

COST Action

Progress Report at 24 months

(27/09/2022 to 27/09/2024)

CA21101: CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS

The Action was approved by the Committee of Senior Officials (CSO) on 27-5-2022 and has the MoU reference COST 015/22.

This report was submitted on 24-10-2024 by the Action Chair on behalf of the Management Committee in fulfilment of the requirements of the rules for COST Action Management, Monitoring and Final Assessment.

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Action leadership and participants

Leadership positions

Position	Name	Contact details	Country*
Chair	Prof María Pilar de Lara-Castells	Pilar.deLara.castells@csic.es +34915616800	Spain

Position	Name	Contact details	Country*
Action Vice-Chair	Prof Cristina Puzzarini	cristina.puzzarini@unibo.it +390512099503	Italy

Working groups

#	WG Title	# of participants	WG Leader	Country*
1	Intermolecular Interactions - Ab initio-Generated Force Fields and Machine Learning	167	Prof Piotr Żuchowski pzuch@fizyka.umk.pl	Poland
2	Molecular Motion in Confined Systems	185	Dr Sonja Grubisic grubisic@chem.bg.ac.rs	Serbia
3	Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale	191	Dr Alessandro Fortunelli alessandro.fortunelli@cnr.it	Italy
4	Helium Nanodroplets in Science and Engineering	68	Prof Marcel Mudrich mudrich@phys.au.dk	Denmark
5	Confined Systems in Astrochemistry: Gas- and Condensed-Phase Spectroscopy and Reactivity	140	Prof Lauri Halonen lauri.halonen@helsinki.fi	Finland

Other key leadership positions

Position	Name	Contact details	Country*
Science Communication Coordinator	Dr Michael Gatchell	gatchell@fysik.su.se	Sweden
GH Scientific Representative	Juan Carlos Hernandez-Garrido	jcarlos.hernandez@uca.es	Spain

* The country displayed is:

- for the Action Chair, the country that nominated that person to the Management Committee before they were elected Action Chair;
- for the Action Vice-Chair the country that nominated the person as a Management Committee Member,
- for all other leadership positions, if the person is a MC Member the country displayed is the country of nomination, otherwise it is the country of the person's primary work affiliation.

Participants

COST members having accepted the MoU

AL	22/06/2022	AM	09/01/2023	AT	22/06/2022	BE	22/06/2022	BA	22/06/2022
BG	22/06/2022	HR	22/06/2022	CY	22/06/2022	CZ	22/06/2022	DK	22/06/2022
EE	22/06/2022	FI	22/06/2022	FR	22/06/2022	GE	22/06/2022	DE	22/06/2022
EL	22/06/2022	HU	22/06/2022	IS	22/06/2022	IE	22/06/2022	IL	22/06/2022
IT	22/06/2022	LV	22/06/2022	LT	22/06/2022	LU	22/06/2022	MT	22/06/2022
MD	22/06/2022	ME	22/06/2022	NL	22/06/2022	MK	22/06/2022	NO	22/06/2022
PL	22/06/2022	PT	22/06/2022	RO	22/06/2022	RS	22/06/2022	SK	22/06/2022
SI	22/06/2022	ZA	22/06/2022	ES	22/06/2022	SE	22/06/2022	CH	22/06/2022
TR	22/06/2022	UA	22/06/2022	UK	22/06/2022				

Other participants

Institution Name	Country
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Summary

The main aim and objective of the Action is to

provide a platform for coordinated efforts among different communities in Europe to redefine the state of the art on confined molecular systems and transfer the new generated knowledge to a sustainable industrial development and to the field of Astrochemistry

During its first two years the Action progressed the achievement of this as described below

The proposers of the COST Action "COSY" have undoubtedly created a leading research and training network focused on confined molecular systems across Europe and beyond, which is composed of over 360 members from over 44 countries. This effort has been carried out through the right combination of cutting-edge basic science and perspectives for real applications to the benefit of the European community. Within our network, the concept of confinement has certainly grown further beyond spatial cage-like confinement and/or pressure-exerted situations restricting molecules to a finite volume. The COST network has cooperatively addressed a broad range of confining environmental conditions, from those relevant in nanomaterials research to those occurring in the interstellar medium, and jointly developed and/or applied a rich variety of experimental and theoretical-computational tools, including progresses on new methods development, clearly surpassing the state-of-the-art, and machine-learned representations. The research achievements have led to over 160 scientific publications on topics of the five Working Groups (WGs) of the COST Action. The clear objectives for each WG have been targeted in a total of fourteen deliverables. Much better than expected the goals in nine deliverables have been achieved, with clear progress on the remaining five deliverables. As expected for the outcomes from a highly creativity and enthusiastic community, our research accomplishments have gone beyond the original deliverables. As a result, five out of six research coordination objectives have been achieved to 76-100%. Similarly, six out of eight capacity building objectives are considered to have been reached to 76-100%. The latter has reflected our commitment to raising the excellence of network research on confined molecular systems with inclusiveness as a catalyst. A variety of measurements such as the celebration of training schools and meetings providing hands-on science communication skills, have allowed that the difficulties due to imbalances in the network of proposers, especially in the proportion of early career researchers (6%), have been successfully overcome. At present, 40% of the WG members are young researchers, having taken 34% of the leadership positions of our COST Action. By enhancing our efforts aimed at a more inclusive scientific community, our COST Action is expanding opportunities for ITC researchers, ensuring that geography or funding limitations do not impede their participation. Thus, the percentage of members from ITCs has increased from 27% in the original proposal to over 40%. Thus, over 54% young researchers from ITCs were supported for transnational mobility through short-term-scientific missions in the second grant period. Moreover, to increase the proportion of female researchers (34% in the proposal), the FemCOSY group has been created, led by a female young researcher from an ITC, with a 48% of the leadership positions having been taken by female researchers. Now the focus is on engaging Small and Medium-sized Enterprises (SMEs) and building academia-industry connections in (sub)nanotechnology (NANOGAP, Hysun, TheNextPangea) and artificial intelligence (Pending AI). Early Career Investigators are creating their own start-ups (nanoKAT), based on methods developed within COSY. To coordinate the SME sector efficiently in upcoming grant periods, the position of SME co-Coordinator is re-opened.

Action website

<https://cost-cosy.eu>

Achievement of MoU objectives, deliverables and additional outputs/ achievements

MoU objectives

The Action reported the following progress in achieving its specific objectives.

