

3rd General Meeting of the “COSY” COST Action

July 9 - July 11, 2025

Aula Tibiletti – 2nd Floor
Via Zamboni, 38

Book of Abstracts



Program of the 3rd General Meeting of the COSY Cost Action

Wednesday 9/7		Thursday 10/7		Friday 11/7	
8:30-9:20	Registration + Opening	8:30-9:00	Registration	9:00-9:30	Registration
9:20-10:00	Mattia Melosso	9:00-9:40	Alessandro Fortunelli		
10:00-10:25	Vladimir Sreckovic	9:40-10:05	A. Sezai Sarac	9:30-10:10	Berta Fernandez Rodriguez
10:25-10:50	Malgorzata Biczysko	10:05-10:30	Michele Reticcioli	10:10-10:35	Piotr Żuchowski
10:50-11:15	Alberto García-Vela	10:30-10:55	Aggelos Avramopoulos	10:35-11:00	Vincenzo Barone
11:15-11:45	Coffee break	10:55-11:25	Coffee break	11:00-11:30	Coffee break
11:45-12:10	Justyna Krupa	11:25-11:50	Stefan Vajda	11:30-11:55	Markus Meuwly
12:10-12:30	Alessandra Savarese (YR-PhD)	11:50-12:30	Maria Pilar de Lara Castells	10:55-12:15	Dennis Dinu (YR)
12:30-12:50	Petra Čechová (YR)	12:30-12:45	Javier Hernández Rodríguez (YR-PhD)	12:15-12:45	Denis Comte (YR)
12:50-13:05	Markéta Paloncýová (YR)	12:45-14:30	LUNCH	12:35-14:30	LUNCH
13:05-14:50	LUNCH				
14:50-15:30	Majdi Hochlaf	14:30-16:30	Management Committee Meeting	14:30-14:50	Luigi Crisci (YR)
15:30-15:55	Jorge Marques			14:50-15:10	Silvia Alessandrini (YR)
15:55-16:20	Kęstutis Aidas			15:10-15:35	Sergiy Perepelytsya
16:20-16:35	Einaras Sipavičius (YR-PhD)			15:35-16:00	Ljiljana Suručić
16:35-17:05	Coffee break	16:30-17:00	Coffee break	16:00-16:10	Closing remarks
17:05-17:30	Sandra Gomez Rodriguez	17:00-18:20	Management Committee Meeting	16:10-18:00	Aperitif & Farewell
17:30-17:55	Miroslav Medved'				

Wednesday 9/7

9:20-10:00	Mattia Melosso	<i>Rotational spectroscopy of potentially detectable interstellar molecules. (E)-1-propenol as an example.</i>
10:00-10:25	Vladimir Sreckovic	<i>Exploring Confined Molecular Systems and Their Role in Astrochemical Processes</i>
10:25-10:50	Malgorzata Biczysko	<i>Reliable modeling of anharmonic spectra from VPT2 and hybrid QM models</i>
10:50-11:15	Alberto García-Vela	<i>Quantum Control of the Dynamical Behavior of Resonance States in Small Organic Molecules with Intense Fields</i>
11:15-11:45	Coffee break	
11:45-12:10	Justyna Krupa	<i>Studies of Weak Complexes with Atmospheric and Astrochemical Relevance in Cryogenic Confinement: Where Experiment Meets Theory</i>
12:10-12:30	Alessandra Savarese (YR-PhD)	<i>Identification of the Best Candidates for Radioastronomical Detection within the C₃H₆O₂ Isomer Family</i>
12:30-12:50	Petra Čechová (YR)	<i>Cholesterol effect on the phase of lipid crowded environment</i>
12:50-13:05	Markéta Paloncýová (YR)	<i>Simulation Insight into Confined Lipid-based Systems</i>
13:05-14:50	LUNCH	
14:50-15:30	Majdi Hochlaf	<i>Molecular confinement induced effects: structures, spectroscopies, reactivity and applications</i>
15:30-15:55	Jorge Marques	<i>From the computational study of protein-ligand confined systems to the design of pesticides-adsorbing materials</i>
15:55-16:20	Kęstutis Aidas	<i>Towards Accurate Modelling of ¹H NMR Spectra of Ionic Liquid</i>
16:20-16:35	Einaras Sipavičius (YR-PhD)	<i>Intermolecular Organization In Aqueous Mixtures Of Choline Lysinate Studied By NMR And Molecular Dynamics/Quantum Mechanics</i>
16:35-17:05	Coffee break	
17:05-17:30	Sandra Gomez Rodriguez	<i>Methods to study deactivation of excited states in condensed systems</i>
17:30-17:55	Miroslav Medved'	<i>Iminothioindoxyls: A New Class of Molecular Photoswitches</i>

Rotational spectroscopy of potentially detectable interstellar molecules. (E)-1-propenol as an example.

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Rotational spectroscopy represents the most important tool to unequivocally identify molecules in the interstellar medium.¹ Therefore, laboratory spectroscopic data are mandatory in order to enable astronomical searches of new molecules that are expected to be present in space. This overview will focus about the experimental techniques used to produce and study molecules of astrochemical interest by means of rotational spectroscopy. Besides giving an idea of the current approaches employed in our laboratory, the recent study of the rotational spectrum of (E)-1-propenol and its astronomical search towards the Galactic Centre will be discussed in detail.

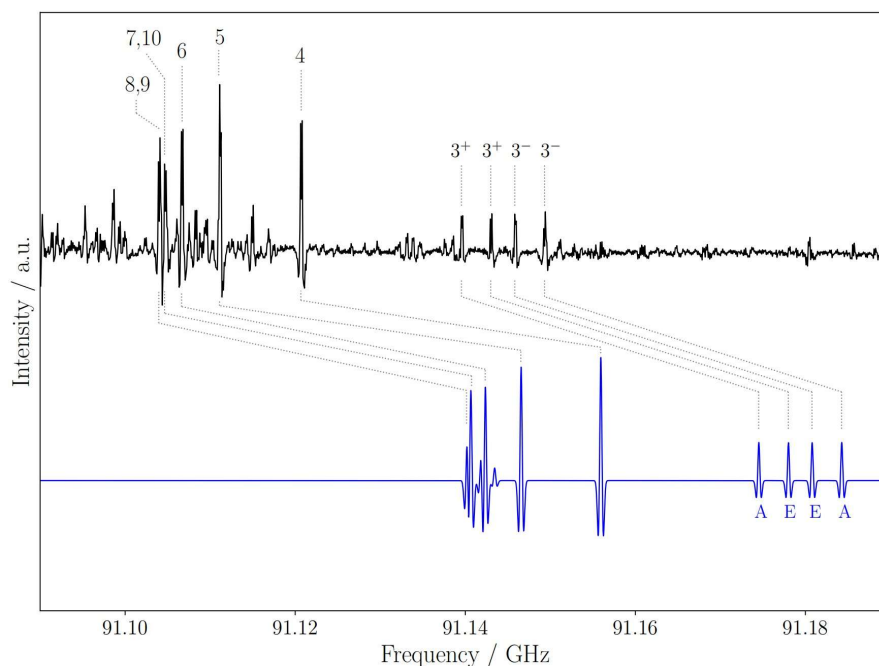


Figure 1. Comparison between the experimental spectrum (black trace) and the simulated one (blue trace) based on computed spectroscopic parameters of 1-propenol. Dotted gray lines provides the correspondence between experimental and predicted transitions.

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Exploring Confined Molecular Systems and Their Role in Astrochemical Processes

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Over the past few decades, computational chemistry has become increasingly important for exploring the behavior and interactions of small molecules within larger structures. Despite their vast size, molecular clouds play a significant yet not fully understood role in enclosed environments. Currently, several hundred molecular species have been identified in interstellar space, including neutral molecules, cations, and anions, with sizes ranging from diatomic molecules to very large ones. Due to the scattering and absorption of interstellar radiation, molecules located deep within these clouds can avoid being broken apart or ionized by light. Therefore, it is essential to investigate both radiative processes and simultaneous collisions. This study focuses on analyzing such interactions involving small molecules — like hydrogen, helium, and silicon molecular ions — and provides data to enhance our understanding of interstellar chemical processes. The findings aim to contribute to the development of more accurate models of molecular behavior in astrophysical environments.



