et al., Reactive collisions between electrons and BeT^+ : Complete set of thermal rate coefficients up to 5000 K, Atomic Data and Nuclear Data Tables, 2021, 139, 101414.
- ⁷S. Niyonzima, et al., Low-energy collisions between electrons and BeD^+ , Plasma Sources Sci. Technol. 2018, 27, 025015.
- ⁸S. Niyonzima, et al., Low-energy collisions between electrons and BeH^+ : Cross sections and rate coefficients for all the vibrational states of the ion, Atomic Data and Nuclear Data Tables, 2017, 115-116, 287.

Photo-transformations of thiazole carboxylic acids in low temperature matrices

Magdalena Sałdyka, Daria Bumażnik

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
magdalena.saldyka@uwr.edu.pl

The structure, spectroscopic properties and photo-induced transformations of two thiazole derivatives, 2-aminothiazole-4-carboxylic acid (ACA) and thiazole-4-carboxylic acid (TCA), isolated in argon and nitrogen matrices were studied using matrix-isolation FTIR spectroscopy and DFT calculations undertaken at the B3LYP-D3/6-311++G(3df,3pd) level of theory.^{a,b} The three most stable structures for both ACA and TCA were identified in matrices after deposition. In the most stable ACA and TCA tautomers the five-membered ring was stabilized by C=C and C=N double bonds and with different arrangement of the carboxyl group. For both compounds, the photo-transformations upon irradiation provided by an Optical Parametric Oscillator (OPO) tunable laser system were studied. Following irradiation at 285 or 1456 nm, a rotation of the OH group around the C–O bond in ACA1 leading to increase of ACA2 was detected. The corresponding reverse photo-rotamerization was detected at 296 or 1434 nm, resulting in the recovery of the initial isomer ACA1. Similar observations were made for TCA, which indicated the ongoing process of TCA1 → TCA2 *trans*–*cis* photo-isomerization at 278 nm (or 1486 nm); when irradiated with a wavelength of 262 nm (or 1434 nm), the opposite process was observed: TCA2 → TCA1.

Selective UV irradiation of matrices with shorter wavelengths led to photolytic decomposition of ACA or TCA compounds and as the first step of photolysis decarboxylation occurred. Subsequent photolysis reactions therefore occurred for 2-aminothiazole or thiazole, during which a number of new molecules, including potential prebiotic carbodiimides or molecular complexes, were identified. Main photoproducts were produced by a cleavage of the CS-CN bond together with hydrogen atom migration. Our results confirm that complex organic compounds undergo photodissociation into simpler prebiotic building blocks.

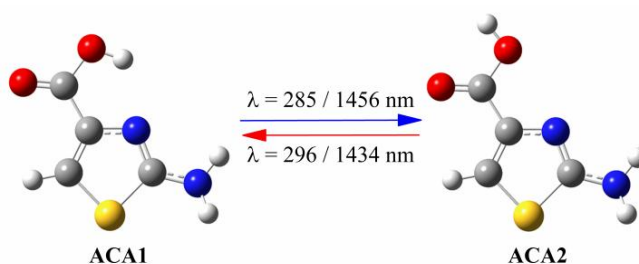


Fig. 1 UV/NIR-induced *cis*–*trans* isomerization reactions between ACA1 and ACA2.

References:

^aBumażnik, D.; Sałdyka, M. Photo-transformations of 2-aminothiazole-4-carboxylic acid in low-temperature matrices. *J. Photochem. Photobiol. A: Chemistry*, 2024, 455, 115766/1–115766/13. <https://doi.org/10.1016/j.jphotochem.2024.115766>

^bBumażnik, D.; Sałdyka, M. UV-Induced Photodegradation of 2-Aminothiazole-4-Carboxylic Acid: Identification of New Carbodiimide Molecules. *Molecules*, 2025, 30, 3713. <https://doi.org/10.3390/molecules30183713>

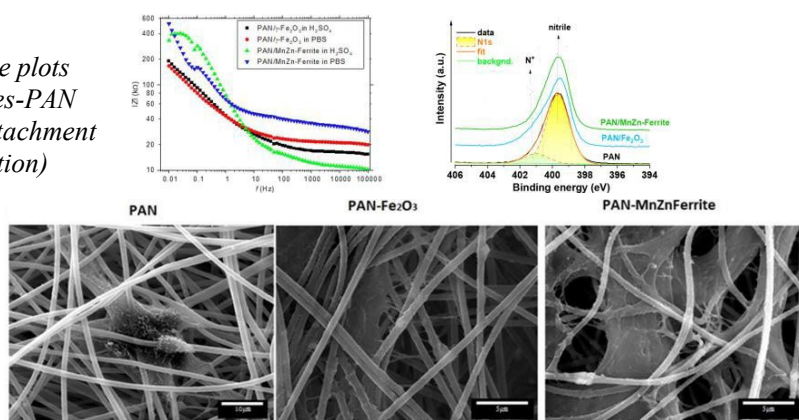
Confined Magnetic Ferrite Nanoparticles in Polyacrylonitrile Nanofibers: Tunable Nanostructures for Tissue Engineering

A. Sezai Sarac^{1*}, Viktor Soprunyuk², Elham Sharifikolouei³, Matej Micusik⁴, Alessandro Scalia³, Baran Sarac⁵, Selin Gümrükçü¹, Eray Yüce⁵, Wilfried Schranz²

¹ Istanbul Technical University, Türkiye, ² University of Vienna, Austria, ³ CAAD, Università del Piemonte Orientale UPO, Italy, ⁴ Polymer Institute, SAS, Bratislava, Slovakia, ⁵ Montanuniversität Leoben, Austria
email * (sarac@itu.edu.tr)

The integration of magnetic nanoparticles into polymer scaffolds has emerged as a promising strategy in tissue engineering, offering the potential for enhanced cell proliferation. In this study, the fabrication and characterization of composite nanofiber membranes composed of ferrite nanoparticles (NPs) and Polyacrylonitrile (PAN), and biocompatible, magnetically active scaffold capable of supporting cellular growth and differentiation was performed. Electrospun PAN Nanofibers embedded Ferrite NPs were characterized using advanced techniques, i.e., FTIR, XPS, HR-SEM, EIS, and XRD [1, 2]. The incorporation of these NPs led to significant changes in the thermal, spectroscopic, and morphological properties of the fibers. Results indicate that the incorporation of MnZn-Ferrite nanoparticles alters the fibers' thermal and morphological properties, enhancing surface chemistry through the formation of new nitrogen functionalities and improved interfacial interactions. Cytocompatibility studies using human mesenchymal stromal cells (hMSCs) revealed no significant impact on cell viability or morphology, confirming the scaffold's biocompatibility. In vitro biological assays using hMSCs demonstrated robust cell attachment and proliferation with no cytotoxic effects, verifying the material's cytocompatibility. By combining the tunable magnetism of MnZn-Ferrites with the mechanical durability of PAN, these scaffolds represent a platform for "smart" regenerative medicine, allowing for non-invasive control over cellular behavior and tissue maturation.

Fig.(a) Bode magnitude plots
(b) XPS N1s of Ferrites-PAN
(c) SEM of hMSC attachment
(48 h of incubation)



References:

1. Sarac, B.; Sharifikolouei, E.; Micusik, M.; Scalia, M. A.; Najmi, Z.; Cochis, A.; Rimondini, L.; Barrera, G.; Coisson, M.; Gümrükçü, S.; Yüce, E.; Sarac, A. S. Development and characterization of (MnZn) ferrite-polyacrylonitrile composite nanofiber membranes for tissue engineering.. Emergent Mater., 2025, <https://doi.org/10.1007/s42247-025-01247-w>
2. Sarac, B.; Soprunyuk, V.; Yüce, E.; Gumrukcu, S.; Schranz, W.; Sarac, A. S. Impact of thermal treatment and magnetic field on the dynamic mechanical behavior of polyacrylonitrile nanofibers with embedded magnetic ferrite nanoparticles. Mater. Adv., 2025, 6, 5475-5485. <https://doi.org/10.1039/D5MA00349K>

Energetic and Spectroscopic Insights into the C₃H₆O₂ Isomer Family for Astrochemical Purposes

Alessandra Savarese¹, Silvia Alessandrini¹, Mattia Melosso¹, Gabriele Panizzi¹,
Michela Nonne², Luca Bizzocchi¹, Cristina Puzzarini¹

¹*Department of Chemistry “Giacomo Ciamician”, University of Bologna, Via P. Gobetti 85,
Bologna 40129, Italy*

²*Scuola Superiore Meridionale, Largo San Marcellino 10, Naples 80138, Italy
alessandra.savarese4@unibo.it*

The interstellar medium (ISM), despite its harsh physical conditions, is known to contain more than 340 molecular species (to date), with new detections being reported on a monthly basis.^a Most of the detected molecules have been identified thanks to radioastronomical signals, which in turn require accurate rotational spectroscopic data for interpretation. One strategy for detecting new interstellar species is to focus on a particular family of isomers, exploiting the connection between the relative stabilities of the isomers and their detectability in the ISM (Minimum Energy Principle, MEP).^b

In the present study,^c a computational protocol based on the MEP has been applied to the C₃H₆O₂ isomer family, providing accurate energetic hierarchies and spectroscopic parameters relevant to astrochemistry. Propanoic acid is predicted as the most stable isomer, followed by methyl acetate, ethyl formate, 1-hydroxyacetone, 2- and 3-hydroxypropanal. All of these species have been experimentally studied and offer the opportunity to benchmark the computed rotational spectroscopic parameters obtained from the protocol. This benchmark has been further extended by including glycidol, a high-energy C₃H₆O₂ isomer, for which new high-frequency rotational spectroscopic measurements have been carried out. This benchmarking strategy establishes reliable uncertainties for the rotational spectroscopic parameters of the species not yet characterized in the laboratory, while the computational protocol indicates that high-energy conformers of propanoic acid should be the focus of future laboratory studies. Finally, the improved set of spectroscopic parameters for glycidol provides data for its radioastronomical search.