MoU objective	Level of progress	Further information (hyperlink or other)
Joint strategy to combine ab initio methods with DFT and ML for describing molecule-environment interactions; integration of multi-scale embedding; extension of selected methods to describe open-shell and highly polarizable systems, charge transfer and excited states; generation of the COSY-INTER dataset; development of training opportunities on composite methods for COSY.	76 - 100%	Understanding the nature of the interaction between atoms/molecules/clusters with their inorganic materials support at the molecular-level is essential. Second-order Møller-Plesset perturbation theory (MP2) is one of the most cost-efficient single-reference (ab initio) post-Hartree-Fock wave-function-based theories that can be applied to these interactions considering adequate molecular models of the support, and thus complementing state-of-the-art dispersion-corrected density functional theory (DFT). However, the resulting cluster-support interaction is typically overestimated with the MP2 method and must be corrected. Within the framework of Working Group 1 (WG1), the coupled MP2 (MP2C) scheme, replacing the uncoupled Hartree-Fock dispersion energy by a coupled dispersion contribution, has proven to describe accurately van-der-Waals (vdW)-dominated interactions between closed-shell atoms/molecules/clusters and carbon-based supports. Within a joint Spain-Poland collaboration, the accuracy of a MP2C-based scheme has been evaluated in modelling open-shell cluster-support interactions that imply charge transfer or other strong attractive energy contributions beyond vdW forces. For this purpose, the interaction of Cu₃ with molecular models of graphene of increasing size (benzene and coronene) has been considered, achieving sub-chemical precision (within 0.1 kcal/mol). The proposed "COSY" open-shell MP2C-based approach is expected to be of general applicability to open-shell atoms, molecules, and clusters interacting with polycyclic aromatic hydrocarbons (PAHs) for regions of the potential landscapes where single-reference electronic structure descriptions suffice (DOI: 10.1039/D4RA05401F). This approach has been extended to excited states, allowing to determine the parameters of an inter-atomic potential model applicable in molecular dynamics (MD) simulations on the nanoseconds scale, and thus contributing to the COSY-INTER dataset. Other methodological developments of WG1 include the creation of a new non-perturbative approach for calculating interaction energies (temporarily named the non-orthogonal Pauli Blockade approach) within the framework of a UK-Poland collaboration. This method captures induction energy to infinite order and generates 'interaction-dressed' orbitals. Additional WG1 developments within Symmetry Adapted Perturbation Theory (SAPT) encompass the application of perturbation theory for interaction-induced properties such as dipole moment surfaces interaction-driven density changes. Moreover, within a China-Poland collaboration, the newly developed multi-configurational SAPT method has been applied to study complexes of a model chromophore in excited states with small molecules, allowing to investigate in detail changes in the inter-molecular interactions upon electronic excitation. Within WG1, additional efforts addressed the improvement of inexpensive semi-empirical methods for non-covalent interactions, utilizing Artificial Intelligence extensively. Within a Poland-France-US-UK-Spain collaboration, the use of Machine Learning has been enhanced for automatic potential generation, developing a family of potentials through the so-named autoPES protocol. These potentials, crucial to astrochemistry, mainly focus on molecular collisions such as those between benzonitrile, H₂Cl⁺, and fragments of carbon chains, with H₂. They have been applied to calculate collision rates for astrochemically relevant systems. Furthermore, studies on molecular dynamics in cometary comae have been initiated, which require more complex potentials, particularly for the interactions between simple molecules (like HCN) and water or CO, to better understand the leading processes in such environments (DOI: 10.1063/5.0173751). Between the activities of WG1, the organization of the meeting "Spectroscopic and Collision Phenomena in Atmospheric Photochemistry, Astrochemistry, and Planetary Sciences" along with Working

		Group 5 stands by.
Development of a common methodology for investigating molecular motion in confined structures; combining multiscale Molecular Dynamics, Monte Carlo treatments and experimental-computational protocols to create new open-access codes for macroscopic studies of confinement effects; generation of the COSY-DYN dataset.	76 - 100%	An in silico method has been proposed to design a new metal-organic framework (MOF), named ZTF (for the zinc triazolate-based framework), exhibiting good adsorption properties for CO₂ capture. Within a Serbia-France-Tunisia collaboration framed in Working Group 2 (WG2) of the COST Action, in the search for new alternatives for the capture of SO₂ and H₂S pollutants, an accurate force field-based approach has been developed for simulations of the adsorption properties of sulfur gases (SO₂ and H₂S) in newly designed ZTF metal organic frameworks (DOI: 10.1039/D2CP04295A), with the article having been featured as the cover of the journal Physical Chemistry Chemical Physics. By carrying out Grand-Canonical Monte Carlo (GCMC) simulations, it has been demonstrated that the recently designed ZTF MOF composed of triazolate as the organic ligand and Zn(II) as the metal linker, as well as MAF-66, exhibits excellent SO₂ and H₂S adsorption capacities at different gas pressures, in agreement with experimental findings. According to the diverse analyses performed, this sequestration is associated with several types of interactions occurring between gas – nanomaterials pores, indicating that sulfur gases are physisorbed rather than chemisorbed avoiding irreversible structural modifications of MOFs and possible drawbacks for recycling these nanomaterials and their subsequent industrial uses. Molecular simulations reveal that these effects are crucial in modulating the selective sequestration of gases. This activity is associated with the creation of open-access data for microscopic studies of confinement effects (COSY-DYN). Further developments are on the way as a joint effort of research groups from Serbia, France, Tunisia and Estonia. In the quest of stabilizing atomically precise metal clusters of sub-nanometer size, within a South Africa-Spain collaboration, ab initio molecular dynamics (AIMD) simulations have been carried out (see DOI: 10.1039/D2CP05843J). The AIMD simulations performed at 400 K illustrated how the intrinsic defects of graphene sheets, carbon vacancies, are capable of sticking individual Cu₅ clusters. Furthermore, the AIMD simulations showed the dimerization of Cu₅ clusters on defect-free graphene, in agreement with high-level ab initio predictions on unsupported clusters (DOI: 10.1039/D2CP03537E). These findings have demonstrated the potential of using graphene-based substrates as an effective platform to stabilize metal clusters of subnanometer size. The study also showed the usefulness of AIMD to provide information on the dynamic behavior and reactivity at the atomic level of confined metal clusters, allowing the understanding of catalytic processes and time-dependent properties. To accelerate them, GPU, machine-learning (ML) accelerators and ab initio-based interatomic potentials (DOI: 10.1039/D4RA05401F) are being developed, contributing to the COSY-DYN dataset. A Training School was organized in Belgrade (Serbia) about current modeling/computational methods and their applications to treat interaction and dynamics of molecular systems either isolated or in confined environments (see book of abstracts at https://cost-cosy.eu/activity/training-school), attracting a large number of young EU scientists. In addition, the first virtual WG2 meeting was organized to gather leading experts in the field of molecular dynamics and electronic spectroscopy. Presentations by young researchers have been encouraged, as well as those addressed specifically Action Goals of the 2nd Grant Period (see book of abstracts at https://cost-cosy.eu/activity/from-quantum-to-classical-dynamics-of-isolated-molecules-and-3d-materials).
Joint strategies to integrate synthesis and theoretical-experimental characterizations of stability, chemical reactivity, diffusion, alloying, magnetic and optoelectronic properties of novel	76 - 100%	Working Group 3 (WG3) researchers have significantly contributed to understanding the structure and behavior of subnanometric metal and metal-oxide clusters. For example, a notable body of work focuses on uniquely stable Cu₅ clusters, their structural fluxionality, and behavior under chemical environments and heat. Remarkably, a Spain-Argentina-France-Italy-Austria collaboration found that Cu₅ clusters undergo reversible oxidation by molecular oxygen, a property, different from bulk Cu material (DOI: 10.1002/chem.202301517). The evidence of the air-stability of Cu₅ clusters opened the door for applications in energy and environmental technologies, such as in visible light photocatalysis. A special issue was published in Physical Chemistry Chemical Physics of the Royal Society of Chemistry (RSC) dedicated