Reliable modeling of anharmonic spectra from VPT2 and hybrid QM models

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Hybrid methods combining different levels of electronic structure quantum mechanical computations with vibrational perturbation theory have been increasingly used in anharmonic simulations of vibrational spectra to achieve accurate results with containable computational costs.¹ However, energy has often been the main focus of these studies, while intensities tended to be overlooked. This situation is largely due to two aspects, stemming from theory and experiment. Theoretically, few implementations were available and standard protocols to identify resonances were not sufficiently robust to handle the complex patterns present in intensities.² Experimentally, high-resolution vibrational spectra of suitable molecular systems, which could really show the effects of different hybrid schemes on the vibrational intensities, remain scarce. In this talk I will discuss the accuracy of anharmonic vibrational wavenumbers, IR intensities and spectral patterns from three different types of hybrid schemes based on the harmonic wavenumbers (Freq), potential energy surface (PES), and both PES and property surface (PS) computed at a higher level than the anharmonic correction.³

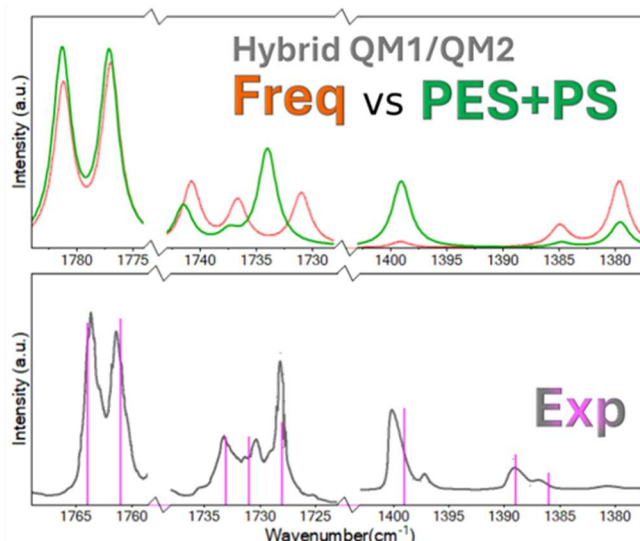


Figure 1. GVPT2 and experimental IR spectra of uracil in the fingerprint regions.

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Quantum Control of the Dynamical Behavior of Resonance States in Small Organic Molecules with Intense Fields

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A variety of molecular reaction processes are governed or mediated by resonance states. Some examples are the photodissociation of intermediate molecular species in chemical cycles, and the resonance-mediated reactive collisions of such intermediate species with other reagents. When these resonance-mediated processes compete, control over the resonance behavior (essentially the resonance lifetime and the product fragment distributions) can be crucial in order to steer the molecular reaction process in a desired direction. In previous works, control schemes using weak laser fields were applied to induce quantum interference in order to modify the lifetime^{1,2} and the product fragment distributions^{3,4} of resonance-mediated molecular photodissociation. Later on, moderately intense (of the order of 10^{11} - 10^{12} W/cm²) laser fields were applied to change (either reduce or increase) the resonance lifetime of a photodissociation process.⁵ In the work presented here, intense fields (of the order of 10^{13} - 10^{14} W/cm²) are applied to modify the product fragment distribution of the photodissociation of the CH₃ radical. The control scheme suggested relies on the creation of a light-induced conical intersection (LICI) that changes the natural couplings between the different electronic states of the radical. Varying the position of the LICI (which is determined by the frequency of the intense laser pulse) allows a large degree of control. It is found that in addition to the product distribution, the resonance lifetime can also be modified (reduced in this case). The scheme appears to be of universal application to resonance-mediated molecular photodissociation.

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Studies of Weak Complexes with Atmospheric and Astrochemical Relevance in Cryogenic Confinement: Where Experiment Meets Theory

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Non-covalent interactions significantly influence atmospheric and astrochemical processes by modifying existing reaction pathways and enabling new ones. Molecular complexes formed in cryogenic environments are particularly relevant to interstellar chemistry and the atmospheres of cold planetary bodies. In this study, we explore weakly bound aggregates and complexes formed by glycolic acid (GA)¹ and isocyanic acid (HNCO)², two molecules of atmospheric and prebiotic interest. Particular attention is given to GA and HNCO aggregates and their complexes with small molecules such as H₂O and N₂.^{3,4} Using matrix isolation infrared spectroscopy (MI-FTIR), we also investigate hetero-complexes formed upon UV-induced photochemistry of GA⁵ in noble gas matrices. The matrix isolation technique provides a unique environment to stabilise and study such weakly interacting systems, simulating conditions similar to those found in interstellar ices or upper atmospheric layers. Experimental results are supported by quantum chemical calculations at the MP2 and B3LYPD3 levels. A direct comparison between experimental and theoretical spectra enables the reliable identification of photoproducts and matrix-isolated complexes. This work highlights the interplay of experimental and theoretical modelling to understand the behaviour of reactive and weakly bound species under cryogenic conditions.

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Identification of the Best Candidates for Radioastronomical Detection within the C₃H₆O₂ Isomer Family

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The interstellar medium (ISM), despite being characterized by harsh physical conditions, is known to contain more than 330 molecular species (to date), with new detections being reported on a monthly basis.¹ One of the strategies for detecting new interstellar complex organic molecules (iCOMs) is to focus on a particular family of isomers, because their chemical formation in the ISM could be related to the same reactive processes.² This idea is at the base of the so-called Minimum Energy Principle (MEP), which states that the most abundant isomers in the ISM are also the most stable ones. This suggests a connection between the relative stabilities of the isomers and their detectability in the ISM, making this empirical principle a possible guiding aid for the search of new iCOMs.³ In the large variety of the possible isomer families, the C₃H₆O₂ class of isomers contains a large number of interstellar candidates, which could serve as a probe for investigating the next step in interstellar chemical complexity.⁴

In this study, the C₃H₆O₂ isomer family has been theoretically characterized, from a structural and energetic point of view, by means of state-of-the-art computational approaches based on Density Functional Theory and Coupled-Cluster Theory. In particular, the use of a computational protocol⁵ based on the MEP has allowed to identify possible candidates for radioastronomical detection within the family. The results obtained in the different steps of the protocol will be presented, along with the final energetic scale.

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Cholesterol effect on the phase of lipid crowded environment

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Biological membranes play a crucial role in the ability of organisms to maintain cellular homeostasis in various environments, making use of the great chemical variability of lipids. However, this incredible diversity in membrane composition poses a great challenge for their use in molecular dynamics. To address this, we compared seven membrane models ranging in from a single-lipid POPC membrane commonly used in MD simulation, to a complex 18-lipid plasma membrane mimetic. We evaluated the impact of lipid composition on membrane properties and the conformational dynamics of an embedded TLR2 protein transmembrane fragment.

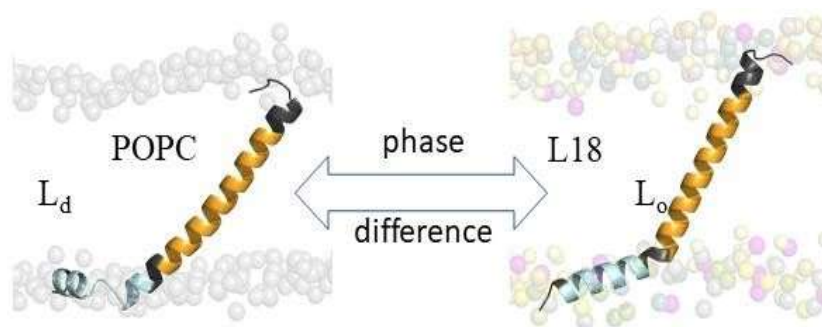


Figure 1: Comparison of the most frequent TLR2 conformation in the simplest (POPC) and the most complex (L18) of studied membranes. The protein is in orange, dark gray and pale cyan cartoon, lipid phosphate groups are depicted as balls with colors corresponding to different lipids. The rest of the membrane, water and ions are hidden for clarity

Our findings show that the main feature that governs membrane model properties is the presence or absence of cholesterol, and the subsequent membrane ordering. This, rather than the number or diversity of lipid species, had the major effect on membrane thickness, rigidity, protein conformational flexibility and its tilt in the membrane.

Simulation Insight into Confined Lipid-based Systems

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Lipid-based systems span a wide range of structures, from bilayers to complex assemblies like lipid nanoparticles (LNPs), each playing a critical role in biological and therapeutic functions. LNPs are at the forefront of nucleic acid (NA) delivery for vaccines and therapies. Their structure—comprising ionizable lipids, helper lipids, PEGylated lipids, and NA cargo—enables efficient encapsulation and pH-triggered release. However, their dynamic behavior inside cells, particularly during endosomal escape, remains poorly understood.