References:

^a<https://cdms.astro.uni-koeln.de/classic/molecules> (CDMS database: Müller, H. S. P; Schlöder, F.; Stutzki, J.; Winnewisser, G. The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists. *Journal of Molecular Structure*, 2005, 742(1-3), 215-227. <https://doi.org/10.1016/j.molstruc.2005.01.027>).

^bLattalais, M.; Pauzat, F.; Ellinger, Y.; Ceccarelli, C. Interstellar complex organic molecules and the minimum energy principle. *The Astrophysical Journal*, 2009, 696(2), L133-L136. <https://doi.org/10.1088/0004-637X/696/2/L1333>.

^cSavarese, A.; Alessandrini, S.; Melosso, M.; Panizzi, G.; Nonne, M.; Bizzocchi, L.; Puzzarini, C. Energetic and Spectroscopic Insights into the C₃H₆O₂ Isomer Family for Astrochemical Purposes. *ACS Earth and Space Chemistry*, 2025, in press. <https://doi.org/10.1021/acsearthspacechem.5c00291>.

First Principal Study of Defects in s-I and s-II Gas Hydrates*

Nevin Uras-Aytemiz¹, F. Mine Balcı², Tuncay Karakurt³

¹ Department of Engineering Basic Science, Bandırma Onyedi Eylül University, 10200
Bandırma-Balıkesir, Türkiye

² Department of Chemistry, Faculty of Engineering and Natural Sciences, Süleyman Demirel
University, Çünür/Isparta, 32260, Turkey

³ Department of Chemical Engineering, Faculty of Engineering–Architecture, Kırşehir Ahi
Evrar University, Kırşehir, 40100, Turkey
naytemiz@bandirma.edu.tr

Clathrate hydrates (CHs) are crystalline materials in which water molecules form cages that encapsulate guest gas molecules. The specific hydrate structure formed is dictated by the size and chemical interactions of the guest molecules with the water network during hydrate formation. This study focuses on the two most common structures: structure I (s-I) and structure II (s-II). The thermodynamic stability of CHs arises from van der Waals interactions between the guest molecules and the host water network. However, certain guest molecules, such as ethylene oxide (EO) and tetrahydrofuran (THF), can form hydrogen bonds with the water molecules within the host cages. The incorporation of these H-bonding guests leads to experimentally observed deviations in various properties compared to CHs formed with nonpolar guests or ice, including dielectric relaxation rates, spin-relaxation times, electrical conductivity, and formation kinetics. These deviations are likely associated with the presence and behavior of distinct types of defects within the CH structure. This study employs first-principles calculations based on Density Functional Theory (DFT) to examine the effects of EO and THF guest molecules on selected protonic and molecular point defects commonly present in ice and ice-like structures. These defects include Bjerrum defects¹, ionic defects ($\text{H}_3\text{O}^+/\text{OH}^-$)², and molecular vacancy defects³. The results of this investigation will be presented in terms of energetics, structural characteristics, and dynamical behavior.

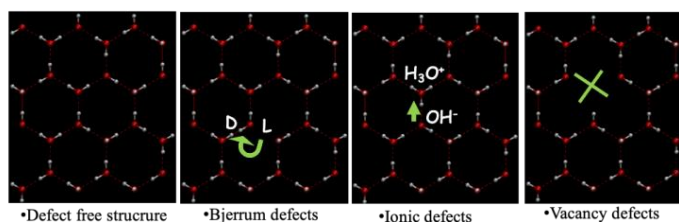


Figure 1. Defects in Clathrate hydrates

References:

- ¹Uras-Aytemiz, N.; Balcı, F. M. Bjerrum defects in s-II gas hydrate. *Journal of Molecular Graphics and Modelling*, 2024, 133, 108878. <https://doi.org/10.1016/j.jmgm.2024.108878>.
- ²Manuscript in preparation.
- ³Balcı, F. M.; Uras-Aytemiz, N. Exploring vacancy defects in s-I clathrate hydrates. *Journal of Molecular Graphics and Modelling*, 2025, 136, 108969. <https://doi.org/10.1016/j.jmgm.2025.108969>.

*This work supported by TÜBİTAK (project number: 119Z880)

Poster Presentations

Grand-canonical DFT investigation of transition-metal sulfide nanoalloys for electrochemical nitrogen reduction

Nawras Abidi¹, Yaovi Holade², Jean-Sébastien Filhol¹, Hazar Guesmi¹

¹ ICGM, University Montpellier, CNRS, ENSCM, 1919 Rte de Mende, 34293 Montpellier Cedex 5, France

² IEM, UMR 5635, Univ Montpellier, ENSCM, CNRS, Montpellier, France
Institut Universitaire de France (IUF), 75005 Paris, France

Ammonia is essential for agriculture and chemical manufacturing, but its industrial production via the Haber–Bosch process is highly energy-intensive and carbon demanding. The electrochemical nitrogen reduction reaction (NRR) provides a sustainable alternative under mild conditions but remains challenging due to the strong stability of the $\text{N}\equiv\text{N}$ bond and competition from hydrogen evolution. Among potential catalysts, transition-metal sulfide nanoalloys are attractive thanks to their tunable electronic properties and surface reactivity.¹ To explore their activity, we performed spin-polarized density functional theory (DFT) calculations using the PBE-dDsC functional with dispersion corrections to investigate stability, adsorption and reaction energetics. Electrochemical effects were included through grand-canonical DFT combined with an implicit solvation model (VASPsol) based on the linearized Poisson–Boltzmann equation.² A systematic screening of Co, Ni, and Fe sulfide hosts and their substitutional nanoalloys identified the most stable composition. We then analyzed its dominant (111) surface, mapping gas-phase adsorption and reaction pathways before incorporating potential-dependent energetics via GC-DFT.

The Fe-Co sulfide nanoalloy exhibits strong N_2 adsorption (-0.65 eV) at the Fe–Co bridge site, leading to clear $\text{N}\equiv\text{N}$ bond elongation and efficient activation. Free-energy profiles reveal an associative-to-dissociative hybrid mechanism: the first protonation ($\text{N}_2 \rightarrow \text{N}_2\text{H}$) is mildly endergonic (0.31 eV), subsequent hydrogenations are exergonic, and NH_3 desorption is the potential-determining step (0.88 eV), which decreases by around 0.2 eV with explicit water coadsorption. Hydrogen adsorption is weak on the most active Fe sites (0.01 eV), indicating low HER activity and enhanced NRR selectivity. Including the applied potential through GC-DFT captures its effect on adsorption and reaction energetics, allowing us to define the operating potential window where NRR is thermodynamically favored over HER.

This work establishes the connection between nanoalloy composition, active sites, and reaction mechanism, providing detailed insights into N_2 activation and NH_3 formation and offering clear design guidelines for developing efficient and selective transition-metal sulfide electrocatalysts for sustainable ammonia synthesis.

References

¹Shen, Y.; Sementa, L.; Johnson, D. D.; et al. J. Am. Chem. Soc. 2025, 147, 14541–14553.

²Mathew, K.; Kolluru, V. S. C.; Mula, S.; Steinmann, S. N.; Hennig, R. G. J. Chem. Phys. 2019, 151, 234101.

The role of Water in Physisorption and Chemisorption of Pollutants within Copper Squarate: A DFT cluster study

Celia Adjal^{1,2, †}, Nabila Guechtouli^{1,3}, Vicente Timón²

¹ USTHB, Laboratory of Thermodynamics and Molecular Modeling, Faculty of Chemistry, BP32, El Alia,

16111, Bab Ezzouar, Algiers; Algeria.

² Instituto de Estructura de la Materia, CSIC, Serrano 121, Madrid 28006, Spain.

³ University of M'hamed Bougara, UMMB, Faculty of Sciences, 35000 Boumerdes, Algeria.

Presenter's email address: vicente.timon@csic.es

[†] Present address (Department of Chemistry, McGill University, 801 Sherbrooke Street West, Montreal, Quebec H3A 0B8, Canada)

The global escalation of atmospheric pollutants presents a critical challenge to public health and biodiversity. To combat this, Metal-Organic Frameworks (MOFs) have emerged as first candidates due to their exceptional adsorption mechanisms skills on various pollutants [1].

We modeled our structures using Density Functional Theory (DFT) at the B3LYP-GD3(BJ) level of theory. To ensure high precision, we employed the LANL2DZ pseudopotential for Cu atoms and the 6-31G** basis set for light atoms, with all adsorption energies refined via the Basis Set Superposition Error (BSSE) counterpoise correction [2]. Our analysis explores energetic profiles by calculation of adsorption energies in both dry and humid environments of CO₂ and SO₂ pollutants to simulate real-world conditions. Structural Parameters as well as vibrational Analysis, with comparison of theoretical IR spectra with experimental data to validate the host-guest interactions.

The results reveal a nuanced interplay between physisorption and chemisorption—details often overlooked in periodic solid-state simulations. By elucidating these distinct capture mechanisms within the framework cavities, this work demonstrates the high efficiency of Copper Squarate as a robust material for targeted pollutant sequestration [3].

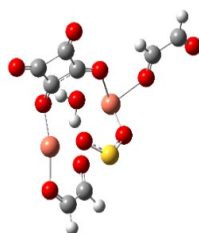


Figure 1: Optimised structure of SO₂ captured by molecular Copper Squarate and water.