nanomaterials; dataset collection with industrial partners in COSY-NANO; dissemination of the research results to public and stakeholder outreach.		to subnanometric metal clusters (DOI: 10.1039/D3CP90063K) and the Action Chair published a Perspective presenting an outlook for their future research (DOI: 10.1002/ssr.202400147). Nanosized oxide clusters exhibit properties different from bulk due to quantum confinement (QC). QC effects in $(\text{ZnO})_n(\text{H}_2\text{O})_4$ (DOI: 10.1007/s00894-023-05641-1) and $(\text{TiO}_2)_n$ clusters (DOI: 10.1039/D3NR06189B) were studied computationally regarding their structural, electronic and optical properties, which can be tuned by varying the cluster size. Small Aun clusters capped by protecting thiolate ligands with well-defined stoichiometry and chemical structure (DOI: 10.1021/acs.jpcllett.2c03923, 10.1039/D4CP00789A) represent an important class of nanomaterials for both fundamental studies and potential applications. Several studies addressed their optical properties, including the synthesis and circular dichroism of intrinsic chiral clusters within an Austria-Finland-USA-Switzerland collaboration (DOI: 10.1021/acs.nano.3c06568). An efficient polTDDFT approach allowed to calculate their optical properties with high accuracy (DOI: 10.1021/acs.jpca.3c05368), having been applied to plasmonic Ag nanoparticles under oxidizing conditions (DOI: 10.1021/acs.jpca.3c05801). The dynamic behavior of CeO₂-supported doped Au₂₅(SR)₁₈ clusters was studied in the water-gas-shift reaction (DOI: 10.1038/s42004-023-01068-0). Many WG3 researchers focused their work on larger nanoparticles or other nanostructures relevant to catalysis (including photo and electrocatalysis). We highlight collaborative works such as cyclohexane oxidative dehydrogenation on graphene-oxide-supported CoFe₂O₄ nanohybrids (Czech Republic-France-Switzerland-Italy, DOI: 10.1021/acscatal.3c02592), low-temperature CO oxidation on Pt/CeO₂ catalysts (Spain-Russia-Czech Republic, DOI: 10.1016/j.jcat.2023.03.004), and dehydrogenative coupling of organosilanes with alcohols on single-atom Au catalysts (Czech Republic-France-Italy-India, DOI: 10.1021/acscatal.3c03937). Other studies include CO₂ reduction by plasmonic photocatalysis (DOI: 10.1021/jacs.3c12470), oxygen reduction reaction by CoOx@Pt (DOI: 10.1038/s41929-024-01180-x) or Zr-doped PtNi nanoparticles (DOI: 10.1063/5.0193848), H₂O₂ photoproduction by carbon dots (DOI: 10.1002/sml.202206587). These works have provided a deeper understanding of catalytic mechanisms and relevant properties, such as nanoparticle-support interactions, the dynamic nature of active sites, charge separation upon photoexcitation, and interactions with adsorbates. Some of the nanoparticle-based systems developed are directly relevant to applications, such as highly stable self-cleaning paints (DOI: 10.1021/acscatal.3c06203), sensors (10.1002/adom.202300750, 10.1016/j.sbsr.2024.100629) and thermoelectric applications (10.1002/adfm.202409216). All the organized WG3 events significantly enhanced the knowledge-exchange, interactions, and collaborations within and outside the Action. The second WG3 online meeting (https://cost-cosy.eu/activity/second-virtual-meeting-of-the-cosy-wg3/) was celebrated on 27 November 2023, achieving good gender and age statistics and strategic discussions. A satellite of the CSI-2024 conference was celebrated on April 10 2024 (https://cost-cosy.eu/activity/cosy-satellite-of-the-clustersurface-interaction-meeting) to strengthen the collaboration with the cluster-surface interaction community. Finally, an international CATCOSY2024 Meeting, co-sponsored by the RSC, was organized in Madrid by the Action Chair on 26-27 September 2024 (https://cost-cosy.eu/activity/workshop-facing-challenges).
Exploitation of quantum fluid properties of helium droplets for technological applications; promoting Europe toward a leadership position in the field; coordinated efforts	76 - 100%	Working Group 4 (WG4) has achieved significant progresses in investigating the quantum fluid properties of helium nanodroplets (HNDs), aiming to utilize them for synthesizing high-purity materials with precise control over size and composition. These materials are promising for applications in nano-catalysis, energy conversion, nano-photonics, nano-plasmonics, and bio-medical fields, particularly in radiotherapies. Collaborations between Austria and Spain have resulted in development of a novel method to aggregate atoms and molecules around multiple charges created in large HNDs (10-100 nm radius) through electron bombardment. This innovation has enabled the production of monodisperse samples of metallic and heterogeneous nanoclusters, including stable dicationic clusters and aggregates not achievable by conventional methods. Specifically,

to synthesize and characterize technologically relevant prototypes of high-purity materials, well controlled in terms of size and composition, for efficient production; integration in the COSY-NANO dataset.		cationic copper clusters, alongside clusters decorated with hydrogen, sodium, and carbon dioxide, were produced and characterized within HNDs to evaluate their nano-catalytic properties under highly controlled conditions (DOIs: 10.1039/D3CP03452F, 10.1016/j.ijhydene.2024.07.425, 10.1039/D4CP01797H). WG4 has contributed to understanding Jahn-Teller distortions in atomically precise metal clusters. A collaboration between Spain and France demonstrated that bipyramidal Cu₅ clusters exhibit Jahn-Teller fluxionality, providing a methodological protocol for studying pentamer metal clusters with conical intersections (10.1002/cphc.202300317). This work was recognized with a front cover feature (DOI: 10.1002/cphc.202300638). Studies on ion solvation dynamics in HNDs further enhanced our understanding of HND dynamics and ionization processes, which are crucial for developing tailored nanomaterials (DOI: 10.1063/5.0205951). Within a Germany-Austria collaboration, the charged-HND technique was used to spectroscopically investigate astrophysically relevant fullerene anions (DOI: 10.1103/PhysRevResearch.6.L012045). Theoretical studies have shown that superfluid HND motion facilitates the soft-landing of both neutral and charged metal atoms on zero-temperature graphene, highlighting how high-density quantum fluctuations can brake charged species during surface deposition (DOI: 10.1039/D3CP01303K). An Austria-Croatia collaboration introduced diamondoid ethers into HNDs, demonstrating their self-assembly driven by London dispersion forces (DOIs: 10.1039/D3CP00489A, 10.1039/D3CP02367B). WG4 has also focused on electronically excited and ionized HNDs, particularly studying resonant interatomic Coulombic decay (ICD) phenomena. Collaborations among Denmark, India, Italy, and Germany explored ICD processes in large He droplets, crucial for understanding energy transfer reactions in quantum environments (DOIs: 10.1103/PhysRevLett.131.023001, 10.1103/PhysRevResearch.6.013019). Studies on double excitation-induced ICD in HNDs have offered new insights into ultrafast electronic interactions in weakly bound confined systems (DOI: 10.1103/PhysRevLett.132.233001). Additionally, research into the fragmentation of water clusters and nano-hydrated biomolecules through charge transfer and Penning ionization in doped HNDs is relevant for catalysis and nanostructure formation in biological systems (DOIs: 10.1063/5.0194098, 10.1039/D3CP02879H). To expand this research, progress has been made in developing ultrafast light sources, particularly bright, continuously tunable vacuum ultraviolet (VUV) femtosecond pulses for ultrafast spectroscopy (DOI: 10.1038/s42005-024-01226-1). This tool enables real-time observation of dynamic processes in the VUV spectral region, advancing time-resolved spectroscopy of HNDs. Reconstructing kinetic energy distributions from time-of-flight mass spectra (10.1063/5.0150934) have also improved the analysis of ionization and fragmentation dynamics. Theoretical studies have focused on quantized vortex nucleation, filament, and jet formation in superfluid HNDs (10.1063/5.0165820, 10.1103/PhysRevA.107.063312, 10.1063/5.0143399), impacting the aggregation processes of new materials in superfluid environments. WG4 also organized a training school targeting young researchers on quantum fluid clusters, particularly HNDs https://www.trainingschool.cost-cosy.eu/, preceding the Quantum Fluid Clusters international conference https://conferences.au.dk/qfc2024, organized by the WG4 leader.
Joint strategy for bio-metal first-principles characterizations and experiments on metal nanoclusters interacting with biologically relevant molecules; common methodology on the integration of solvent effects, charge transfer, and transport through the metal-	51 - 75%	The first step in studying the intermolecular interactions between open-shell metal clusters and aromatic systems has been completed, including the development of a theoretical and practical framework for their characterization, as well as pairwise potentials that form the basis for creating force fields (DOI: 10.1039/D4RA05401F). These force fields are essential for molecular dynamics simulations, which are often used to explore large-scale biological systems on long timescales. This research lays the groundwork for investigating more complex biological interactions, such as those involving the aromatic systems in DNA's nitrogenous bases and certain amino acids, the building blocks of proteins. Additionally, studies on the photoactivation and optical properties of metal clusters (DOIs: 10.1016/j.jcis.2021.12.186, 10.1002/ssr.202400147) have revealed their importance not only in understanding catalytic processes but also in potential cancer treatments, particularly in photodynamic therapy. By using light-activated metal clusters to selectively target cancer cells, this work could play a role in developing novel cancer therapies. As a starting point, the effect of an aromatic system in the conical intersections featured by Jahn-Teller fluxional metal clusters has been addressed by applying and further enhancing multi-state