Multiscale molecular dynamics simulations address this challenge, offering insights into LNP structure, stability, and lipid phase behavior. All-atom models capture molecular interactions, while coarse-grained simulations reveal mesoscale organization and composition-dependent properties, guiding the in-silico design of next-generation LNPs.

In parallel, carbon nanomaterials like carbon dots and graphene show promise in biomedical applications but raise questions about biocompatibility. Simulations of their interactions with lipid membranes and generally cell models reveal binding mechanisms and structural perturbations, essential for safe and targeted use.

Together, these simulation approaches illuminate the structure–function relationships in confined lipid systems and at bio-nano interfaces, enabling predictive, mechanism-driven development of therapeutic platforms and biocompatibility assessment.



Molecular confinement induced effects: structures, spectroscopies, reactivity and applications

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Using first principles methodologies, we determine the structural and spectroscopic properties of molecules, either isolated or interacting with various substrates (rare gas or metallic cluster, metallic surface, rare gas matrices, cavity of MOFs, ...). We focus on the study of interactions between these substrates and these molecules, where we determine their binding energies or adsorption energies. Diverse analyses are also performed to characterize the strong and weak intermolecular interactions, the charge and/or proton transfers and the induced spectroscopic shifts (both vibrational and electronic).

Probing the intermonomer interactions in play provides a wealth of information on confinement induced effects on the molecular properties and also on how these properties are modified by their environments. We show that, although these interactions are weak, where the molecular properties are only slightly perturbed by the surrounding environment, the resulting spectroscopic and structural parameters of the molecule and its reactivity are strongly affected. In sum, we show that the longrange interactions play crucial roles with important applications in several chemical, physical, biological, environmental and industrial domains. In particular, they modulate the physical chemical processes at interfaces such as the selective adsorption / solvation / sequestration of molecular species. Several examples will be presented.



From the computational study of protein-ligand confined systems to the design of pesticides-adsorbing materials

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The design of new materials with effective adsorbing properties for a target molecule may benefit from the application of computational techniques. In the present project, we are interested in materials that can adsorb pesticides so that they can be employed for water remediation purposes. The main idea behind this work is to take advantage of the acquired knowledge about pesticides-proteins interactions in order to select key amino acids that can be used to improve the adsorption properties of chitosan. This type of material has shown to be effective for pesticide adsorption¹ and it has the advantage of being derived from chitin, which is an abundant and biodegradable natural resource.^{2,3} Thus, we describe a multi-stage computational strategy, based on docking, molecular dynamics (MD) simulations and electronic-structure calculations to unveil the most relevant interactions between pesticides and amino acids from target proteins. To test the present methodology, this was first applied to imidacloprid (IMI), an insecticide used worldwide, and the *Aplysia californica* acetylcholine-binding protein (AChBP) as the target molecule, since a crystal structure is already available for such pesticide-protein complex. We have also shown that the methodology can be generalized to other neonicotinoids, *i.e.*, acetamiprid and thiacloprid, the former of which does not possess a resolved crystal structure. The most promising amino acids selected according to our strategy were then used to functionalize monomers and trimers of chitosan and the ability of these model systems to adsorb the neonicotinoids was assessed by MD simulations. The results indicate a significant improvement of the adsorption of the three pesticides when chitosan is functionalized with tyrosine and tryptophan.

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Towards Accurate Modelling of ^1H NMR Spectra of Ionic Liquid

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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. MD simulations are employed to sample the phase space of molecular system of interest under specific thermodynamic conditions, and then QM/MM calculations of electronic properties are performed where the central part of the molecular system is described by an electronic structure method and the rest of the system is modelled by a classical force field. The final results of electronic properties are obtained as statistical averages over a set of molecular snapshots taken from the MD trajectory.

Relative ^1H NMR spectra of 1-butyl-3-methyl-imidazolium tetrafluoroborate, $[\text{C4mim}][\text{BF}_4]$, ionic liquid (IL) and its aqueous mixtures were recently computed using classical MD simulations with IL-specific force field, and the entire first solvation shell of the C4mim^+ cations had to be treated quantum mechanically in the QM/MM calculations. The ^1H NMR chemical shifts of imidazolium cations have been reproduced with the overall root-mean-square deviation of 0.2 ppm in aqueous IL mixtures with molar fraction of the IL in the range of 0.17 to 1.00.¹ The previously troublesome chemical shift of the proton at position 2 in the imidazolium ring² was also predicted very accurately. Computations confirm that ^1H NMR spectrum of aqueous mixtures of $[\text{C4mim}][\text{BF}_4]$ is very little dependent on the composition of the mixture, even though considerable alterations in the composition of the first solvation shell of the cation were observed with the increasing content of water in the mixture.¹

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Intermolecular Organization In Aqueous Mixtures Of Choline Lysinate Studied By NMR And Molecular Dynamics/Quantum Mechanics

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Choline lysinate (ChoLys) is a biocompatible ionic liquid (IL) belonging to ChoAA (choline-amino acid) family of ILs. They are potential green solvents¹, lubricators², CO₂ absorbers in carbon capture technologies³, but most importantly, ChoAA ILs can effectively solubilize various materials in aqueous media, such as lignin⁴ and various drugs, like glibenclamide⁵. They have lowered toxicity compared with well-investigated classical synthetic ILs, thus making them promising materials in pharmaceutical and clinical fields. Yet only a few theoretical studies on ChoAA:water mixtures intermolecular structure and solubilization mechanism of drug molecules are published.^{4,6} Without fundamental understanding of this phenomenon, all solubilization experiments and potential applications will be restricted to trial-and-error methods with no possible prediction beforehand.

We investigated ChoLys and its aqueous mixtures using a combination of molecular dynamics (MD) simulations, quantum mechanics / molecular mechanics (QM/MM) calculations and ¹H NMR and NMR DOSY measurements. We described intermolecular structure of such systems using radial distribution functions and by performing water and ion aggregation analysis. Validity of the results was checked in two ways: calculated diffusion coefficients were compared with NMR DOSY results and QM/MM-calculated NMR shielding constants was compared with ¹H NMR experimental spectra.

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Methods to study deactivation of excited states in condensed systems

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Understanding how excited states deactivate in condensed systems is crucial for unraveling the mechanisms behind photostability, photoswitching, and energy transfer in complex environments. This talk will present a range of computational approaches used to investigate the relaxation pathways of electronically excited molecules in condensed phases, such as solution¹ and extended PAH systems.² Emphasis will be placed on nonadiabatic quantum dynamics simulations, which allow us to capture the interplay between electronic and nuclear motions and to model the influence of the environment on deactivation processes. I will discuss strategies to address the challenges posed by the large number of degrees of freedom and the wide range of timescales involved, including the use of grid-based wavepacket methods and multilayer techniques implemented in the Quantics program package.³ Examples will highlight how these methods complement experimental observations, providing molecular-level insight into ultrafast relaxation phenomena observed with spectroscopic techniques.⁴

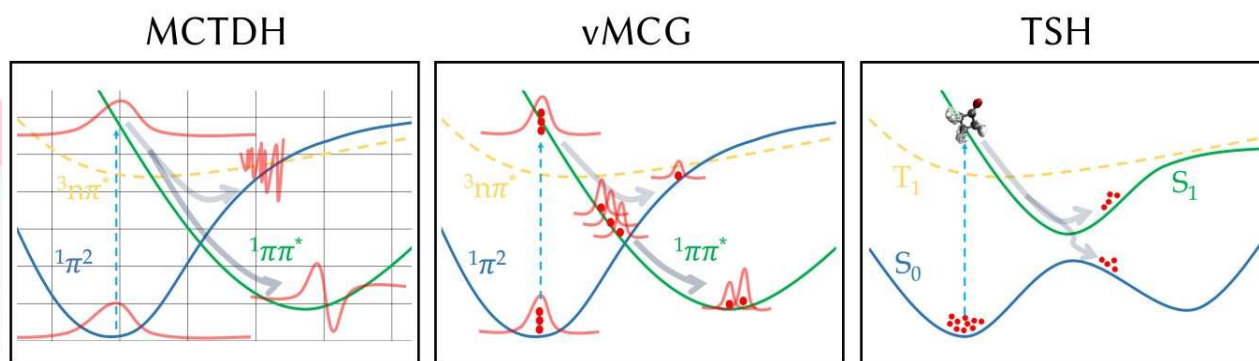


Figure 1. Depiction of three of the most used non-adiabatic molecular dynamics methods to study photoinitiated systems.