References:

- [1] Timón, V.; Senent, M. L.; Hochlaf, M. Structural single and multiple molecular adsorption of CO₂ and H₂O in zeolitic imidazolate framework (ZIF) crystals. *Microporous and Mesoporous Materials* 2015. doi:10.1016/j.micromeso.2015.06.035.
- [2] Becke, A. D. A new mixing of Hartree-Fock and local density-functional theories. *The Journal of Chemical Physics* 1993. doi:10.1063/1.464304.
- [3] Adjal, C.; Guechtouli, N.; Timón, V.; Colmenero, F.; Hammoutène, D. Theoretical Study of Copper Squarate as a Promising Adsorbent for Small Gases Pollutants. *Molecules* 2024. doi:10.3390/molecules29133140.

Dynamics and Binding Behavior in Light-Responsive HDAC Inhibitors

Ana Paola Leyva Aizpuru¹, Sandra Gómez¹, Javier Camarillo Cisneros², Juan José Nogueira^{1,3}

¹Department of Chemistry, Universidad Autónoma de Madrid, 28049, Madrid, Spain

²Computational Physical Chemistry Laboratory Universidad Autónoma de Chihuahua, 31125, Mexico.

³Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain.

Conventional anticancer therapies are known for damaging not only tumorous cells but also the surrounding tissue. This poor spatial selectivity leads to adverse effects that significantly compromise patient well-being. Photoswitchable therapy offers an alternative by enabling external, light controlled activation and localized drug activity, thereby reducing systemic toxicity. Histone deacetylases (HDACs) are well-established anticancer targets due to their involvement in gene expression regulation. Azobenzene-modified derivatives from the FDA-approved inhibitor vorinostat have demonstrated reversible, light dependent inhibition. Notably, the Z isomer shows roughly 50 fold greater potency toward HDAC1 than its E counterpart, as reported in in situ assays¹. Computational studies have mapped binding poses and proposed intermediates associated with the switching behavior, but the direct photoisomerization process within the enzyme environment is not yet fully characterized². In this study, we perform classical molecular dynamics simulations complemented by MM/GBSA calculations to evaluate the stability and energetics of enzyme–inhibitor interactions³. The next stage will incorporate non-adiabatic molecular dynamics to follow excited-state evolution and the photoisomerization pathway in real time⁴. Together, these approaches elucidate the mechanistic basis for the experimentally observed differences in isomer stability inside the HDAC active site and provide computational insights that may guide the rational design of photoswitchable HDAC inhibitors with enhanced photochemical performance.

References:

- ¹Josa-Culleré, L.; Llebaria, A. *Visible-Light-Controlled Histone Deacetylase Inhibitors for Targeted Cancer Therapy*. *J. Med. Chem.*, 2023, 66(3), 1909–1927. <https://doi.org/10.1021/acs.jmedchem.2c01713>
- ²Queizán, C. M.; Teijeira, M.; Hermida-Ramon, J. M. *Molecular basis of the activity of a photoswitchable histone deacetylase inhibitor*. *J. Mol. Liq.*, 2025, 437(B), 128488. <https://doi.org/10.1016/j.molliq.2025.128488>
- ³Miller III, B. R.; McGee Jr, T. D.; Swails, J. M.; Homeyer, N.; Gohlke, H.; Roitberg, A. E. *MMPBSA.py: An Efficient Program for End-State Free Energy Calculations*. *J. Chem. Theory Comput.*, 2012, 8(9), 3314–3321. <https://doi.org/10.1021/ct300418h>
- ⁴Mallo, M.; Gómez-Carrasco, S.; Gómez, S. *Delayed photoisomerisation of the trans-PSB3 retinal toy model using on-the-fly quantum dynamics*. *Phys. Chem. Chem. Phys.*, 2025, 27(34), 17770–17778. <https://doi.org/10.1039/d5cp02117k>

Vacancy Bjerrum Defects in s-II type Clathrate Hydrates*

F. Mine BALCI¹, Nevin Uras-Aytemiz²

¹ *Department of Chemistry, Faculty of Engineering and Natural Sciences, Süleyman Demirel University, Çünür/Isparta, 32260, Turkey*

² *Department of Engineering Basic Science, Bandırma Onyedi Eylül University, 10200 Bandırma – Balıkesir, Turkey*
minebalci@sdu.edu.tr

Clathrate hydrates are crystalline, cage-like structures formed by hydrogen-bonded water molecules that encapsulate guest gas molecules. The hydrate structure that forms depends strongly on the size of the guest species and its chemical interactions with water or ice¹. One of the most common and widely studied hydrate phases is structure II (sII). In this work, we present a density functional theory (DFT) investigation of vacancy–Bjerrum defect complexes in sII hydrates, focusing on their structure, energetics, and dynamics. These defects are believed to play a crucial role in hydrate formation processes and in facilitating the transport of guest gas molecules through the water cages²⁻⁴.

References:

¹Sloan, E. D.; Koh, C. A. Clathrate hydrates of Natural Gases. 3rd. ed., CRC Press: Boca Raton, FL., 2008.

²Buch, V.; Devlin, J. P.; Monreal, I. A.; Jagoda-Cwiklik, B.; Uras-Aytemiz, N.; Cwiklik, L. Clathrate Hydrates with Hydrogen-Bonding Guests. *Physical Chemistry Chemical Physics*, 2009, 11, 10245–10265. <https://doi.org/10.1039/B911600C>.

³Uras-Aytemiz, N.; Balci, F. M. Bjerrum defects in s-II gas hydrate. *Journal of Molecular Graphics and Modelling*, 2024, 133, 108878. <https://doi.org/10.1016/j.jmgm.2024.108878>.

⁴Balci, F. M.; Uras-Aytemiz, N. Exploring vacancy defects in s-I clathrate hydrates. *Journal of Molecular Graphics and Modelling*, 2025, 136, 108969. <https://doi.org/10.1016/j.jmgm.2025.108969>.

* This manuscript is in preparation and supported by TÜBİTAK (project number: 119Z880)

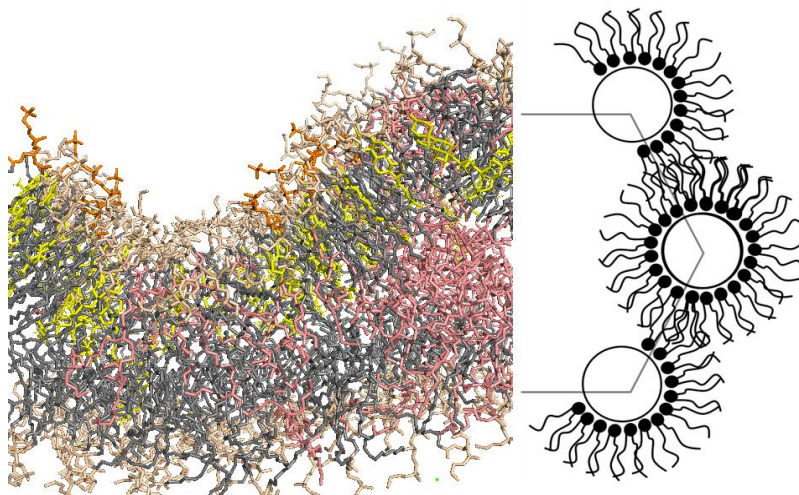
Geometry and phase behaviour of nonlamellar lipids in confined environments

Petra Čechová^{1*}, Martin Šrejber¹, Markéta Paloncýová¹, Michal Otyepka^{1,2}

¹Czech Advanced Technology and Research Institute (CATRIN), Palacký University
Olomouc, Křížkovského 511/8, 779 00 Olomouc, Czech Republic

²IT4Innovations, VŠB – Technical University of Ostrava, Studentská 6231/1B
708 00 Ostrava, Czech Republic

Lipid confined environments are the basis of many structures both in nature^a and in biotechnologies^b. In both of these cases, non-lamellar lipids bring conformational flexibility required for the system to transition from a planar bilayer to more complex three-dimensional structures – be it a simple curved membrane or a system in the inverted hexagonal or cubic phases. The interplay between the lipid geometry and charge^c is a fundamental property that decides the shape of its molecular assembly, with consequences for various mixtures containing these nonlamellar lipids.



A curved membrane of POPE and nonlamellar lipid, a schematic of a hexagonal phase

References:

^aČechová P., Kührová P., Šrejber M., Valério M., Borbuliak M., Souza P. C. T., Otyepka M., Paloncýová M. Computational Microscopy of Lipid Confined Systems: Challenges and Opportunities. *Small Structures*, 2026, X(X), XX–XX. <https://doi.org/10.1002/sstr.202500697>

^bPaloncýová M., Valério M., Nascimento Dos Santos R., Čechová P., Dobchev D. A., Balsubramani A., Banáš P., Agarwal V., Souza P. C. T., Otyepka M. Computational Methods for Modeling Lipid-Mediated Active Pharmaceutical Ingredient Delivery. *Molecular Pharmaceutics*, 2025, 22 (3), 1110–1141, doi.org/10.1021/acs.molpharmaceut.4c00744

^cČechová, P., Paloncýová, M., Šrejber, M., & Otyepka, M. Mechanistic insights into interactions between ionizable lipid nanodroplets and biomembranes. *Journal of Biomolecular Structure and Dynamics*, 2025, 43(17), 9983–9993. <https://doi.org/10.1080/07391102.2024.2329307>

On the use of theoretical models as tools for the stability prediction of actinide extractants

Colmenero F.^{1*}, Sánchez-García, I.¹, Vacas-Arquero, P.¹, Timón V.², Galán H.¹

¹Dpto. de Fisión Nuclear, CIEMAT, Avda. Complutense, 40, 28040 Madrid, Spain.