bio contact; identification of quantum effects in the contact; integration in the COSY-NANO dataset.		multireference ab initio theory (DOI: 10.1039/D4CP03271C). Besides demonstrating that the identity of an isolated Jahn-Teller metal cluster can be preserved against complexation with an aromatic system at a physisorption state and lifted out at a chemisorption state, the results indicated that a correlation exists between conical intersection topography and fluxionality in the metal cluster's atom-atom motifs as well as the possibility of a photo-induced boosting of structural fluxionality and photo-reactivity. This study is also important for bioapplications due to its influence on photochemical and catalytic processes. Conical intersections play a key role in tuning the electronic properties of metal clusters, which impacts photostability, enzyme-mimetic catalysis, and oxidative stress responses in biomolecules. Understanding these effects is essential for optimizing catalytic efficiency, developing light-activated drugs, and enhancing photodynamic therapy. Additionally, investigating how support interactions affect conical intersections helps control energy dissipation in biomolecules, offering potential for advancements in bioelectronic devices, biosensors, and bio-inspired materials. The 2nd Scientific Workshop for Students "Computational Physics of DNA" in Kyiv, Ukraine was organized within the COSY network to train early career investigators in biosimulations. The results of this event were published in the Biophysical Bulletin (https://periodicals.karazin.ua/biophysvisnyk/article/view/24324/22044). This workshop not only provided essential training but also contributed to the creation of a joint strategy for advancing bio-metal simulations, focusing on the integration of solvent effects, charge transfer, and quantum phenomena.
Creation of a platform for identification of confined molecular systems relevant to astrochemistry; development of common experimental and computational tools for the characterization of interstellar chemistry; accomplishment evaluation of experimental and computational tools; performance assessment of helium-droplet mediated spectroscopy for astrochemistry; development of the COSY-ASTRO dataset; dissemination of research results.	76 - 100%	During the 1st Grant Period (GP), Working Group 5 (WG5) achieved significant results, including studying quantum delocalization and its rovibrational fingerprints in van der Waals complexes through a Hungary-Germany collaboration (DOI: 10.1002/anie.202306744). WG5 developed a general method for producing and investigating unstable/reactive species, determining accurate spectroscopic parameters used to create precise line catalogs for astronomical searches (DOI: 10.1039/d3fd00052d). A collaboration between Poland and Finland focused on low-temperature molecular aggregation and nucleation processes related to atmospheric and astrochemistry (DOI: 10.3390/molecules28031430), while a Tunisia-Spain collaboration explored photodissociation of species that affect chemical processes in the atmosphere (DOI: 10.1039/d3cp01460f). In the 2nd GP, WG5 concentrated on characterizing molecular systems and their dynamics in astrophysical environments, setting up tools and strategies for these investigations (DOI: 10.3389/fspas.2023.1211784). They contributed to astrochemical database collection (DOIs: 10.3847/1538-4357/ad5007, 10.3847/1538-4357/ad11dd) and explored radiative and collisional processes in interstellar molecular clouds. Results included automated learning models for spectroscopic characterization (DOI: 10.1016/j.aichem.2024.100059) and multidimensional potential energy surfaces applied to molecular collisions at ISM temperatures and high-energy plasma environments. Noteworthy studies involved propargyl cation collisions with helium (DOI: 10.1093/mnras/stae1824), electron-BeH⁺ collisions for fusion plasma modeling (DOI: 10.1039/d4cp01736f), PO⁺ excitation by para-H₂ (DOI: 10.1093/mnras/stad3140), and PAH molecules forming hydrogenated fullerenes in circumstellar environments (DOI: 10.1039/D4CP01147C). New data for cyclopentadiene excitation by helium impacts enabled improved interpretations of astronomical detections of large cyclic species (DOI: 10.1039/D4CP01380H). Short-term scientific missions (STSMs) produced new collisional data for cyclic molecules in the ISM, dissociative recombination in H₂⁺/HD⁺ systems, and machine learning PES for MgC₂-H₂ collisions. Czechia-France collaborations focused on acetonitrile fragmentation, Italy-France explored PAH reactions, and Turkey-France studied NO⁺ + H₂ collisions. AColnode, a versatile database for excitation, ionization, and recombination data, was created. Thermochemical and kinetic calculations offered insights into PO formation (DOI: 10.3847/1538-4357/ad1ffa) and CH₂SO isomers (DOI: 10.1093/mnras/stad2253), alongside studies of reactions between methanimine and small radicals (10.3847/1538-4357/ad11dd). Photodecomposition processes of CH₂Br (DOI:

		10.1063/5.0187546) and acetaldehyde (DOI: 10.1063/5.0207362) were explored, while new reactivity studies include glycolamide formation in icy mantles via STSMs. Spectroscopic characterization during the 2nd GP involved collaborations on high-resolution spectra of species relevant to Earth-like exoplanets, with new transitions for $^{13}\text{C}^{16}\text{O}_2$ (DOI: 10.1002/jcc.27266), $^{16}\text{O}^{12}\text{C}^{18}\text{O}$ (DOI: 10.1002/jcc.27453), and N_2O (DOI: 10.1016/j.jqsrt.2024.108902). Additionally, high-resolution ro-vibrational lines were reported for molecular complexes such as $(\text{HF})_2$ (DOI: 10.1080/00268976.2024.2341106), including highly-excited vibrational states (DOI: 10.1002/ijch.202300092). Focusing on the ISM, rotational spectroscopy measurements enabled characterizations of deuterated (DOI: 10.1021/acs.jpca.4c02533) and hetero-aromatic species (DOI: 10.1039/d3cp03984f), as well as ions (DOI: 10.3847/1538-4357/ad5007). WG5 studies extended molecular collision data to new species, contributed to the COSY-ASTRO datasets, and worked on the IUPAC definition of physicochemical quantities (10.1039/9781839163180). They explored PAH complexes' contributions to diffuse interstellar bands, revealing vibrational distortions in PAH systems (10.1039/D4CP03271C). Efforts also focused on detecting organic molecules in Martian soil (10.1038/s41598-024-66669-8, 10.1089/ast.2023.0088), identifying cyano-astroCOMs (10.3389/fchem.2024.1439194), and predicting spectral data for carbamic acid dimers in $\text{NH}_3\text{-CO}_2$ ices (10.1002/jcc.27442). Concerning the dissemination of research results, besides the presentations at the conferences attended by WG5 members, a position paper is in preparation. A joint WG1-WG5 meeting was held in Poland (https://cost-cosy.eu/activity/spectroscopic-and-collision-phenomena-in-atmospheric-photochemistry-astrochemistry-and-planetary-sciences/).
Creation of a leading research and training network in Europe that is uniquely focused on confined molecular systems.	76 - 100%	The proposers of the COST Action "COSY" have undoubtedly created a leading research and training network focused on confined molecular systems in Europe, which is composed of over 370 members from 45 countries. This effort has been carried out through the right combination between cutting basic science and perspectives for real applications to the benefit of the community. Within the network, our concept of confinement has certainly grown further beyond spatial cage-like confinement and/or pressure-exerted situations restricting molecules to a finite volume. The COST network has cooperatively addressed a broad range of confining environmental conditions, from those relevant in nanomaterials research to those occurring in the interstellar medium. The research achievements have led to over 160 scientific publications of the five Working Groups (WGs) of the COST Action. Thus, efforts within a Spain-Poland collaboration in WG1 have resulted into the development of new approaches for the interaction between a molecule and its confinement environment, reaching sub-chemical accuracy (DOI: 10.1039/D4RA05401F). Within a WG2 Serbia-France-Tunisia collaboration, Metal-Organic Frameworks (MOF) have been uniquely designed for capturing and sequestering pollutants and toxic gases through molecular dynamics simulations (DOI: 10.1039/D2CP04295A). Remarkably, a Spain-Argentina-France-Italy-Austria WG3 collaboration found that the smallest copper clusters undergo reversible oxidation by molecular oxygen (DOI: 10.1002/chem.202301517), opening the door for applications in energy and environmental technologies. COSY members from Spain, Italy, Czech Republic and Croatia have acted as guest editors of a Royal Society of Chemistry special collection dedicated to subnanometric metal clusters (DOI: 10.1039/D3CP90063K), followed up with a Perspective on their future research (DOI: 10.1002/ssr.202400147). A joint Czech Republic-Denmark-Germany effort within WG4 resulted into the development of a new tunable vacuum ultraviolet source for ultrafast spectroscopy (DOI: 10.1038/s42005-023-01513), assessing the tunability in an experiment probing the interatomic Coulombic decay in doped He nanodroplets across the He absorption bands. Within WG5, STSMs (involving mostly young researchers) have contributed to new collisional data for cyclic molecules in the interstellar medium (ISM), dissociative recombinations, and machine-learned potential representations for addressing collisions of astrochemical relevance through collaborations including Czech Republic, France, Italy, and Turkey. As another example of collaborative effort within WG5,