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Iminothioindoxyls: A New Class of Molecular Photoswitches

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Light is an exceptional external stimulus offering precise control over the properties and functions of chemical and biological systems. This is enabled through the use of materials exhibiting photochromism, *i.e.*, a reversible change of color upon the light irradiation. This change usually also affects other properties such as, *e.g.*, dielectric constants, surface wettability, and refractive index. Molecular photoswitches have diverse applications including control of surface properties, data/energy storage, and drug delivery. For each application, there are specific requirements on their photochromic characteristics. For medicinal applications, ideal photoswitches should operate in the VIS region, show good addressability and thermal half-life ~ 0.1 -1 s, and be functional in water.

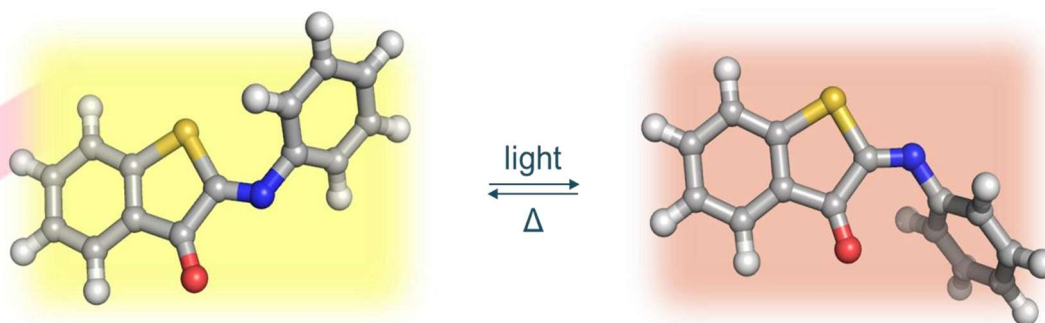


Figure 1. Photoswitching of Iminothioindoxyls

In close collaboration with experimentalists, we reported a new class of molecular photoswitches called iminothioindoxyls (ITIs) that meet most of these requirements,^{1,2} but typically thermally relax on the ms timescale. With the help of theory, we very recently successfully designed new ITI derivatives with thermal half-lives exceeding 0.1 s.³ In the talk, several exemplars of how computational tools can be used to gain insights into molecular photochromism will be provided.

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Thursday 10/7		
9:00-9:40	Alessandro Fortunelli	<i>High-Throughput and Conformal Funnels in NanoCatalytic Processes</i>
9:40-10:05	A. Sezai Sarac	<i>Polyacrylonitrile Composite Nanofibers with Confined Magnetic Ferrite Nanoparticles</i>
10:05-10:30	Michele Reticcioli	<i>Machine Learning for Polaronic Materials: TiO₂(110) at the nanoscale</i>
10:30-10:55	Aggelos Avramopoulos	<i>Hyperpolarization Effects in Molecular Materials</i>
10:55-11:25	Coffee break	
11:25-11:50	Stefan Vajda	<i>Addressing Size, Composition and Support Effects in Nanocatalysis: Subnanometer Mono- and Bimetallic Clusters in CO Oxidation</i>
11:50-12:30	Maria Pilar de Lara Castells	<i>Unsupported and surface-supported subnanometric metal clusters as fluxional Jahn-Teller molecules</i>
12:30-12:45	Javier Hernández Rodríguez (YR-PhD)	<i>Non-Adiabatic Dynamics of Excited States in Tetraphenylpyrazine: From Monomer to Dimer</i>
12:45-14:30	LUNCH	
14:30-16:30	Management Committee Meeting	
14:30-16:30	Coffee break	
17:00-18:20	Management Committee Meeting	

High-Throughput and Conformal Funnels in NanoCatalytic Processes

Alessandro Fortunelli,^{1*} Thantip Roongcharoen,¹ Giorgio Conter,¹ Giacomo Melani,¹ Luca Sementa¹

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I will discuss general principles, challenges, and recent advances in theoretical and computational modeling of heterogeneous nano-catalysts as confined systems. Starting from the dramatically urgent societal need of novel, more active, more selective, cheaper, and sustainable catalysts for all of the critical mass-scale catalytic processes used in chemical industry, I will discuss the opportunities offered by confinement and nano-structuration, the challenges presented to approaches aiming at efficient and practical high-throughput catalysts screening, and some recent advances.^{1,2,3} that promise to provide a possible solution to this important problem.

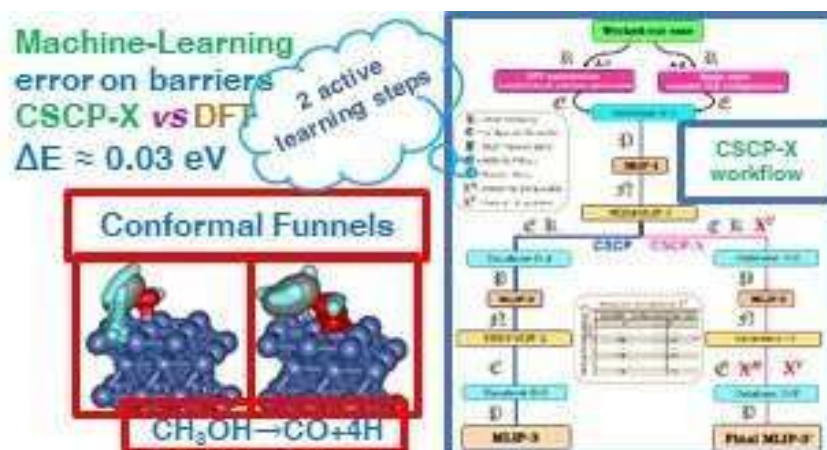


Figure 1. Illustrative Depiction and Workflow of Conformal Catalyst Sampling

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Polyacrylonitrile Composite Nanofibers with Confined Magnetic Ferrite Nanoparticles

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Ferrite-polymer nanofiber composites, of polyacrylonitrile (PAN), show promise in biomedical applications and energy conversion, due to their unique electronic and material properties, which allow for customizable functions.¹ In this study, electrospinning was used to create well-defined PAN nanofibers blended with various ferrite nanoparticles, *i.e.*, γ -Fe₂O₃, MnZnFe₂O₄,² and CoFe₂O₄. Well-dispersed nanoparticles in PAN exhibit the inherent electronic characteristics of the polymers and respond to external magnetic fields. Application of an external magnetic during dynamic mechanical measurements (DMA), the storage modulus of PAN/ γ -Fe₂O₃ at its glass transition (T_g) increases at the expense of the loss modulus. HRSEM, XRD, DMA and spectroscopic analyses, provided insight into the interaction mechanism between the ferrite nanoparticles and the polymer matrix. SEM imaging and EDX mapping confirmed well dispersion of ferrite nanoparticles within the PAN composite nanofibers, with minimal bead formation (Fig.1). Electrochemical Impedance Spectroscopic (EIS) data was analyzed using an equivalent circuit modelling [$R_s(Q_1(R_1(Q_2R_2)))$] to better understand the interface between the metal oxide/PAN hybrid polymeric nanofiber

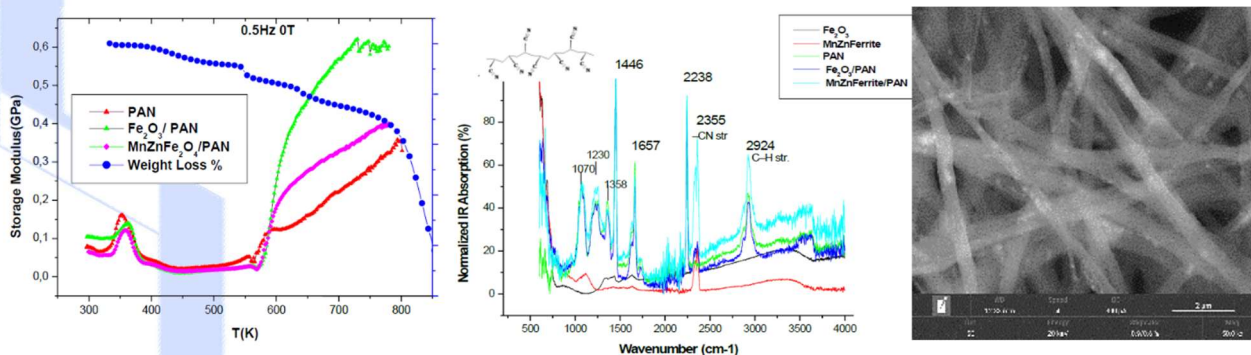


Figure 1. Thermomechanical (DMA), FTIR, and SEM results of nanofibers

mat/solution. C≡N functional groups in PAN nanofibers can immobilize magnetic nanoparticles through hydrogen bonding and coordination interactions.