²Instituto de Estructura de la Materia, CSIC, C/ Serrano 121, 28006 Madrid, Spain.

*francisco.colmenero@ciemat.es

Organic extractant molecules (EM) enable the selective separation of Am(III) from lanthanides and Cm(III) within the AmSel process [1]. Due to the harsh working conditions in these processes, organic molecules undergo hydrolytic and radiolytic degradation. Thus, the selection of suitable ligands strongly depends on the rigorous assessment of their stability. Here, the study of the stability of the novel ligands proposed to enhance the selective separation through the AmSel process, such as PrOH-BPTD, SO₃-Ph-BTBP and TODGA molecules, through a combination of experimental and theoretical techniques is illustrated.

In the experimental side, Raman spectroscopy and HPLC-MS techniques, which have effectively employed for this purpose [2], are used. Nuclear Magnetic Resonance (NMR) technique is also explored. In the theoretical side, computer simulations based in Density Functional Theory (DFT) are performed to determine the 3D structure, bond orders, Raman and NMR spectra, and Molecular Electrostatic Potential Maps (MEP) of these molecules. Furthermore, a series of molecular fragments (MF) of these molecules and a set of potential degradation compounds (DC), hypothesized from HPLC-MS analyses were also studied using Gaussian, DMOL3 and CASTEP computer codes [3]. The theoretical methodology allow to consider the EMs and DCs separately, an important advantage since the isolated study of the compounds involved is very difficult or impossible experimentally. The use of theoretical methods in the characterization of complex materials, with the aim of interpreting experimental results, and their predictive value are well known [4].

In this work, the following tasks were carried out: (1) Optimization of the 3D structures of the EMs, MFs and DCs. These structures are necessary as input for the subsequent theoretical determination of their properties and spectra; (2) Determination of EM bond orders. The bond orders between the atoms in the EMs indicate the bonds most susceptible to breakage when these molecules are exposed to gamma radiation fields. Therefore, they are useful for predicting the mechanisms and products of radiolytic degradation; (3) Computation of Raman spectra of MEs, FM, and CDs. The knowledge of the spectra of MEs is useful for investigating possible degradation mechanisms. The modification of Raman bands after degradation indicates a structural perturbation whose origin can be unraveled through the assignment of the corresponding bands. Raman spectra of each CD leads to their unique band fingerprints which can confirm if they are present in the ME spectrum under radiation. Assignment of the Raman bands of the FM can aid in assigning the bands of the MEs; (4) Calculation of the NMR spectra of the EM and CDs. These spectra provide distinctive chemical shifts allowing to identify the CDs; (4) MPEs provide a topological characterization of the MEs useful for the recognition of new extractant molecules and for identifying the sites for actinide complexation.

References:

[1] Weßling, P., et al., *Inorg. Chem.* **2022**, 61, 17719; [2] Sánchez-García, I., et al., *Progr. Nucl. Energy* **2026**, 191, 106114; [3] Colmenero, F., et al., Proceedings of the 51^a Reunión Anual de la Sociedad Nuclear Española, Septiembre, **2025**, Cáceres, Spain; [4] Colmenero, F. In *Minerals*. Essa, K.S ed. Chapter 4. Pp. 66-94. InTech, **2018**.

Gaussian Approximation Potentials for Adsorbate-Functionalized Pt–Cu Nanoparticles

Ilker Demiroglu^{1*}

¹*Eskisehir Technical University, Turkey*

Bimetallic Pt–Cu nanoparticles are attractive catalysts for oxidation and hydrogenation reactions due to their tunable electronic structure, reduced noble metal content, and enhanced resistance to surface poisoning. However, first-principles modeling of realistic nanoparticle sizes and morphologies remains computationally demanding. Here, we develop high-fidelity Gaussian Approximation Potential (GAP) models for Pt–Cu nanoparticles functionalized with single O₂ and CO molecules, enabling near–DFT-accurate simulations at a fraction of the computational cost. The training dataset was generated from ab initio molecular dynamics trajectories spanning temperatures from 300 to 1000 K and includes multiple particle sizes (38–260 atoms) and morphologies, such as pure, core–shell, Janus, and ordered alloy structures. The resulting GAP models reproduce DFT reference energies and forces with high accuracy, achieving root-mean-square errors below 0.4 meV atom^{−1} for energies and 70 meV Å^{−1} for forces, while remaining transferable across different structural motifs. Large-scale molecular dynamics simulations reveal that alloying Pt with Cu significantly improves thermal and mechanical stability. In particular, core–shell and Janus nanoparticles maintain ordered atomic coordination up to 1000 K, whereas monometallic counterparts exhibit increased surface disorder. Radial distribution function analysis confirms the persistence of short-range order under elevated temperatures and adsorbate presence. These results demonstrate that machine-learning-based interatomic potentials provide a robust and efficient framework for investigating adsorption-driven restructuring, morphology evolution, and thermal stability in bimetallic nanoparticles. The developed GAP models bridge the gap between quantum-mechanical accuracy and realistic length and time scales, offering valuable insights into composition–structure–stability relationships and supporting the rational design of cost-effective Pt–Cu catalysts for energy and environmental applications.

Emergent Stability of 2D Metal Oxides at the Nanoscale

Andreu A. de Donato,^{1*} Albert Bruix¹ and Stefan T. Bromley^{1,2}

¹*Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, C/Martí i Franquès 1, Barcelona, Spain.*

²*Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, Barcelona, Spain.*
adedonpe7@alumnes.ub.edu

Two-dimensional (2D) oxides are a novel type of material with significant potential in several technologically relevant applications such as electrocatalysis. However, the structure, properties, and stability of these systems is often unclear. In this work, we investigate the competing 2D and 3D morphologies of various MO₂ (M = Ir, Ti, Ru, Sn, Os, Pd, Ce, Pb) oxides. We build nanoparticle models across a size range of 45 to 813 atoms using calculations based on the density functional theory (DFT) and develop an efficient computational screening strategy to predict 2D nanostructure stability. We thus reveal a surprising preference of some dioxides, such as IrO₂, for forming planar systems at the nanoscale. Because these planar structures have distinct electronic and chemical properties, our work shows that novel 2D materials with enhanced physical and chemical properties can be produced by carefully selecting particle size.

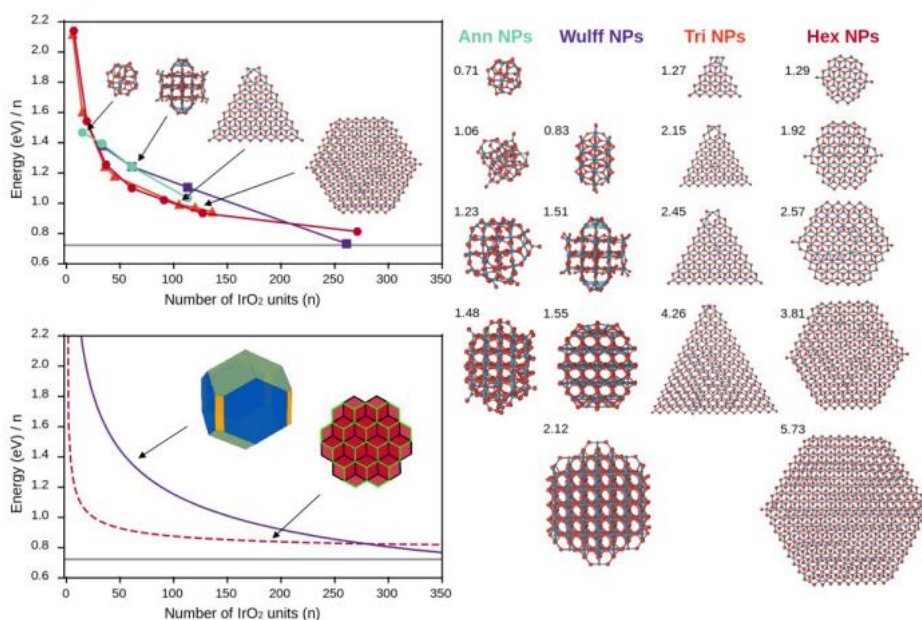


Figure 1: In the upper left corner, we show the relative energy per IrO₂ unit for annealed Wulff constructed, Wulff constructed, triangular and hexagonal nanoparticles ranging from ~50 to ~800 atoms. In the lower left corner, we show the theoretical framework that estimates the stability/size crossover point between 2D and 3D IrO₂. The right half shows the different DFT relaxed structures of IrO₂ nanoparticles with their diameter in nanometers.

Towards Accurate Description of Intermolecular Induction

Humahuti Dihingia¹, Bartosz Tyrcha¹,
Konrad Patkowski², Piotr S. Żuchowski¹, Alston J. Misquitta³

¹*Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in
Toruń, Grudziądzka 5, 87-100, Poland*

²*Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama
36849, USA*

³*School of Physical and Chemical Sciences, Queen Mary University of London, Mile
End Road, E1 4NS, United Kingdom*
humahuti@umk.pl

A key feature of Symmetry-Adapted Perturbation Theory (SAPT)¹ is the composition of the interaction energy in terms of physically significant terms such as: electrostatics, exchange, induction and dispersion. Among these, the induction energy plays a significant role, specially for strongly bonded systems. However, the induction terms in perturbation theory diverge and the lowest order terms do not recover the total induction. The missing higher order induction can be incorporated with delta-HF correction, resulting into a hybrid theory². While the delta-HF correction is important for H-bonded systems, but it is also known to overbind dispersion-dominated complexes. Therefore, it would be ideal to recover the induction effect in a consistent theory. One such approach is Pauli-Blockade^{3,4} method, which offers a variational framework for infinite-order induction. However, because of the orthogonalization step and subsequent loss of monomer identity, this theory is not useful for further SAPT-like development.