		a Hungary-Germany collaboration made possible to reveal quantum nuclear delocalization effects and their rovibrational fingerprints for van der Waals complexes (DOI: 10.1002/anie.202306744). The training of young researchers on confined molecular systems has been one of the most important goals. Thus, two Training Schools (TSs) have been organized in Belgrade (Serbia) and Prague (Czech Republic), with the earliest TS having uniquely addressing helium nanodroplets. In addition to scientific training, the COSY Action emphasized hands-on activities to improve communication skills. Key events, such as the Listen-to-My-Presentation event (https://cost-cosy.eu/activity/the-1st-listen-to-my-presentation-event), encouraged early-stage participants to present complex topics clearly and effectively, and receive constructive feedback from the Science Communication Team. The “Improve Your Presentation Skills” session, featured in the Second COSY Training School (https://www.trainingschool.cost-cosy.eu/), also provided tailored guidance on refining presentation techniques, boosting confidence, and ensuring clarity. These initiatives empowered early-stage researchers to share their work more effectively within the COSY network and beyond, complementing the scientific achievements.
Providing a unique and urgently needed platform for exchange and collaboration between research groups working on confined molecular systems scattered over many countries and over various scientific areas, including theoretical and experimental groups in the fields of atomic and molecular physics, physical chemistry, biology, material science, and astrochemistry.	76 - 100%	The COSY Action has provided a platform for exchange and collaboration among research groups working on confined molecular systems. Spanning over 370 participants from 45 countries, the Action brought together theoretical and experimental groups in fields such as atomic and molecular physics, physical chemistry, biology, material science, and astrochemistry. By fostering a collaborative environment, the Action enabled significant advancements in the understanding and control of confined molecular systems, with impacts stretching from fundamental science to applications. General and dedicated meetings have been organized with the main purpose of offering a forum for leading research groups on confined molecular systems in Europe. The two General Meetings (see, e.g., https://cost-cosy.eu/activity/the-second-cosy-general-meeting/) served as platforms for knowledge exchange between Working Groups (WG) members and external participants, fostering interdisciplinary collaboration. CATCOSY2024 (https://cost-cosy.eu/activity/workshop-facing-challenges) brought together worldwide experts in both theoretical and experimental metal and metal oxide (photo)catalysis. WG-focused meetings (for the 2nd Grant Period, see, https://cost-cosy.eu/activity/second-virtual-meeting-of-the-cosy-wg3, https://cost-cosy.eu/activity/from-quantum-to-classical-dynamics-of-isolated-molecules-and-3d-materials, https://cost-cosy.eu/activity/spectroscopic-and-collision-phenomena-in-atmospheric-photochemistry-astrochemistry-and-planetary-sciences) allowed for deeper dives into specialized research areas such as intermolecular interactions, theoretical methods development and machine-learning (WG1), molecular motion in confined systems and biosystems (WG2), (sub)nanomaterials science and (photo)catalysis (WG3), (superfluid) helium nanodroplets as confining environments (WG4), and Astrochemistry (WG5). These meetings were crucial for accelerating progress in the field, allowing for real-time discussions and collaborative problem-solving. The combination of theoretical and experimental approaches helped to build a comprehensive understanding of the behavior of molecules in confined environments, which is central to both scientific discovery and practical applications. The First and the Second COSY Training Schools (see, e.g., https://www.trainingschool.cost-cosy.eu) were essential for building capacity among early-career investigators, providing hands-on learning opportunities from both senior and early-stage tutors, as well as soft-skills training. STSMs promoted knowledge exchange across countries, mobility and professional development of early-career investigators (ECIs), while an inclusive approach ensured broad participation, prioritizing scientists from Inclusiveness Target Countries (ITCs). Moreover, collaborations between WG played an important role in the Action's success and was further supported by structured interactions during the meetings, leading to the development of shared datasets (e.g. COSY-INTER-NANO: https://github.com/piotrzuchowski/COSY_Inter_Nano) and methodologies (e.g. https://patents.justia.com/patent/12068147 - patented method for producing