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Machine Learning for Polaronic Materials: $\text{TiO}_2(110)$ at the nanoscale

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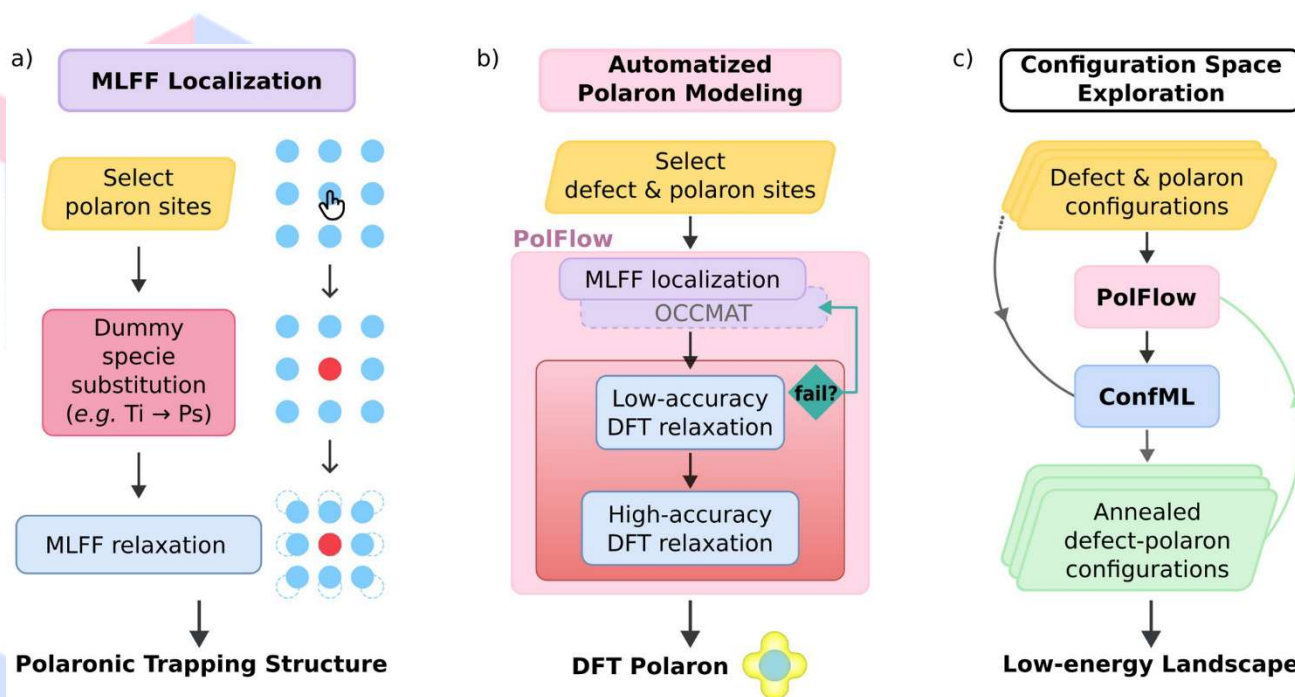
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The combination of machine learning (ML) with density functional theory accelerates material simulations, expanding both spatial and temporal scales. However, current ML methods struggle to address polaron trapping. We present a novel machine learning force field (MLFF) approach that incorporates polaron trapping descriptors, enabling large-scale studies of polaronic materials.

Using $\text{TiO}_2(110)$ as a case study, we reveal how dopants and atomic vacancies affect polaron configurations and drive catalytic CO adsorption. Additionally, our method captures the dynamic evolution of polarons with unprecedented statistical robustness.

This work advances fundamental understanding of defect-polaron interactions while offering a fully automated and efficient computational suite for the study of polaronic materials, facilitating characterization and design of metal oxide catalysts [COSY GAPG-5].



Hyperpolarization Effects in Molecular Materials

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Design at the molecular level is an important issue for material science. One specific challenge is the understanding of factors that govern light-matter interactions and how one can tune them in an efficient way. The Linear and Non-Linear (L&NLO) properties are of great current interest, because they allow to advance our understanding of the electronic and vibrational structure of the molecules. In addition, they are key parameters for the design of materials with many applications (e.g., fiber optic communication, all optical switching).

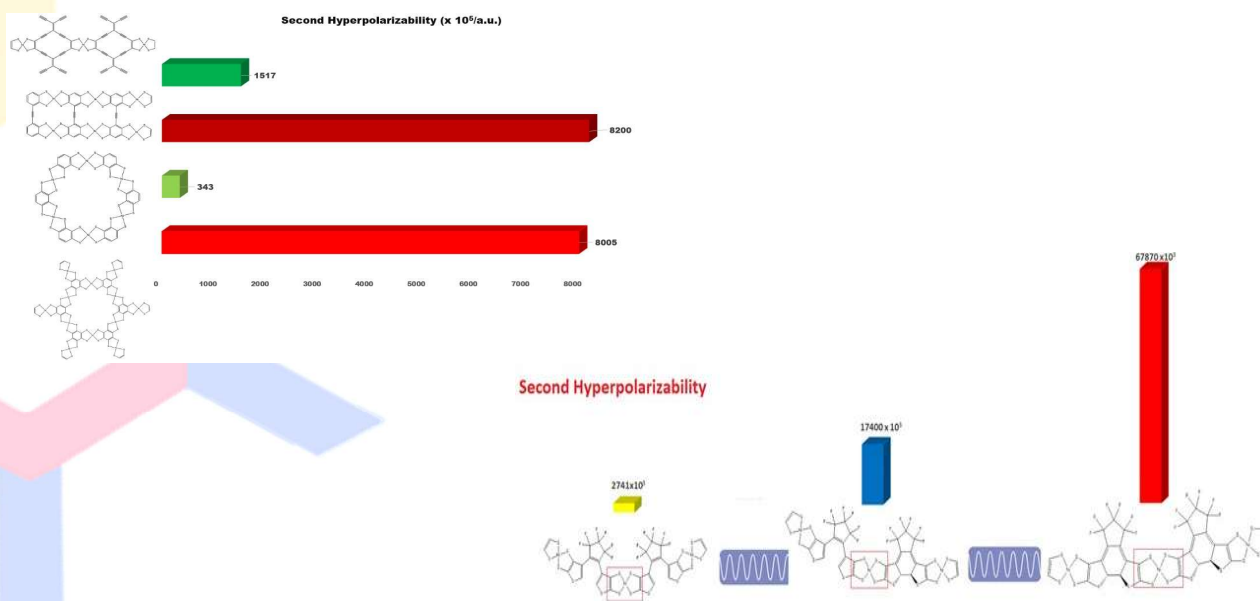


Figure 1. Structures and non-linear optical properties of a series of molecular materials.

A series of molecular materials were computationally designed with the aid of Density Functional Theory (DFT), having with exceptional high NLO properties. These include (Fig. 1): **I**) 1D and 2D coordination polymers (nanosheets), based on nickel bis(dithiolene) and benzene (), **II**) Oligomer of (RA-NiBDT)_n, RA = radiaannulene, **III**) Polycyclic Aromatic Hydrocarbons (PAH) (0D graphene quantum dots). **IV**) Molecular Switches based on the 1,2-diarylethenes (DAE) Main objectives are: I) to demonstrate the superior non-linear optical (NLO) performance of the proposed materials in terms of their electronic structure character and II) the understanding of factors that govern hyperpolarization effects in molecular materials.

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Addressing Size, Composition and Support Effects in Nanocatalysis: Subnanometer Mono- and Bimetallic Clusters in CO Oxidation

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Using mono- and bimetallic clusters supported on amorphous and crystalline supports, the following points will be discussed: (i) bridging the materials gap between amorphous and crystalline alumina support using Pt₁₀ clusters¹; (ii) bridging the subnanometer and nanometer size range of clusters^{1,3}; (iii) substitution of atoms of precious metals with alternatives;^{2,3} (iv) support effects on catalytic performance by using alumina, tin oxide, titania and zirconia support; and (v) evolution of the nature of the catalyst's components during reaction conditions.