In this work, we explore intermolecular interactions through a potentially infinite-order induction, dispersion-free and many-body variational approach termed as Symmetry-Adapted Relaxation Theory, which is motivated by Pauli-Blockade but maintains monomer identity, therefore retaining SAPT-like character. Our methodology formulated in second quantization, is implemented using Psi4NumPy⁵, a Python-based interface for the computational chemistry software Psi4. We report the agreement between interaction energy computed using our approach and supermolecular Hartree-Fock energy, demonstrating that variationally relaxed monomers effectively capture induction effects to infinite-order in the interaction operator.

References:

- [1] Jeziorski B., Moszynski R. and Szalewicz K., Perturbation theory approach to intermolecular potential energy surfaces of van der Waals complexes, Chemical Reviews,(1994)
- [2] Patkowski K., Szalewicz K. and Jeziorski B., Orbital relaxation and the third-order induction energy in symmetry-adapted perturbation theory, Theor Chem Acc (2010)
- [3] Gutowski M., Piela L., Interpretation of the Hartree-Fock interaction energy between closed shell systems, Mol. Phys. 64 (1988)
- [4] Rajchel Ł., Żuchowski P. S., Szczęśniak M. M. and Chałasiński G., Interpretation of the Hartree-Fock interaction energy between closed shell systems, Phys. Rev. Lett. 104 (2010)
- [5] Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development, J. Chem. Theory Comput. (2018)

Machine learning modeling for infrared spectra of titanium carbide nanoparticles

Jorge Fabila¹, Stefan T. Bromley²

¹*Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Spain*

²*Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain*

Titanium carbide (TiC) nanoparticles are believed to be among the first solid compounds to condense in the outflows of carbon rich evolved stars, acting as nucleation seeds for cosmic carbonaceous dust. These tiny but crucial grains may influence the chemical evolution of galaxies by catalyzing the formation of complex organic molecules in space. A key challenge is identifying such grains observationally and that hinges on the accurate prediction of their infrared (IR) spectral signatures. While density functional theory (DFT) has been a powerful tool for simulating the vibrational and IR spectra of nanostructures, it remains computationally demanding, especially for large or dynamic systems. Machine learning (ML) emerges as a compelling alternative, promising accurate predictions at a fraction of the cost. Yet, its adoption in astrochemistry remains limited, in part due to concerns about the reliability of ML models in reproducing detailed physical behavior. In this contribution, we present a machine-learned interatomic potential trained on DFT molecular dynamics trajectories of TiC nanoparticles, using the MACE architecture. The ML-generated IR spectra show excellent agreement with DFT benchmarks and are transferable to larger nanoparticle sizes. This opens up exciting possibilities for simulating astrophysical dust populations with realistic dynamics and scale a necessary step toward bridging the gap between theoretical modeling and observational astronomy.

Methodological Perspectives on Modeling Photo-Induced Interactions at the Silver Nanoparticle-Bio Interface

S. Hajizada¹, A. Karimova², H. Shirinova³, Christoph Reissfelder¹ and Vugar Yagublu¹

¹*Department of Surgery, Medical Faculty Mannheim, University of Heidelberg, 68167 Mannheim, Germany*

²*Department of Chemistry of High Molecular Weight Compounds, Baku State University, Baku AZ 1148, Azerbaijan*

³*Department of Chemical Physics of the Nanomaterials, Baku State University, Baku, AZ 1148, Azerbaijan*

The application of silver nanoparticles (AgNPs) in targeted therapies relies strongly on their optical response under controlled irradiation, particularly within the blue light spectrum (400–480 nm). At bio-nano interfaces, the interaction between metallic surfaces and biomolecules is governed by complex electronic phenomena that remain challenging to describe using standard computational protocols [1]. These limitations become especially pronounced under photo-activation, where plasmonic excitations and interfacial charge transfer processes jointly determine the stability and reactivity of hybrid bio–nano systems [2] (Figure 1).

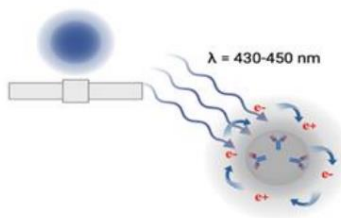


Figure 1: Schematic representation of localized surface plasmon resonance (LSPR) and biomolecular interactions at the AgNP interface under 430–450 nm irradiation (Created in BioRender (2026)).

In this context, the present work proposes a systematic benchmarking framework aimed at assessing the reliability of theoretical methods for modeling photo-activated AgNP–biomolecule assemblies. Due to the size, flexibility, and chemical heterogeneity of these systems, accurate modeling requires not only robust excited-state methodologies but also extensive structural sampling and multi-scale treatment of the interfacial environment [3]. Particular attention is given to systems involving DNA, where photosensitization and aggregation phenomena play a critical role in governing electronic processes and photochemical outcomes [4].

The methodological challenges addressed in this framework are structured as follows:

- **Spectral Sensitivity:** Assessing the capability of time-dependent density functional theory (TD-DFT) and related excited-state approaches to accurately reproduce electronic transitions of AgNP-based systems in the visible region (400–480 nm), particularly when functionalized with biological ligands, where plasmonic resonances and metal-ligand coupling strongly influence excitation profiles [1, 2].
- **Confinement and Charge Transfer:** Evaluating how spatial confinement at nanoparticle surfaces modulates charge-transfer pathways and energy transfer efficiency at the bio–nano

interface, with a focus on the photostability and reactivity of DNA-AgNP complexes under irradiation [2, 5].

- **Methodological Benchmarking:** Systematically comparing exchange–correlation functionals and excited-state methodologies to identify computational strategies that optimally balance accuracy and feasibility for largescale hybrid bio–nano models [1, 3].

- **Implementation and Preliminary Experimental Insights**

Wavelength-Dependent Modulation of Cell Fate: Our findings demonstrate that 433 nm irradiation, when combined with AgNPs, predominantly biases cancer cell fate toward programmed mitochondrial apoptosis, whereas 450 nm irradiation results in a cell death profile dominated by non-programmed, necrosis-associated mechanisms.

- **Irradiation Dynamics and Temporal Profile:** We observed that at 433 nm, even short irradiation durations are sufficient to trigger an efficient apoptotic response, while treatment under 450 nm requires more prolonged exposure to induce significant cytotoxicity.

- **Differential Oxidative Stress Induction:** Our results indicate that 433 nm light exhibits higher photochemical efficiency, leading to rapid and pronounced generation of intracellular Reactive Oxygen Species (ROS), while 450 nm irradiation produces a significantly slower and less intense oxidative response.

- **Transcriptional Regulation and Gene Expression:** Through qPCR analysis, we confirmed that the 433 nm + AgNP combination triggers a coordinated molecular cascade, significantly upregulating pro-apoptotic genes (such as BAX and CASP3), whereas 450 nm irradiation fails to consistently activate these structured apoptotic gene programs.

In conclusion, we have established a mechanistic framework demonstrating that the choice of blue light wavelength (433 nm vs. 450 nm) is a critical determinant that programs the specific intracellular stress-response pathway and the subsequent mode of cancer cell death.

- **Conformational Sampling:**

Implementing efficient global potential energy surface exploration and conformational sampling strategies on nanoparticle facets to identify representative interfacial structures and capture realistic molecular arrangements governing photo-induced behavior [3]. By addressing these interconnected challenges, this benchmarking framework directly contributes to the objectives of Working Group 1 and Working Group 4 of the COSY Action. The proposed methodological roadmap aims to support the rational design of photoresponsive silver-based nanomaterials while providing fundamental insight into the molecular mechanisms underlying light-driven processes at complex bio–nano interfaces.

References:

- ¹Melo, R.M., et al., Recent Advances in the Application of Silver Nanoparticles for Enhancing Phototherapy Outcomes. *Pharmaceuticals*, 2025. 18(7): p. 970.
- ²Zhang, Y., et al., Surface-plasmon-driven hot electron photochemistry. *Chemical reviews*, 2017. 118(6): p. 2927-2954.
- ³Casalini, T., et al., Molecular modeling for nanomaterial–biology interactions: Opportunities, challenges, and perspectives. *Frontiers in bioengineering and biotechnology*, 2019. 7: p. 268.
- ⁴Gattuso, H., et al., Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. *Physical Chemistry Chemical Physics*, 2016. 18(27): p. 18598-18606.
- ⁵Dumont, E. and A. Monari, Understanding DNA under oxidative stress and sensitization: The role of molecular modeling. *Frontiers in chemistry*, 2015. 3: p. 43.

Confined Drug Organization in Fe₃O₄@Dextran Nanostructures: Effect of Nanocarrier–Drug Ratio

Karimova Aynura¹, Mehdiyeva Aygun²

¹Department Chemistry of High Molecular Weight Compounds, Baku State University, Zahid Khalilov 33, AZ 1148, Baku, Azerbaijan

²Nanoresearch Laboratory, Baku State University, Zahid Khalilov 33, AZ 1148 Baku, Azerbaijan

Presenter's email address: aynurakarimova@bsu.edu.az

Dextran-coated magnetite nanoparticles (Fe₃O₄@Dextran) represent a model hybrid confined molecular system in which drug molecules are spatially restricted within a polysaccharide shell and at the organic-inorganic interface. In this study, the influence of the Fe₃O₄@Dextran-to-drug ratio on molecular confinement, interfacial interactions, and structural organization was systematically investigated in order to elucidate the mechanisms governing ratio-dependent loading behavior.