		charged clusters and nanoparticles out of the helium nanodroplets). This interdisciplinary exchange directly contributed to advances in areas such as the synthesis of new nanomaterials, the understanding chemical reactivity under extreme conditions, and the characterization of quantum effects in confined systems and interstellar medium. These results were disseminated widely through high-impact publications (over 160, https://cost-cosy.eu/cosy-papers, https://cost-cosy.eu/articles) and presentations at international conferences. Furthermore, five podcasts (one by each Working Group) will be launched at the end of the 2nd Grant Period to disseminate our results to a general audience.
Promotion of the exchange of knowledge, technical know-how and ideas, as well as establishing long-lasting collaborations between academic and industrial partners.	26 - 50%	Within the FemCOSY initiative we have established contact with Dr Tatiana Lopez, CEO of the company Nanogap & Hysun, which participated to the event, kindly sharing her knowledge and experience through a talk at the 2nd FemCOSY event and subsequent round-table discussion. Representatives from TheNextPangea company attended the CATCOSY2024 meeting, expressing interest in the COSY Action's scientific objectives.
Offering a platform for establishing and exploiting a direct connection to industry, including: high-valued markets in sustainable energy and life science, companies developing software for computational chemistry and physics, and those generating deep knowledge through artificial intelligence and machine learning tools.	51 - 75%	A collaboration was established with the "Pending AI" (a company developing machine learning protocols for life-sciences, working on the world-wide scale with units in Australia, Europe and US) enabling efficient studies of bio-polymers confined architectures (DOI:10.1007/s00214-023-03046-0; DOI:10.1101/2024.07.21.604493). Within a COST Action research group, the nanoKAT project has been proposed to define the groundwork for a new generation of nanoparticle catalysts, offering the potential to make chemical processes more efficient, resource-conserving, and less emissions-intensive. In fact, over 80% of all chemical products are produced using catalysts, forming the basis of our modern standard of living. In order to optimize the current status quo, precise control over nanoparticles' sizes and distributions is necessary. As this requirement is an ongoing challenge in conventional nanoparticle production, a technique has been proposed based on multiply charged helium droplets for the generation of monodisperse nanoparticles. Helium droplets can stabilize several charge centers, which act as nucleation centers for cluster growth when doped with atoms or molecules. As the dopants distribute evenly on these nucleation sides and the ionization probability of the helium droplets, as well as their pick-up probability scale with the droplets' geometric cross-section, nanoparticles with a uniquely narrow size distribution can grow (see "USA - Patent Nr. 12,068,147" in "Other Outputs").
Targeting the problem of research limitations in Inclusiveness Target Countries (ITCs) due to unequal access to funding, knowledge, infrastructure, and resources by prioritizing their participation in all COSY initiatives, including joint proposal preparation in response to high-level European calls, and engaging in dialog with the	76 - 100%	During the 2nd Grant Period (GP), the COSY Network placed significant emphasis on increasing participation and inclusivity, particularly for researchers from Inclusiveness Target Countries (ITCs). Two major events—the 2nd Training School and the 2nd General Meeting—were hosted in ITCs, specifically Czech Republic and Poland. These events were co-organized by early-stage investigators and other researchers from ITCs, highlighting the network's commitment to promoting diverse contributions. Moreover, the 2nd Scientific Workshop for Students "Computational Physics of DNA" was organized in Kyiv, Ukraine. To further expand accessibility, COSY introduced several online meetings, allowing ITC participants to participate without the need for travel funding. This initiative enabled participants to receive training and contribute to COSY's efforts remotely. For example, the meetings of Working Group 2 (WG2) and Working Group 3 (WG3) were held successfully online. During the General Meeting, the Ukraine Management Committee (MC) member was also able to fully participate online, including delivering an invited lecture. The 2nd Training School featured a fully virtual session on intermolecular interactions in helium nanodroplet systems and molecular dynamics, delivered by the AC Team. Additionally, transversal meetings for the Early Career Researchers and Innovators (ECIs), Science Communication, and FemCOSY groups were also held online, reflecting COSY's commitment to inclusivity and accessibility. One of the notable initiatives during this GP was the "Listen-my-presentation" event.

respective national funding agencies.		Designed to help ECIs enhance their scientific presentation skills, this event was largely attended by ECIs from ITC countries. After receiving overwhelmingly positive feedback, plans are underway to repeat this event in the 3rd GP. This approach ensures that COSY events are accessible to a wider range of participants, regardless of funding or travel restrictions. Throughout the Grant Period, ITC-affiliated researchers played an active role in COSY's activities. Whether at the General Meeting or the CATCOSY conference, a significant number of ITC researchers contributed by attending, presenting lectures, presenting their research, and chairing sessions. By continuing these efforts, COSY is expanding opportunities for ITC researchers, fostering a more inclusive scientific community, and ensuring that geography or funding limitations do not impede participation. As a result of all our measurements, the percentage of members from ITCs has been increased from 27% in the original proposal to 43% (according to the draft of the Working and Budget Plan of the 3rd Grant Period).
Promoting efficient use of common resources in COST-member countries by favoring the transnational mobility of young researchers through Short-Term Scientific Missions.	76 - 100%	Transnational mobility and support of scientific training for young researchers through Short-Term Scientific Missions has been in both the First and the Second Grant Period one of the highlights of our Action's achievements. COSY has supported 16 successful STSMs in the 1st GP and over 20 successful STSMs in the 2nd GP, while at the same time taking into consideration general COST inclusiveness policies. Therefore, we supported over 40% young researchers from ITCs and over 30% female researchers in the 1st GP, while increasing both categories to 54% and 43%, respectively, in the 2nd GP. It should also be mentioned that in the 2nd GP we also supported 2 researchers from COST Near Neighbour Countries (NNC). In that way, COSY gave to our junior members an equal and invaluable opportunity for scientific growth and training in state-of-the-art scientific fields, despite their previous possibly less privileged background, with an emphasis on scientific excellence and quality. By providing access to the scientific infrastructure and to the exiting know-how of well-established research groups in COST-member countries to young scientists from ITCs, COSY effectively promoted direct hands-on knowledge transfer and growth development, with a long term goal to facilitate future high level scientific endeavors in those countries. Collaborations formed through such STSM research visits guarantee continued joint research efforts and the pursuit of excellent science in a transnational environment.
Helping Early Career Investigators (ECIs) to promote their careers by entrusting them with positions of responsibility within the Action, like including them as trainers in the organized Training Schools and as Chairs in the organization of focused meetings.	76 - 100%	During the 2nd Grant Period (GP), the involvement of Early Career Investigators (ECIs) in the COSY Network expanded significantly, creating an environment that not only supported their career development but also nurtured leadership skills and fostered collaborations. New leadership positions, such as the Social Media Team and FemCOSY Coordinator, were entrusted fully to ECIs, underscoring the network's commitment to empowering emerging researchers. Additionally, every COSY event included dedicated sections for ECIs to ensure their active participation. In the Working Groups (WGs), as well as the General and CATCOSY Meetings, special sessions were created for short, hot topic or flash poster presentations, allowing ECIs to showcase their work. ECIs were also involved in co-organizing these events and took on responsibilities such as chairing sessions or meetings, for example the Local Organizing Committee (LOC) Chair of the General Meeting in Wroclaw was a ECI female researcher. Similarly, two of the three organizers of the CATCOSY2024 Meeting were young researchers. This involvement not only enhanced their visibility within the network but also honed their organizational skills. The 2nd Training School (TS) was fully focused on providing both scientific and soft-skills training for ECIs, offering a platform for knowledge sharing and networking. A new and valuable aspect of the TS, held in the Czech Republic, was the role ECIs played not only as trainees but also as trainers. By delivering practical tutorials to their peers, ECIs had the opportunity to showcase their expertise and build confidence, while fostering a collaborative atmosphere of mutual growth and scientific exchange. This model, which promotes both collaborative development and professional leadership, will continue in future GPs and is already integrated into upcoming COSY Academy events, where ECIs will participate as both trainers and trainees. The 2nd Scientific Workshop for Students "Computational Physics of DNA" was organized in Ukraine. This workshop not only provided training but also contributed to the creation of a joint strategy for advancing biosimulations. A standout initiative for ECIs was the launch of the "Listen-my-presentation" event,