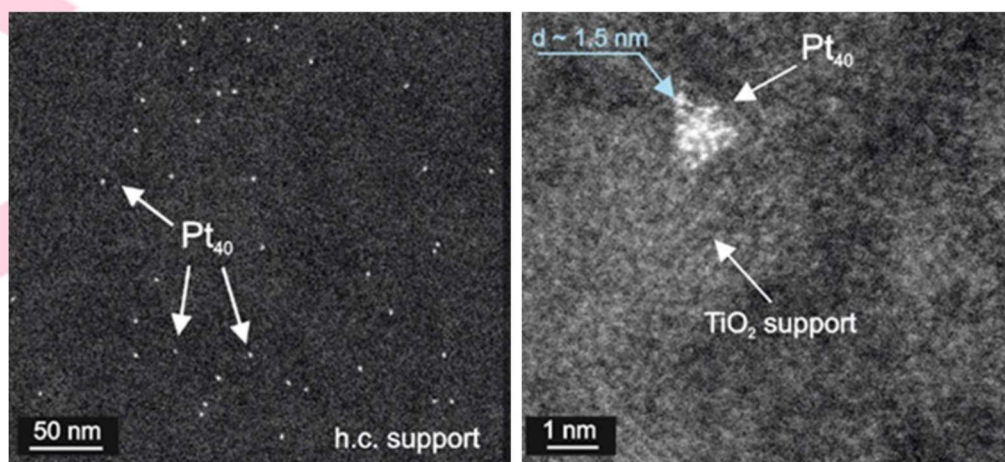


Figure 1. Image of a 13- and 40-atom Pt cluster

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Unsupported and surface-supported subnanometric metal clusters as fluxional Jahn-Teller molecules

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Current advances in synthesizing and characterizing atomically precise monodisperse metal clusters (AMCs) composed of just one to ten atoms are allowing to deepen our physical and chemical insights into the structure of matter. Their quantized ‘molecule-like’ electronic structure showcases unique stability and properties different from those of nanoparticles and bulk materials. When integrated into materials that interact with environmental molecules and sunlight, AMCs exhibit enhanced (photo)catalytic activity, electronic properties, and even optical behavior.¹⁻¹² The concept of fluxionality has been invoked to explain the enriched catalytic properties of AMCs. In this lecture, starting with studies of metal clusters, and even single metal atoms, embedded in helium nanodroplets as ultra-cold nanolabs, I will present an overview of recent COSY studies¹⁻¹² with a focus on *ab initio* evidences of copper and silver clusters as fluxional Jahn-Teller molecules as well as the influence of intermolecular cluster-support interactions on the associated conical intersections, considering benzene and coronene as model supports. A support-induced transition from a Jahn-Teller to a pseudo-Jahn-Teller distortion will be uncovered as well.

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Non-Adiabatic Dynamics of Excited States in Tetraphenylpyrazine: From Monomer to Dimer

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Fluorescent organic chromophores are crucial for applications like cellular imaging and OLEDs, where performance depends on their gas-phase and solid-state behaviour. Unlike traditional fluorophores suffering from Aggregation-Caused Quenching (ACQ), Tetraphenylpyrazine (TPP) exhibits solid-state luminescence enhancement (SLE), showing stronger emission in aggregates due to suppressed non-radiative decay.^{1,2}

This study delves into the excited-state quantum dynamics of the TPP monomer, and the dimer configuration extracted from the X-ray crystal structure. We employed Overdia to approximate the potential energy surfaces (PESs) by constructing Linear Vibronic Coupling (LVC) Hamiltonians, performing diabatic state diagonalisation, and implementing charge-transfer states for the dimer. Nuclear dynamics were simulated using ML-MCTDH, as implemented in QUANTICS package,³ across 144 (monomer) and 288 (dimer) vibrational normal modes. Results reveal how aggregation restricts intramolecular motions elucidating SLE at the quantum level by the absorption spectra and the deactivation pathways.

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Friday 11/7

9:00-9:30	Registration	
9:30-10:10	Berta Fernandez Rodriguez	<i>Pursuing Accuracy in the Evaluation of Intermolecular Potentials</i>
10:10-10:35	Piotr Żuchowski	<i>Response theory and molecular interactions</i>
10:35-11:00	Vincenzo Barone	<i>Next-Gen Computational Spectroscopy with VMS2.0: Accurate, AI-Enhanced, Scalable, and User-Friendly</i>
11:00-11:30	Coffee break	
11:30-11:55	Markus Meuwly	<i>Machine Learning Based Potential Energy Surfaces for Chemical Reactions</i>
10:55-12:15	Dennis Dinu (YR)	<i>Seven Years in the Matrix: A Personal Journey Through Cryogenic Spectroscopy and Vibrational Theory</i>
12:15-12:45	Denis Comte (YR)	<i>Protonated Dimers as Gateways to Interstellar Chemical Evolution</i>
12:35-14:30	LUNCH	
14:30-14:50	Luigi Crisci (YR)	<i>DDCI-Augmented PCS Protocol: Unlocking Size-Consistent, Near-Full-CI Accuracy in Bond Dissociation Reactions</i>
14:50-15:10	Silvia Alessandrini (YR)	<i>Formation of glycolamide (NH₂C(=O)CH₂OH) on interstellar ice grains: Insights from atomistic simulations</i>
15:10-15:35	Sergiy Perepelytsya	<i>Counterion-induced DNA confinement: Modeling and simulation insights for biological and nanotechnological applications</i>
15:35-16:00	Ljiljana Suručić	<i>Bridging the Gap: Challenges and Opportunities for Bosnian-Herzegovinian Participation in COST Actions</i>
16:00-16:10	Closing remarks	
16:10-18:00	Aperitif & Farewell	

Pursuing Accuracy in the Evaluation of Intermolecular Potentials

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I will give an overview on the work we have been carrying out in the last years, regarding the evaluation of intermolecular interactions and potentials. In the field of intermolecular interactions dispersion is the most demanding contribution to determine. Its accurate description is a challenge from the theoretical point of view. Van der Waals complexes exhibit low dissociation energies, large bond lengths and low-frequency vibrational modes, while retaining many of the individual monomer properties. These clusters are ideal for investigating the accurate evaluation of intermolecular interactions, as the weak bonding between nonpolar systems primarily relies on dispersion forces. An accurate description of the dispersion can be achieved through the use of coupled cluster methods, that allow the obtention of state-of-the-art intermolecular potentials, providing results that can be considered predictive and can compete with experimental determinations. Some examples will be presented.

Recently we studied larger systems and developed analytical corrections to improve the accuracy of the PM6 and GFN2-xTB semiempirical quantum mechanical methods for the evaluation of noncovalent interaction energies in alkanes and alkenes.¹ We followed the approach of functional group corrections (FGC),² wherein the atom–atom pair corrections depend on the nature of the interacting functional groups. In general, for the systems included in the training and validation sets, the errors obtained with the PM6-FGC and xTB-FGC methods are within chemical accuracy. The FGC results were compared to those obtained using recently developed Machine Learning (ML) approaches, in particular AIQM1-2³ and PM6-ML.⁴

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Response theory and molecular interactions

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This talk will highlight the significance of response theory in the study of molecular interactions. Some time ago we have introduced Hermitian formulation of Coupled Cluster theory using the expectation-value CC approach¹. Building on this foundation, several new methodologies were introduced, notably the CCSD-based SAPT, which significantly improves the description of intramonomer correlation effects in the induction and dispersion interactions^{2,3}.

An important contribution by Jeziorski and collaborators was the direct calculation of some of the properties of the H₂ molecule (including relativistic corrections) without relying on the subtraction of monomer properties⁴. I will show how this concept can be incorporated into the SAPT framework to directly compute interaction-induced properties, such as the dipole moment of a van der Waals complex⁵. Furthermore, I will present how the new tool helps to understand how the electrostatic potential of the monomers should be corrected to account for Pauli exchange effects an insight that leads to a new scheme for treating induction interactions to infinite order.