Crystallite size analysis based on the Debye-Scherrer equation revealed a progressive decrease from 17.1 nm for Fe₃O₄@Dextran to 15.69 nm (D1) and 13.7 nm (D2), followed by a slight increase to 14.96 nm at the highest drug ratio (D3), indicating that drug incorporation limits crystal growth and that surface saturation is reached at higher loadings [1]. FTIR spectroscopy further confirmed the involvement of dextran hydroxyl groups and surface Fe-O sites in hydrogen bonding and coordination with drug molecules. Electron microscopy evidenced well-dispersed magnetic cores embedded in an amorphous dextran matrix, forming nanoscale cavities and interfacial domains that act as confinement sites. Variation of the Fe₃O₄@Dextran/drug ratio resulted in pronounced changes in adsorption efficiency, interfacial packing density, and molecular distribution within the polymer shell.

The ratio-dependent loading behavior is attributed to the balance between available surface binding sites, polymer chain mobility, and steric crowding effects under confined conditions [2]. At lower drug ratios, adsorption is dominated by specific hydrogen bonding and coordination to Fe-O and -OH groups, whereas at higher ratios, saturation of interfacial sites and confinement-induced packing led to cooperative and competitive interactions, in line with theoretical descriptions of molecular organization in restricted polymeric environments.

These findings demonstrate that molecular confinement within Fe₃O₄@Dextran nanostructures can be finely tuned by the nanoparticle-drug ratio, providing fundamental insight into structure-interaction-confinement relationships in soft-hard hybrid systems.

References

1. Karimova, A., Hajizada, S., Shirinova, H., Nuriyeva, S., Gahramanli, L., Yusuf, M. M., et al. Surface modification strategies for chrysin-loaded iron oxide nanoparticles to boost their anti-tumor efficacy in human colon carcinoma cells. *J. Funct. Biomaterials*, 2024, 15 (2), 43. doi:10.3390/jfb15020043
2. Najafipour, I., Emami, N., Sadeh, P., Amoli, A., Mosleh-Shirazi, S., Amani, A. M., et al. Synthesis of Fe₃O₄@ MIL-101-OH/Chitosan for adsorption and release of doxorubicin. *Polym. Test.*, 2025, 142, 108659. doi:10.1016/j.polymertesting.2024.108659

When two worlds collide: what happens when silicate and carbonaceous dust grains meet?

A. Kyriazis^{*1,2}, S. T. Bromley^{2,3} and A. Rimola¹

¹*Departament de Química, Universitat Autònoma de Barcelona, Bellaterra, Spain*

²*Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Spain*

³*Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain*

Alexandros.kyriazis@uab.cat

Silicate and carbonaceous grains originate from distinct circumstellar environments and are often treated as two separate populations. Low temperature environments, potentially relevant for interstellar dust (re)formation, also appear to favour the production of separate and carbonaceous dust families [1]. Models of dust evolution, however, suggest that there should be some significant interactions between these two worlds [2]. In this study, we model collisions between nanosized grains of amorphous hydrogenated carbon (a-C:H) and magnesium silicate. For both grain types we employ atomistically detailed models using carefully prepared realistic structures and compositions [3,4]. We examine both the physical and chemical outcomes of the collisions for a systematic scan of astrophysically relevant impact velocities. Our results reveal that production of silicate-carbonaceous mixed grains is generally not favoured but can occur for a narrow range of conditions. However, collision-induced interactions between these distinct grain types can drive a wide range of chemically rich processes (e.g production of ICOMs). As such, collisions between silicate and carbonaceous grains could provide a novel route to chemical complexity in interstellar environments.

References:

¹G. Rouillé, C. Jäger, T. Henning, *Astrophys. J.*, 892, 96 (2020).

²N. Ysard, A. P. Jones, V. Guillet, K. Demyk, M. Decleir, L. Verstraete, I. Choubani, M.-A. Miville-Deschenes, L. Fanciullo, *Astron. Astrophys.*, 684, A34 (2024).

³A. M. Escatllar, T. Lazaukas, S. M. Woodley, S. T. Bromley, *ACS Earth Space Chem.*, 3, 2390 (2019).

⁴R. Ranganathan, S. Rokkam, T. Desai, P. Koblinski, *Carbon*, 113, 87 (2017).

Elastic electron scattering on the inhalation anaesthetic molecules in gas phase at medium energy range

Jelena Maljković¹, Jelena Vukalović, Gustavo García, Francisco Blanco and Bratislav P. Marinković

¹ *Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

² *Faculty of Science, University of Banja Luka, Mladena Stojanovića 2, 78000 Banja Luka, Republic of Srpska, Bosnia and Herzegovina*

³ *Departamento de Física Atómica Molecular y Nuclear, Facultad de Ciencias Físicas, Universidad Complutense, Avda. Complutense s/n, E-28040 Madrid, Spain*

⁴ *Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 121, 28006 Madrid, Spain*

jelenam@ipb.ac.rs

We performed both experimental and theoretical investigations, motivated by the significant contribution of anaesthetic molecules to global warming and ozone depletion (*References^a*). Halogenated anaesthetics halothane, isoflurane, sevoflurane and desfluran have been investigated due their important role in environment impact. Absolute differential cross sections (DCSs) for elastic electron scattering on halogenated anaesthetics (*References^b*, *References^{c,d}*) have been determined on electron spectrometer UGRA settled in Laboratory of atomic collision processes in the Institute of Physics in Belgrade. Cross beam apparatus consist of electron gun producing electrons energy of 50-300 eV crossed perpendicular with gas produced from capillary gas needle and a channeltron detection system. Electron gun can be rotated around gas needle which allows us to measure DCSs in the function of scattering angle (25°-125°). To normalize the measured relative cross sections, we employed the relative-flow method with argon as the reference gas. Theoretical calculations of the differential cross sections were carried out using the Independent Atom Model combined with the Screening Corrected Additivity Rule and interference effects (IAM-SCAR+I). The experimental and theoretical values for absolute differential cross sections have very good agreement both, on the absolute scale and in shape.

Acknowledgement: The work is funded by Science Fund of Serbia, ATMOLCOL project #6821.

References:

^aLangbein T., Sonntag H., Trapp D., Hoffmann A., Malms W., Röth E.P., Mörs V., Zellner R, Volatile anaesthetics and the atmosphere, Br. J. Anaesth, 1999, **82**, 62-73. <https://doi.org/10.1093/bja/82.1.66>

^bMaljković J.B., Vukalović J., Pešić Z. D., Blanco F., García G., Marinković B. P., Experimental and theoretical study on elastic electron interaction with halothane molecule in the intermediate energy range, Eur. Phys. J. Plus, 2023, **138**, 349, <https://doi.org/10.1140/epjp/s13360-023-03967-6>

^cVukalović J., Maljković J.B., Blanco F., García G., Predojević B., Marinković B.P., Absolute differential cross-sections for elastic electron scattering from sevoflurane molecule in the energy range from 50-300 eV, Int. J. Mol. Sci, 2022, **23**, 21 <https://doi.org/10.3390/ijms23010021>

^dVukalović J., Marinković B. P., Rosado J., Blanco F., García G., Maljković J.B., Investigating Theoretical and Experimental Cross Sections for Elastic Electron Scattering from Isoflurane, Phys. Chem. Chem. Phys, 2024, **26**, 985-991, <https://doi.org/10.1039/D3CP05052A>

Machine learning interatomic potentials for hydrogen adsorption/desorption on transition-metal-carbon platforms

Luis Martín-Encinar¹, Alberto Castro¹, Estefanía Germán¹, María J. López¹

¹*Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, 47011, Valladolid, Spain*

Presenter's email address: luis.martin.encinar@uva.es

Carbon-based nanoporous and layered materials doped with transition metals (TM) are promising candidates for hydrogen storage platforms according to Density Functional Theory (DFT) studies.^{a,b} However, modelling the adsorption/desorption of hydrogen under realistic conditions requires large-scale Ab Initio Molecular Dynamics (AIMD) simulations that are computationally prohibitive. In this context, universal Machine Learning Interatomic Potentials (uMLIPs) provide transferable and computationally efficient models capable of capturing DFT accuracy across large systems and long timescales.^c

In this work, we tested different uMLIPs on TM-carbon platforms. In particular, we examined its performance on properties such as thermal stability, radial distribution function, adsorption energies and geometries of TM atoms/clusters, diffusion pathways and migration barriers, and vibrational properties. Our results showed that MACE-MH_OC20 and NequIP-OAM-XL models, despite not being specifically trained on our target TM-carbon platforms, agree with the main structural, energetic, and dynamical properties observed in DFT. Then, we fine-tuned both uMLIPs models using a large and diverse dataset that includes a wide range of TM clusters and carbon-based layers (including defective ones), mostly generated from AIMD simulations covering near- and out-of-equilibrium structures. Our aim is to train a model that can be reliably transferred for dynamic catalytic studies. Finally, extensive MD simulations of hydrogen adsorption and desorption will be performed to evaluate the hydrogen storage capacity of TM-carbon platforms under practical conditions.

This work was supported by MCIN/AEI/10.13039/501100011033 and FSE+ (PID2022-138340OB-I00); Junta de Castilla y León - Apoyo a GIR (VA029G24); University of Valladolid; RES: BSC in MareNostrum 5 (FI-2024-2-0031); RES: CSUC in Pirineus III (FI-2025-1-0029, FI-2025-2-0004).