		developed on an idea from the AC. Fully organized by ECIs for ECIs, the event provided a platform for participants to receive constructive feedback from the Science Communication Team on their presentation skills and tips on how to enhance them. This event was highly successful and will be repeated during the 3rd GP. It serves as an example of how ECIs can take charge of their own development, while benefiting from peer support and expert guidance. In transversal activities, ECIs have also been actively engaged, particularly within the FemCOSY Board. ECIs played a role in organizing events and contributing to the gender balance survey as part of the broader COSY gender study. These experiences not only allowed ECIs to contribute to the network's diversity initiatives but also helped them develop valuable project management and collaborative skills. Moreover, in order to further motivate YRIs involvement in the COST Action, a "COSY Young Scientist Prize" is planned to be delivered in the Final General Meeting in 2026.
Helping under-represented genders to highlight their careers and favoring their access to senior academic positions.	76 - 100%	A focus of the COSY Network has been to promote gender equity, particularly by supporting underrepresented genders in advancing their academic careers. The FemCOSY initiative, launched to address these challenges, has become a vital platform for discussion, collaboration, and action toward achieving gender balance in science. Through a series of meetings and activities, FemCOSY has created a supportive environment aimed at empowering female researchers while fostering a more inclusive research culture. One of the major achievements of FemCOSY has been the steady increase in female participation within the network, as evidenced by a rise in the proportion of female researchers from 33% in the initial group of proposers to 37% by the time of the second FemCOSY meeting. In addition to its success in increasing female participation, FemCOSY is hosting a series of online meetings that engage researchers in meaningful discussions on gender imbalance. These meetings have featured invited lectures from distinguished guests and provided platforms for both male and female researchers to contribute to gender equity initiatives. One of the core activities has been the development of a comprehensive gender imbalance survey, aimed at understanding the factors that contribute to gender disparities within the scientific fields covered by the COST Action. The survey explored a range of factors influencing career choices, including mentorship, peer support, and family encouragement, and divided the analysis by gender and career stage (early-stage vs. experienced researchers). Out of the 90 respondents of the survey, 62% were women and 54% were young researchers. Another key achievement of FemCOSY has been the creation of leadership opportunities for underrepresented genders. By involving female and gender-diverse researchers in organizing meetings, chairing sessions, and leading initiatives such as the survey, FemCOSY has empowered these researchers to take on leadership roles and gain visibility within the scientific community. This active participation has helped build leadership and project management skills, further supporting career advancement. FemCOSY's efforts have also extended beyond the meetings. The initiative has promoted gender equity through the development of online resources, including a dedicated webpage and promotional materials, ensuring that the discussions and outcomes reach a broad audience. Additionally, plans are underway to publish the findings of the gender imbalance survey in a specialized journal, further contributing to the broader academic discourse on gender equity in science.

Deliverables

The Action reported the following progress with achieving its deliverables

Deliverable	Month deliverable due	Delivery status	Further information (hyperlink or other)
Working Group 1. Creation of new protocols for excited state calculations (M12); Results of test calculations for ground- and excited-states of confined systems (M24); Creation of diverse datasets (M36); Assessment of methods against created datasets (M48).	48	Not delivered, but expected before end of Action	
Working Group 1. Descriptors of systems under confinement (M24); Development of Force-Fields using Machine-Learning (M48); Development of embedding potentials describing confining environments along with Working Group 3 (M36).	48	Not delivered, but expected before end of Action	
Working Group 2. Description of gas adsorption, separation, and storage in MOFs along with Working Group 1 (M24); Optimized encapsulation of different active entities in MOFs along with Working Group 1 (M24); Catalytically active COF materials with pore-incorporated catalysts along with Working Group 3 (M36).	36	Not delivered, but expected before end of Action	
Working Group 2. New protocols to characterize nucleic acids in crowded environments (M36); Quantification of binding specificity between organic compounds and confining environments (M36); Study of metal clusters in biological environments: optical/non-optical properties and charge transfer along with Working Group 3 (M36); Quantum dynamics of molecules under electromagnetic fields (M48).	48	Delivered	https://cost-cosy.eu/wg2-reporting
Working Group 3: Mono- and bi-metallic nanoparticles and clusters with potential applications synthesized and spectroscopically characterized on various supports along with Working Group 4 (M48); Screening of specific electrochemical/photocatalytic reactivity of clusters by experiment and theory along with Working Group 4 (M48).	48	Delivered	https://cost-cosy.eu/wg3-reporting
Working Group 3. Analysis of metal clusters interaction with biologically relevant molecules and involved reactivity (M42); Analysis of diffusion and aggregation of supported size-selected metal clusters along with Working Group 4 (M48).	48	Not delivered, but expected before end of Action	
Working Group 3. Ab initio descriptions of the interaction between open-shell molecules and supported metal clusters along with Working Group 1 (M42).	42	Delivered	https://cost-cosy.eu/wg3-reporting
Working Group 3. Links to SMEs - e.g., datasets and big data analysis by AI and ML	48	Delivered	https://cost-cosy.eu/wg3-reporting

technologies along with Working Groups 1 and 5, and generation of relevant prototypes of new materials for large-scale production along with Working Groups 3 and 4 - (M48).			
Working Group 4. Controlled low-temperature aggregation and substrate-deposition of multicomponent metal nanostructures along with Working Group 3 (M26); Deposition and ex-situ characterization of relevant organo-metallic nanoparticles (M48).	48	Delivered	https://cost-cosy.eu/wg4-reporting
Working Group 4. Spectroscopic characterization of helium droplet-aggregated organic light-harvesting complexes (M48); New routes for enhancing energy conversion using helium droplets (M48).	48	Delivered	https://cost-cosy.eu/wg4-reporting
Working Group 4. Detailed analysis of astrophysically relevant cold reactions using helium droplets along with Working Group 5 (M48) ; Controlled low-temperature formation of cosmic dust nanoparticles (M48).	48	Not delivered, but expected before end of Action	https://cost-cosy.eu/wg4-reporting
Working Group 5. Definition of the computational protocol for grain-chemistry and results along with Working Group 4 (M36); Thermochemical and kinetic database for grain-chemistry along with Working Group 1 (M48); Physical and chemical properties of adsorbed/desorbed molecules on/from interstellar grains (M48).	48	Not delivered, but expected before end of Action	
Working Group 5. Spectroscopic characterization of energetic processes on grains and of different nanoparticles along with Working Group 3 (M48); Definition of the computational protocol for gas-phase chemistry and results along with Working Group 1 (M36).	48	Not delivered, but expected before end of Action	https://cost-cosy.eu/wg5-reporting
Working Group 5. Thermochemical and kinetic database for gas-phase chemistry in the interstellar medium (M48); Spectroscopic characterization of astrochemical molecules and set-up of a database along with Working Group 2 (M48).	48	Delivered	https://cost-cosy.eu/wg5-reporting

Additional outputs/ achievements

The Action reported 100 publications on the topic of the Action, co-authored by at least two Action participants from two countries participating in the Action, and for which the Action networking was necessary.

The Action has also produced the outputs/ achievements described below.

Co-authored Action publications - peer-reviewed

1. [doi:10.1021/acscatal.3c04578](https://doi.org/10.1021/acscatal.3c04578)

Title	Partial Oxidation of Methanol on Gold: How Selectivity Is Steered by Low-Coordinated Sites
Authors	Salma Eltayeb; Lenard L. Carroll; Lukas Dippel ; Mersad Mostaghimi; Wiebke Riedel ; Lyudmila V. Moskaleva ; Thomas Risse
DOI	doi:10.1021/acscatal.3c04578
Type	Journal article
Published in	ACS Catalysis
Published by	American Chemical Society (ACS)
ISSNs	2155-5435 ; 2155-5435
Link	https://pubs.acs.org/doi/pdf/10.1021/acscatal.3c04578

2. [doi:10.1021/acscatal.3c02748](https://doi.org/10.1021/acscatal.3c02748)

Title	Impact of the Warhead of Dipeptidyl Keto Michael Acceptors on the Inhibition Mechanism of Cysteine Protease Cathepsin L
Authors	Adrián Fernández-de-la-Pradilla; Santiago Royo ; Tanja Schirmeister; Fabian Barthels; Katarzyna Świderek ; Florenci V. González ; Vicent Moliner
DOI	doi:10.1021/acscatal.3c02748
Type	Journal article
Published in	ACS Catalysis
Published by	American Chemical Society (ACS)
ISSNs	2155-5435 ; 2155-5435
Link	https://pubs.acs.org/doi/pdf/10.1021/acscatal.3c02748

3. [doi:10.1021/acsnano.3c06568](https://doi.org/10.1021/acsnano.3c06568)