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Next-Gen Computational Spectroscopy with VMS2.0: Accurate, AI-Enhanced, Scalable, and User-Friendly

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To fully exploit the wealth of information offered by high-resolution spectroscopic techniques, accurate and efficient quantum mechanical tools are essential — especially for medium — to large-sized molecular systems, where spectral congestion hampers standard approaches. Although components of a general exploration/exploitation strategy exist in specialized codes, a robust and user friendly platform for unbiased comparison of experimental and theoretical spectra is still lacking. To address this need, we are developing version 2.0 of our Virtual Multifrequency Spectrometer (VMS2.0), integrating advances in quantum chemistry, machine learning (ML), and visualization. The platform includes pre- and post-processing utilities, high-resolution graphics, and immersive VR interfaces. In the initial stage, non-redundant generalized natural internal coordinates enable a clear separation of molecular motions, while ML algorithms based on continuous features (synthons) guide efficient quantum methods across soft-mode-dominated potential energy surfaces. Then, the family of Pisa Composite Schemes (PCSs)¹ optimizes the cost/accuracy ratio for systems of different size. For molecules with up to ~20 atoms, explicitly correlated coupled-cluster approaches (PCS3 and PCS2), including core–valence correlation and basis set extrapolation, are employed. For larger systems (~50 atoms), similar accuracy is achieved via frozen natural orbitals (FPCS3) for energies and bond corrections applied to DFT geometries (BDPCS3). Vibrational contributions to rotational constants, partition functions, and IR/Raman spectra are computed using dual-level VPT2. A new flexible engine combines multiple coordinate systems with analytical Hessians and gradients, enabling highly accurate reduced-dimensionality models. Additionally, effective strategies are implemented to treat systems with strong static correlation. A panel of biologically relevant molecules demonstrates that our integrated approach rivals the accuracy of high-end quantum methods for small semi-rigid systems, while extending applicability to significantly larger ones. By encompassing the entire computational workflow—from preprocessing to spectral simulation—VMS2.0 provides accurate yet affordable characterization of medium- to large-sized molecules through an intuitive, black-box interface accessible even to experimentalists. This paves the way for the simulation of even more complex molecular systems.

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Machine Learning Based Potential Energy Surfaces for Chemical Reactions

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In this contribution I will describe neural network and kernel-based methods suitable to construct full-dimensional, reactive potential energy surfaces for 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.



Seven Years in the Matrix: A Personal Journey Through Cryogenic Spectroscopy and Vibrational Theory

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Seven years ago, we set out to study the vibrational features of the stable reduction intermediates of carbon dioxide (CO₂),^{1,2} formic acid (HCOOH), formaldehyde (H₂CO), methanol (CH₃OH),³ methane (CH₄)¹, and water (H₂O).⁴ On this journey, we combined matrix isolation IR spectroscopy with anharmonic calculations using vibrational configuration interaction.^{5,6} After extensive explorations of potential energy surfaces and changing a fair share of Swagelok fittings, we now see why formaldehyde wins theoreticians' hearts and tests experimentalists' patience. In other words, our studies¹⁻⁶ pushed the limits of both theory and experiment to better understand molecular vibrations in cryogenic matrices, *i.e.*, confined host-guest systems. Conclusion: Each host-guest system exhibits unique peculiarities that cannot be transferred from one to another (cf. Figure 1). For example, the rotation of water or methane, cage splitting of carbon dioxide, torsional splitting of methanol, formic acid dimerization, and the challenge of isolating pure formaldehyde.

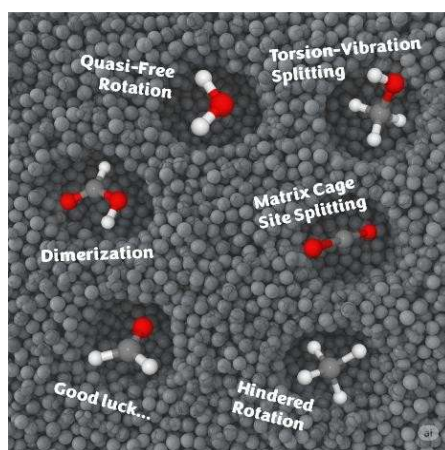


Figure 1. The most important peculiarities of different molecules isolated in cryogenic matrices.

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Protonated Dimers as Gateways to Interstellar Chemical Evolution

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The formation and evolution of complex organic molecules under abiotic conditions remains a central question in both physical chemistry and astrochemistry. Here, I present combined experimental and theoretical works that highlight the key role of protonated molecular dimers in driving molecular complexity in the gas phase under astrophysically relevant conditions. Using glycine and other prebiotic species, we show that new bonds, especially peptide ones, can form via unimolecular dehydration reactions within cluster ions, without the need for catalytic surfaces. Experiments performed with the DIAM device,^{1,2} mimicking cosmic-ray energy deposition reveal that these dimers act both as stabilizing frameworks and as reactive intermediates, guiding energy relaxation through evaporation, covalent bond cleavage, and unimolecular reaction. Notably, for glycine-containing clusters, the results indicate a tendency toward preferential formation of mixed dimers (e.g., a dipeptide paired with a glycine molecule), which appear more reactive and more prone to undergo further chain-elongation reactions. This suggests a potential mechanism for further peptide growth in the gas phase, offering new insights into how molecular complexity could emerge in cold extraterrestrial environments relevant to the origins of life.

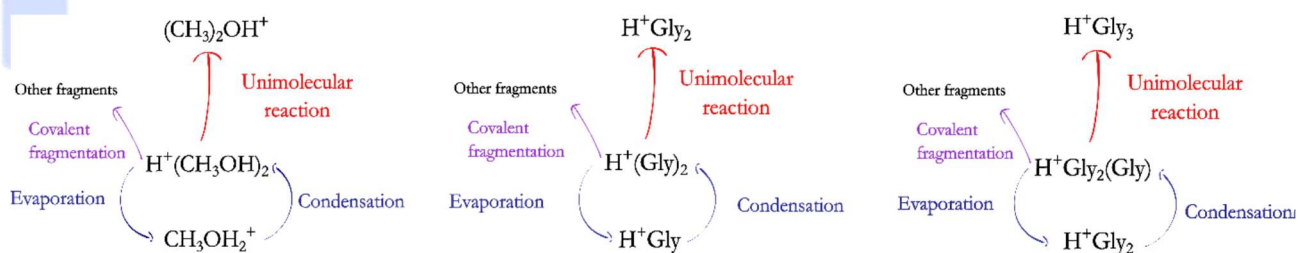


Figure 1. Relaxation mechanisms of protonated dimers for methanol, glycine, and diglycine, as observed after a single collision with the DIAM device.

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DDCI-Augmented PCS Protocol: Unlocking Size-Consistent, Near-Full-CI Accuracy in Bond Dissociation Reactions

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Recent theoretical and hardware developments have turned computational investigations into valuable assets for every chemist's toolkit. Advanced versions of Transition State Theory (TST), Variational Transition State Theory (VTST), and Variable Reaction Coordinate Transition State Theory (VRC-TST)¹ are at the forefront of addressing the complexities of chemical kinetics. While both approaches mitigate the non-recrossing approximation, their effectiveness strongly hinges on the quality of the underlying potential energy surface, with this aspect being particularly daunting for VRC-TST, which relies on a Monte Carlo (MC) phase-space sampling. In this connection, state-of-the-art approaches employ *on-the-fly* one-dimensional corrections for geometrical and electronic errors. The first correction aims to alleviate the bias induced by the use of rigid fragments in all the MC steps, whereas the latter correction tries to overcome the intrinsic inaccuracy of cheap quantum chemical models. This approach strengthens the role of robust and reliable quantum chemical models in the generation of accurate reference dissociation curves also for pathological multireference situations. Here, we propose an efficient yet accurate solution to tackle this aspect. After the determination of a suitable wave-function for the single-reference high-spin state by employing the Pisa composite scheme (PCS),² the *reference potential* is obtained by adding the energy difference between the high- and low-spin states (*spin-splitting* correction)³ computed by the Iterative Difference Dedicated Configuration Interaction (I-DDCI)⁴ or its perturbative version (I-DDCI-PT2) presented here for the first time. This embodies a rapid basis-set convergence, reduced number of doubly excited configurations, lack of intruder states interferences and a nearly exact recovery of size consistency. Then, the validity of the proposed reference potential is tested against the obtained rate constants. To this end, the multiconfigurational pair density functional theory represents the method of choice for the MC sampling, provided that the amount of exact exchange is carefully selected. Here, we propose a black-box procedure to find the most appropriate contribution of Hartree-Fock exchange to be used in different regions of the whole dissociation path. The results for C₂H₄ and CH₄ hydrogen dissociation are compared with accurate quantum mechanical calculations and experimental data showcasing the reliability of the presented approach.