References:

^aRaja K., K.; Anusuya, T.; Kumar, V. DFT study of hydrogen interaction with transition metal doped graphene for efficient hydrogen storage: effect of d-orbital occupancy and Kubas interaction. *Physical Chemistry Chemical Physics*, 2023, 25(1), 262–273. <https://doi.org/10.1039/D2CP03794G>

^bSandoval Menjivar, J.; Germán, E.; Alonso, J.A.; López, M.J. Building single-atom and single-cluster metal catalysts supported on graphdiyne and boron-graphdiyne. *Small Structures*, 2026, 7, e202500508. <https://doi.org/10.1002/ssstr.202500508>

^cKraß, H.; Huang, J.; Moosavi, S.M. MOFSimBench: evaluating universal machine learning interatomic potentials in metal-organic framework molecular modeling. *npj Comput Mater*, 2026, 12(1), 4. <https://doi.org/10.1038/s41524-025-01872-3>.

Theoretical Study of Oxygen Reduction Reaction (ORR) on Graphene and Pt-Supported Catalysts

Edgard Alejandro Miranda Sáenz¹, Fernando Aguilar-Galindo Rodríguez¹²

¹*Department of Chemistry, Autonomous University of Madrid, Spain*

²*Institute for Advanced Research in Chemical Sciences (IAdChem), Autonomous University of Madrid, Spain*

edgard.miranda@edu.uah.es

The global energy demand has risen sharply in recent decades due to population growth and increasing per-capita consumption. To achieve sustainable development and meet decarbonization goals, the transition toward clean and efficient energy conversion systems has become essential. Within this framework, the oxygen reduction reaction (ORR) plays a central role in electrochemical devices such as fuel cells and metal–air batteries, as highlighted by extensive experimental research on platinum-based catalysts^a.

However, the ORR is a kinetically sluggish process, requiring efficient catalysts to overcome its high activation barriers. Platinum remains the benchmark catalyst for this reaction, yet its scarcity and cost drive the search for more sustainable alternatives or configurations that enhance Pt utilization. Theoretical studies have provided critical insight into the origin of the ORR overpotential and the adsorption energetics of key intermediates^b. In this work, a comparative theoretical study of pristine graphene (Gr) and Pt-doped graphene (Gr–Pt) was conducted under neutral and anionic conditions to evaluate their catalytic behavior toward the ORR.

Several intermediates were characterized along the reaction pathway, revealing distinct structural and electronic trends between both systems. Analytical tools such as the projected density of states (pDOS), differential charge density ($\Delta\rho$), and Bader charge analysis provided insight into the interaction between oxygenated intermediates and the catalyst surface, as well as the effect of electronic injection on reaction energetics.

These results contribute to a deeper understanding of the structure–activity relationship in carbon-based and Pt-modified materials, offering valuable guidelines for the rational design of next-generation ORR catalysts and related electrochemical processes.

References:

^aSteele, B. C. H.; Heinzel, A. Materials for fuel-cell technologies. *Nature*, 2001, 414(6861), 345–352.

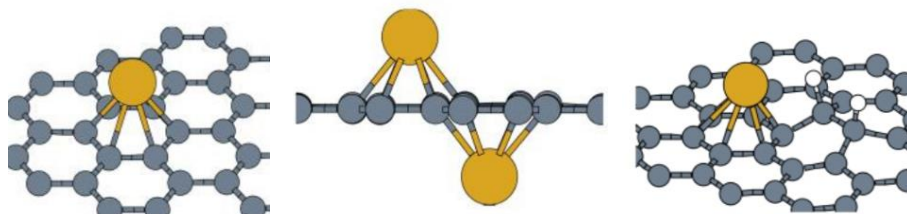
^bNørskov, J. K.; Rossmeisl, J.; Logadottir, A.; Lindqvist, L.; Kitchin, J. R.; Bligaard, T.; Jónsson, H. Origin of the overpotential for oxygen reduction at a fuel-cell cathode. *Journal of Physical Chemistry B*, 2004, 108(46), 17886–17892. <https://doi.org/10.1021/jp047349j>

Hydrogen adsorption at graphene layers doped with transition metals: Insight from DFT simulations.

Luis M. Molina¹, Gabriel Navarrete¹

¹*Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid (Spain)*

The interaction of hydrogen with graphitic systems has been extensively studied, searching for novel materials capable of adsorbing high quantities of hydrogen. In this study, we have employed DFT simulations to analyze the dissociation of hydrogen at graphene layers doped with various types of metal atoms, such as Li, Mg, Al, Cu, Zr and Ru. Also, we have studied the tendency of these metal atoms to form clusters in the surface of graphene. Depending on the element, strong differences are found in the trends for clustering, with dispersion on the graphene layer strongly favoured for s-p metals such as Li or Al. Then, we have investigated the energetics of the dissociative adsorption of H₂ in the neighbourhood of adsorbed metal atoms. While reactive d-electron metals easily break the H-H bond, transfer of the dissociated hydrogen atoms to the graphene layer is hampered by large barriers. Finally, we have also studied the interaction between dissociating hydrogen with metal atoms adsorbed at the other side of a graphene layer. The presence of the metal induces sizable variations in the H-C binding strength.



Adsorption of Zr atoms at graphene

Acknowledgements:

This work was supported by Ministerio de Ciencia e Innovación of Spain (Grant PID2022-138340OB-I00 funded by MCIN/AEI/10.13039/501100011033 and FSE+). This work is also based upon work from the COST Action CA21101 – Confined Molecular Systems: From a New Generation of Materials to the Stars (COSY), supported by COST (European Cooperation in Science and Technology).

Size-Dependent Structural and Optical Behavior of ZnO/MWCNT Nanocomposites toward Optoelectronic Applications

Sevinj Nuriyeva^{1*}

¹*Nano Research Laboratory, Center of Excellence in Research, Development and Innovation, Baku State University, Baku 1148, Azerbaijan.*

In this study, nanocomposites based on zinc oxide (ZnO) nanoparticles of different sizes and acid-functionalized multi-walled carbon nanotubes (F-MWCNTs) were synthesized, and their structural and optical properties were systematically investigated. The ZnO/MWCNT nanocomposite films were prepared by a solution-mixing approach using various MWCNT mass fractions. Surface morphology and structural characteristics were examined by atomic force microscopy (AFM) and X-ray diffraction (XRD). AFM analysis revealed that although both small- and large-sized ZnO nanoparticles exhibit a certain degree of agglomeration, their primary particle sizes remain within the nanoscale range, ensuring a high specific surface area. XRD results confirmed the preservation of the wurtzite crystal structure of ZnO, while the appearance of a characteristic carbon-related diffraction peak indicated the successful incorporation of MWCNTs into the nanocomposites. Fourier transform infrared (FTIR) spectroscopy revealed the presence of oxygen-containing functional groups and ZnO–MWCNT interfacial interactions, confirming effective functionalization and composite formation. Optical properties were investigated using UV–Vis absorption and photoluminescence (PL) spectroscopy. The UV–Vis spectra showed that the fundamental absorption features of ZnO were retained in the nanocomposites, accompanied by a pronounced enhancement in absorption intensity. PL measurements demonstrated that, depending on ZnO particle size and MWCNT loading, either luminescence quenching or emission enhancement occurred, reflecting differences in interfacial charge-transfer efficiency and electron–hole recombination behavior.

From Methanol to C₂ Products: Active Surface Oxygen–Mediated Pathways in Methane Conversion over Ce–LaO_x Catalysts

Junjie Shi¹, Wen Li², Thomas Haunold¹, Nevzat Yigit¹, Leonard Atzl¹, Esko Kokkonen⁴, Yong Qin³, Günther Rupprechter¹

¹*Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria.*

²*State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, 030001 Taiyuan, China.*

³*College of Materials Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, Shandong, China.*

⁴*MAX IV Laboratory, Lund University, SE-221 00 Lund, Sweden.*

junjieshiding@gmail.com

Methane (CH₄) is abundant but also a potent greenhouse gas, with a global warming potential ~85 times higher than CO₂. Selective conversion of CH₄ into value-added products such as CH₃OH or C₂ hydrocarbons could mitigate its environmental impact while offering economic value. However, the high inertness of the C–H bond and the propensity for over-oxidation make selective oxidation highly challenging.¹ Ce–LaO_x mixed oxides have emerged as promising catalysts due to their excellent oxygen mobility and tunable surface properties, yet the mechanisms governing product selectivity remain poorly understood.

Our recent studies show that Ce–LaO_x exhibits strong dependence of product selectivity on temperature and gas atmosphere: Methanol prevails at 250–400 °C, whereas C₂ products dominate above 450 °C. The presence of water vapor further alters the product distribution, suggesting distinct pathways at low vs. high temperature regimes.

To elucidate the origin of this selectivity, we combine operando DRIFTS and time-resolved AP-XPS to track the evolution of surface intermediates and oxidation states under reaction conditions. TPD–MS is used to probe the adsorption, activation, and desorption behavior of reactants (CH₄, H₂O, O₂) and products (CH₃OH). Systematic comparison of atmospheres with and without O₂ and water vapor directly links surface chemistry to product selectivity, providing mechanistic insights into methane activation and C–C coupling on Ce–LaO_x catalysts.