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Formation of glycolamide ($\text{NH}_2\text{C}(=\text{O})\text{CH}_2\text{OH}$) on interstellar ice grains: Insights from atomistic simulations

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In 2023, Rivilla et al.¹ reported the observation of syn-glycolamide in the G+0.693-0.027 molecular cloud. This species plays an important prebiotic role, as it is one of the few amides observed in space and a stable isomer of glycine. The detection of this species required interpretation in terms of chemical reactivity, which was the main topic of my STSM. Since the G+0.693 region undergoes cloud-cloud collisions that induce large-scale shocks, dust grains are sputtered, releasing molecules into gas phase². For this reason, the synthesis of glycolamide on a water cluster mimicking interstellar ice mantles is particularly relevant. The proposed reaction pathway for the formation of glycolamide on icy mantles consists of two steps:³

- (1) $\text{H}_2\text{CO} + \text{NH}_2\text{CO}\cdot \rightarrow \text{NH}_2\text{C}(\text{O})\text{CH}_2\text{O}\cdot$
- (2) $\text{NH}_2\text{C}(\text{O})\text{CH}_2\text{O}\cdot + \text{H}\cdot \rightarrow \text{NH}_2\text{C}(\text{O})\text{CH}_2\text{OH}$

In the first step, a radical intermediate is formed, which is then hydrogenated to yield the target molecule. While the simulations based on an 18 water molecules cluster indicate that glycolamide can be formed on ice mantles from this process, a competing product -- $\text{NH}_2\text{C}(\text{O})\text{CHO}$ -- is also observed. At the same time, the water model appears to selectively form anti-glycolamide, suggesting that a conformational rearrangement should occur upon desorption into the gas phase.

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Counterion-induced DNA confinement: Modeling and simulation insights for biological and nanotechnological applications

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In aqueous solution, DNA adopts a double helical structure, with each phosphate groups along its backbone carrying a single negative charge ($-1e$). These charges are neutralized by positively charged counterions from the surrounding medium. Experimental studies show that, at sufficiently high concentrations, multivalent counterions, especially trivalent ($3+$) and higher, can induce condensation.¹ Molecular dynamics simulation have provided insights into the underlying mechanism, showing that DNA condensation is driven by the formation of stable, counterion-mediated DNA-DNA contacts.² In these structures, counterions are confined in the interhelical space and effectively screen the phosphate charges. Condensation is generally considered unlikely in the presence of monovalent ions, as polyelectrolyte models predict that in their presence the electrostatic attraction between DNA molecules is too weak to induce condensation.³ However, recent findings suggests that monovalent ions can influence the stability of the DNA double helix and facilitate the formation of intermolecular crosslinks.^{4,5} This is of particular relevance for DNA-based technologies.⁴ In this talk, we will revisit the molecular mechanisms of counterion confinement and DNA condensation, highlighting how recent simulation results challenge classical views and offer new perspectives for biological and nanotechnological applications.

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Bridging the Gap: Challenges and Opportunities for Bosnian-Herzegovinian Participation in COST Actions

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Attraction of young researchers from Inclusiveness Target Countries (ITC), particularly Bosnia and Herzegovina in COST Actions, which is in line with the COST overall mission, has been our priority in the framework of implementation of the COSY COST Action. In this light we launched the survey among 60 researchers from the University of Banja Luka, alongside with additional input from Tuzla and Sarajevo universities. This survey attracted 67% researchers that had not yet participated in any COST Action and 33% of those who have experience with COST programme (Figure 1). The survey identified three primary barriers to participation: limited awareness of opportunities, time constraints due to teaching and administrative duties, and insufficient funding for international engagement due to the COST reimbursement model. To address these challenges, and with the support of the Ministry of Civil Affairs of Bosnia and Herzegovina, a webinar titled "Funding Opportunities through COST Actions: Research Stays, Conferences, and Support for Young Researchers" was organized, with a special focus on COSY COST Action. The webinar covered topics such as joining active COST Actions, available financial support schemes, and networking strategies, with a particular emphasis on early-career researchers. The initiative targeted academic staff, doctoral candidates, and postdoctoral researchers. Key factors identified in order to increase activity included the need for more information through workshops and guides (36.7%), institutional financial support (26.7%), and greater visibility of participation calls (21.7%).

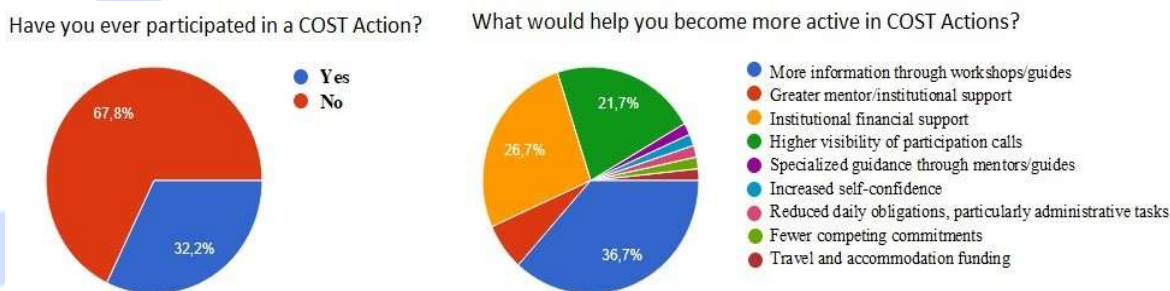


Figure 1. Survey results on COST Action participation and factors for increased activity

Lunch Menu on Wednesday 9/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Bocconcini soffici alle olive farciti con crudo dolce di Parma
Soft mini-bread with Parma Ham and olives
3. Rombetti di frittata ai sapori di campo 🌿
Small slices of omelette with spinach
4. Piccoli tramezzini assortiti
Small sandwiches
5. Torta salata vegetariana con ricotta e spinaci 🌿
Quiche with ricotta and spinach
6. Crocchettine di patata 🌿
Potato croquettes
7. Crostini dorati ai sapori di bosco 🌿
Tosted bread with veggies and mushrooms

Main Course:

1. Mezze maniche con pomodorini ciliegini, basilico e bruciatini di pancetta
Pasta with cherry tomato, basil and bacon
2. Rosette verdi con fontina, melanzane e basilico 🌿
Oven cooked egg and spinach pasta with cheese, aubergines and basil

Desserts:

1. Frutta fresca di stagione 🌿
Seasonal fruit
2. Ciotolini di mousse al pistacchio di Bronte 🌿
Small bowls of pistachio mousse

Lunch Menu on Thursday 10/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Piccoli sandwich a bocca di lupo farciti con salumi e salsine
Small sandwiches with cold cuts and sauces
3. Bicchierino con tarallini pugliesi, stracchino, basilico e pomodorini confit 🌿
Bowls with "tarallini", soft cheese, basil and confit tomatoes
4. Mini calzoncini vegetariani con ricotta e spinaci 🌿
Toasted bread with ricotta and spinach
5. Focaccine farcite con melanzane grigliate e mozzarella 🌿
Focaccia bread with aubergine and mozzarella
6. Bruschettine dorate con speck e zucchine marinate
Toasted bread with speck and courgette
7. Piccolo stecchino alla bolognese pastellato
Fried Bologna-meat skewers

Main Course:

1. Pennette con fiammiferi di speck, asparagi e zafferano
Pasta with speck, asparagus and saffron
2. Crespelle delicate ai sapori di bosco su fonduta di Parmigiano Reggiano 🌿
Oven-cooked crepes with mushrooms and parmesan

Desserts:

1. Frutta fresca di stagione
Seasonal fruit
2. Ciotolini di tiramisù
Small bowls of tiramisù

Lunch Menu on Friday 11/7 (Vegetarian Option indicated with 🌿)

Finger Food:

1. Piccoli spiedini di mozzarelline di bufala e pomodorini ciliegini 🌿
Vegetarian skewers with mozzarella and cherry tomatoes
2. Piccoli sandwich a bocca di lupo farciti con salumi e salsine
Small sandwiches with cold cuts and sauces
3. Mini calzoncini con prosciutto cotto e fontina
Small stuffed "calzone" with ham and cheese
4. Rombetti di frittata ai sapori di campo 🌿
Small slices of omelette with spinach
5. Quiche Lorraine con mozzarella, funghi e prosciutto cotto
Quiche with mozzarella, mushrooms and ham
6. Bruschettine dorate con speck e zucchine marinate
Toasted bread with speck and courgette
7. Crocchettine di patata 🌿
Potato croquettes

Main Course

1. Cous cous con ratatouille di verdure ripassate al forno 🌿
Cous Cous with roasted veggies
2. Nidi di rondine alla Romagnola con prosciutto cotto e fontina
Roasted egg-pasta with ham and cheese

Desserts:

1. Frutta fresca di stagione 🌿
Seasonal fruit
2. Sacher torte monoporzione 🌿
Sacher torte

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