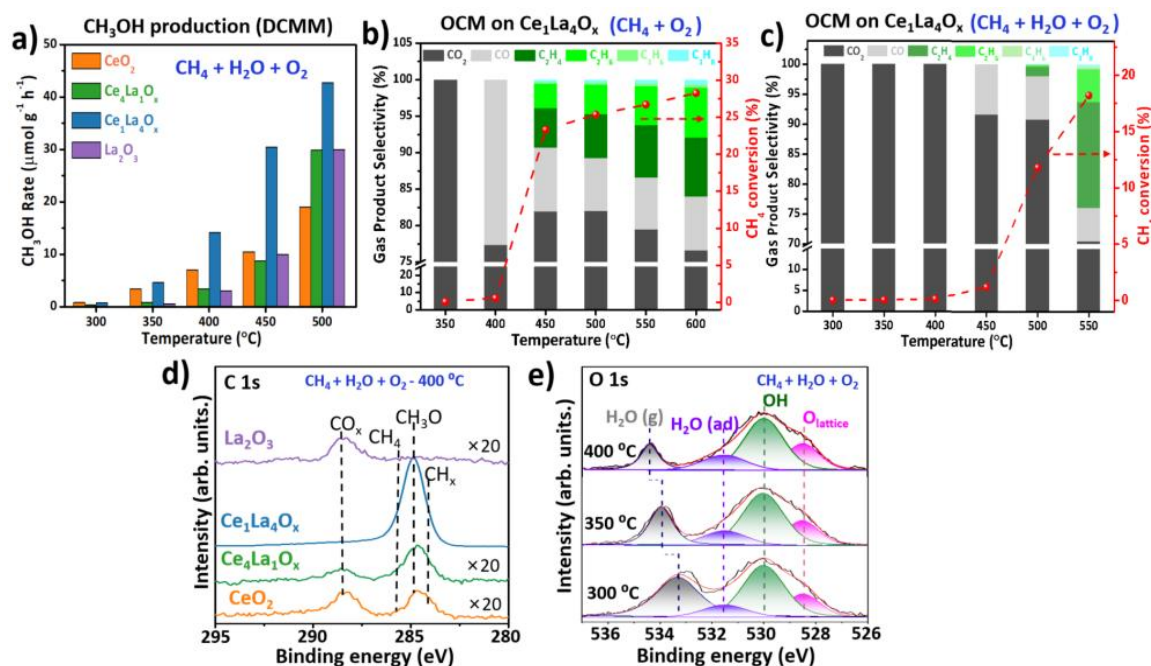


Fig. 1. (a) CH₃OH yields over Ce-LaO_x; OCM selectivity and CH₄ conversion of Ce₁La₄O_x under (b) CH₄ + O₂ and (c) CH₄ + H₂O + O₂; (d) AP-XPS C 1s spectra of Ce-LaO_x under CH₄ + O₂ + H₂O at 400 °C; (e) Temperature-dependent AP-XPS O 1s spectra of Ce₁La₄O_x under CH₄ + H₂O + O₂ at 300–400 °C.

References:

1. Li, W.; Shi, J.; Tangpakonsab, P. L.; Zhang, B.; Haunold, T.; Genest, A.; Yigit, N.; Atzl, L.; Kokkonen, E.; Qin, Y.; Rupprechter, G. *ACS Catalysis* **2025**, 15, (24), 20496-20511.

Na⁺/Cu⁺ rivalry in neutral organic solvents and on an inert surface
Veronika Petkova^{1,2}, Hristo Rashev¹, Radostina Stoyanova², Alia Tadjer¹

¹ Faculty of Chemistry and Pharmacy, University of Sofia, 1164 Sofia, Bulgaria

² Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113, Sofia,
Bulgaria
tadjer@chem.uni-sofia.bg

Copper is utilized not only as the perfect current collector but also as a supporting frame for graphene (or rGO) sheets used as anodes in sodium-ion batteries. However, the solvent's polarity influences the efficiency of the cell and since XPS studies prove the emergence of copper on the electrode surface, its origin in the system and the dependence on the solvent used call for elucidation. The present study aims to provide a comparative theoretical (DFT) analysis of the interactions of the monovalent cations Na⁺ and Cu⁺ in neutral organic solvents with different polarity – diglyme ($\epsilon = 7.3$) and propylene carbonate ($\epsilon = 64.9$). The main objective is to evaluate the energetics of solvation and adsorption to the end of rationalizing the experimental findings.

Integration of Molecular Dissociative Recombination Theoretical Data into the ACol VAMDC Node for Confined Molecular Systems

Veljko Vujčić¹, Felix Iacob², Vladimir Srećković³

¹*Astronomical Observatory, Volgina 7, 11060 Belgrade, Serbia*

²*West University of Timișoara, Vasile Părvan Boulevard, 300233, Romania*

³*Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

Presenter's email address: veljko@aob.rs

This work enhances data interoperability for the study of confined molecular systems by integrating a high-precision theoretical dataset on molecular dissociative recombination into the Atomic and Molecular Collisions (ACol) node of the Virtual Atomic and Molecular Data Centre^a (VAMDC). The integrated pilot data^{b,c,d}, generated using advanced quantum chemical methods (MQDT, R-matrix), provides critical cross-sections and rate coefficients for processes governing molecular ions in low-temperature, low-density environments, such as the interstellar medium and laboratory analogues.

The core technical achievements include mapping the dataset to the VAMDC XSAMS schema, extending the ACol^e node's data model to support reactive collision data, and implementing a validated pilot dataset with prototype visualization tools. This integration directly supports the COST Action COSY (Confined Molecular Systems) by contributing to shared astrochemical datasets, promoting FAIR data principles, and bridging theoretical data with experimental efforts to understand molecule-environment interactions and motion in confined systems.



References:

^aAlbert, D., Antony, B.K., Ba, Y.A., Babikov, Y.L., Bollard, P., Boudon, V., Delahaye, F., Del Zanna, G., Dimitrijević, M.S., Drouin, B.J. and Dubernet, M.L., 2020. A decade with VAMDC: Results and ambitions. *Atoms*, 8(4), p.76. <https://doi.org/10.3390/atoms8040076>

^bEpée Epée, M.D., Motapon, O., Pop, N., Iacob, F., Roueff, E., Schneider, I.F. and Mezei, J.Z., 2022. Dissociative recombination and rotational transitions of $D^+ 2$ in collisions with slow electrons. *Monthly Notices of the Royal Astronomical Society*, 512(1), pp.424-429. <https://doi.org/10.48550/arXiv.2202.09143>

^cHassaine, R., Djuissi, E., Pop, N., Iacob, F., Epée, M.D., Motapon, O., Laporta, V., Bogdan, R., Ayouz, M., Telmini, M. and Coppola, C.M., 2025. Electron impact ro-vibrational transitions and dissociative recombination of H_2^+ and HD^+ : Rate coefficients and astrophysical implications. arXiv preprint arXiv:2507.14602. <https://doi.org/10.48550/arXiv.2507.14602>

^dIacob, F., Pop, N., Mezei, J.Z., Epée, M.E., Motapon, O., Niyonzima, S., Laporta, V. and Schneider, I.F., 2019, January. Recombination and excitation of molecular cations with electrons: Application to $H^+ 2$, BeD^+ and BeT^+ . In *AIP Conference Proceedings* (Vol. 2071, No. 1, p. 020007). AIP Publishing LLC. <https://doi.org/10.1063/1.5090054>

^eVujčić, V., Marinković, B.P., Srećković, V.A., Tošić, S., Jevremović, D., Ignjatović, L.M., Rabasović, M.S., Šević, D., Simonović, N. and Mason, N.J., 2023. Current stage and future development of Belgrade collisional and radiative databases/datasets of importance for molecular dynamics. *Physical Chemistry Chemical Physics*, 25(40), pp.26972-26985. <https://doi.org/10.1039/D3CP03752E>

Development of Fluorescent Gold Nanoparticles using Rhodamine 6G, Sulforhodamine B, Rhodamine 101, Fluorescein and Coumarin dyes for sensing applications

İdris Yazgan¹, Selin Çeter¹

¹*Department of Biology, Kastamonu University, Kastamonu, 37150 Türkiye*

Fluorescence based sensing approaches have become popular for their sensitivity and high signal/noise ratio in biomedical applications. It is critical to keep the fluorescence character when the sensing agents interact with the analyte's matrix, which is currently a challenge since the fluorescent moiety loses its intrinsic character upon the interaction with proteins and certain organic groups (e.g. ascorbic acid)^a. In this study, we developed a synthetic route to introduce fluorescent moieties on the gold nanoparticles, which decreases the loss of the fluorescent character of the agents when they interact with proteins (e.g. 20 mg/mL BSA) and such organic groups as ascorbic acid and carboxylic acid. We utilized cellobiose derivatives to initiate the gold nanoparticle synthesis, which was encapsulated into lab-made chitosan nanobeads (<200 nm) and used as the substrate for the fluorescent dye (i.e. Rhodamine 6G, Sulforhodamine B, Rhodamine 101, Fluorescein and Coumarin dyes) loading. The fluorescence characterization revealed that except Rhodamine 6G, the rest of the dyes can effectively strictly bind to the gold nanoparticles within the chitosan beads. Ongoing studies are to utilize the developed formulations for the detection of bacterial pathogens in water and food samples.

References:

^aKırbay, F.Ö., Yazgan, İ., Demirkol, D.O.. Comparison of Direct and Sandwich Type Immunoassays on Electrospun Nanofibers Using of Metal Organic Frameworks as a Fluorescence Probe, *Sensors Actuators B. Chem.* (2022) 132621.
<https://doi.org/10.1016/j.snb.2022.132621>.

Sponsors & Acknowledgements

This meeting is supported by:

COST (European Cooperation in Science and Technology)

COST Action CA21101 – COSY

<https://www.cost.eu/actions/CA21101/>

Event Sponsors:

- **Physical Chemistry Chemical Physics (PCCP)** – Royal Society of Chemistry
<https://www.rsc.org/publishing/journals/pccp>
- **Small Structures** – Wiley
<https://onlinelibrary.wiley.com/journal/26884062>

COST is funded by the Horizon Europe Framework Programme of the European Union.