Title	Directing Intrinsic Chirality in Gold Nanoclusters: Preferential Formation of Stable Enantiopure Clusters in High Yield and Experimentally Unveiling the “Super” Chirality of Au ₁₄₄
Authors	Vera Truttmann; Adea Loxha; Rareș Banu; Ernst Pittenauer ; Sami Malola; María Francisca Matus ; Yuchen Wang ; Elizabeth A. Ploetz ; Günther Rupprechter ; Thomas Bürgi ; Hannu Häkkinen ; Christine Aikens ; Noelia Barrabés
DOI	doi:10.1021/acsnano.3c06568
Type	Journal article
Published in	ACS Nano
Published by	American Chemical Society (ACS)
ISSNs	1936-0851 ; 1936-086X
Link	https://pubs.acs.org/doi/pdf/10.1021/acsnano.3c06568

4. [doi:10.1021/acscatal.3c02592](https://doi.org/10.1021/acscatal.3c02592)

Title

Cyclohexane Oxidative Dehydrogenation on Graphene-Oxide-Supported Cobalt Ferrite Nanohybrids: Effect of Dynamic Nature of Active Sites on Reaction Selectivity

Authors

[Shashikant A. Kadam](#); Stefania Sandoval; Zdeněk Bastl; Karolína Simkovičová; [Libor Kvítek](#); [Juraj Jašík](#); Joanna Elżbieta Olszówka; Stanislav Valtera; Mykhailo Vaidulych; Jaroslava Morávková; [Petr Sazama](#); [David Kubička](#); [Arnaud Travert](#); [Jeroen A. van Bokhoven](#); [Alessandro Fortunelli](#); [Armin Kleibert](#); [Martin Kalbáč](#); [Štefan Vajda](#)

DOI

[doi:10.1021/acscatal.3c02592](https://doi.org/10.1021/acscatal.3c02592)

Type

Journal article

Published in

ACS Catalysis

Published by

American Chemical Society (ACS)

ISSNs

[2155-5435](#); [2155-5435](#)

Link

<https://pubs.acs.org/doi/pdf/10.1021/acscatal.3c02592>

5. [doi:10.1021/acscatal.3c06203](https://doi.org/10.1021/acscatal.3c06203)

Title

Highly Stable Self-Cleaning Paints Based on Waste-Valorized PNC-Doped TiO₂ Nanoparticles

Authors

[Qaisar Maqbool](#); Orlando Favoni; Thomas Wicht; [Niusha Lasemi](#); Simona Sabbatini; Michael Stöger-Pollach; Maria Letizia Ruella; [Francesca Tittarelli](#); [Günther Rupprechter](#)

DOI

[doi:10.1021/acscatal.3c06203](https://doi.org/10.1021/acscatal.3c06203)

Type

Journal article

Published in

ACS Catalysis

Published by

American Chemical Society (ACS)

ISSNs

[2155-5435](#); [2155-5435](#)

Link

<https://pubs.acs.org/doi/pdf/10.1021/acscatal.3c06203>

6. [doi:10.1021/acscatal.3c03937](https://doi.org/10.1021/acscatal.3c03937)

Title

Linear-Structure Single-Atom Gold(I) Catalyst for Dehydrogenative Coupling of Organosilanes with Alcohols

Authors

Ravishankar G. Kadam; [Miroslav Medved'](#); [Subodh Kumar](#); Dagmar Zaoralová; Giorgio Zoppellaro; Zdeněk Bad'ura; [Tiziano Montini](#); [Aristides Bakandritsos](#); [Emiliano Fonda](#); Ondřej Tomanec; [Michal Otyepka](#); [Rajender S. Varma](#); Manoj B. Gawande; [Paolo Fornasiero](#); [Radek Zbořil](#)

DOI

[doi:10.1021/acscatal.3c03937](https://doi.org/10.1021/acscatal.3c03937)

Type

Journal article

Published in

ACS Catalysis

Published by

American Chemical Society (ACS)

ISSNs

[2155-5435](#); [2155-5435](#)

Link

<https://pubs.acs.org/doi/pdf/10.1021/acscatal.3c03937>

7. [doi:10.1002/adfm.202409216](https://doi.org/10.1002/adfm.202409216)

Title

PbSe Quantum Dot Superlattice Thin Films for Thermoelectric Applications

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| <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Viviana Sousa; Masahiro Goto; Marcel S. Claro; Sergey Pyrlin; Luis Marques; Evgeny B. Modin; Oleg I. Lebedev; Siavash M. Alizadeh; Cátia Freitas; Eliana M. F. Vieira; Kirill Kovnir; Pedro Alpuim; Takao Mori; Yury V. Kolen'ko
doi:10.1002/adfm.202409216</p> <p>Journal article</p> <p>Advanced Functional Materials</p> <p>Wiley</p> <p>1616-301X; 1616-3028
https://onlinelibrary.wiley.com/doi/pdf/10.1002/adfm.202409216</p> |
| <p>8. doi:10.1002/adom.202300750</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Carbon Dots Enabling Parts□Per□Billion Sensitive and Ultraselective Photoluminescence Lifetime□Based Sensing of Inorganic Mercury Lukáš Zdražil; David Panáček; Veronika Šedajová; Zdeněk Baďura; Michal Langer; Miroslav Medved'; Markéta Paloncýová; Magdalena Scheibe; Sergii Kalytchuk; Giorgio Zoppellaro; Štěpán Kment; Alejandro Cadanel; Aristides Bakandritsos; Dirk M. Guldi; Michal Otyepka; Radek Zbořil
doi:10.1002/adom.202300750</p> <p>Journal article</p> <p>Advanced Optical Materials</p> <p>Wiley</p> <p>2195-1071; 2195-1071
https://onlinelibrary.wiley.com/doi/pdf/10.1002/adom.202300750</p> |
| <p>9. doi:10.1002/anie.202306744</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Quantum Nuclear Delocalization and its Rovibrational Fingerprints Irén Simkó; Christoph Schran; Fabien Briec; Csaba Fábrí; Oskar Asvany; Stephan Schlemmer; Dominik Marx; Attila G. Császár
doi:10.1002/anie.202306744</p> <p>Journal article</p> <p>Angewandte Chemie International Edition</p> <p>Wiley</p> <p>1433-7851; 1521-3773
https://onlinelibrary.wiley.com/doi/pdf/10.1002/anie.202306744</p> |
| <p>10. doi:10.1016/j.apsusc.2024.160578</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSN</p> <p>Links</p> | <p>Detailed work function and structural investigations of layered MoO₃ onto SiO₂ and MoS₂ in air Saeed Sovizi; Sergio Tosoni; Tomasz Zdunek; Robert Szoszkiewicz
doi:10.1016/j.apsusc.2024.160578</p> <p>Journal article</p> <p>Applied Surface Science</p> <p>Elsevier BV</p> <p>0169-4332
https://api.elsevier.com/content/article/PII:S01694</p> |

- 33224012911?httpAccept=text/xml;
<https://api.elsevier.com/content/article/PII:S0169433224012911?httpAccept=text/plain>
11. [doi:10.1016/j.aichem.2024.100059](https://doi.org/10.1016/j.aichem.2024.100059)
 Title
 Automated learning data-driven potential models for spectroscopic characterization of astrophysical interest noble gas-containing NgH₂⁺ molecules
 Authors
 María Judit Montes de Oca-Estévez; Rita Prosmi
 DOI
[doi:10.1016/j.aichem.2024.100059](https://doi.org/10.1016/j.aichem.2024.100059)
 Type
 Journal article
 Published in
 Artificial Intelligence Chemistry
 Published by
 Elsevier BV
 ISSN
[2949-7477](https://doi.org/10.1016/j.aichem.2024.100059)
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<https://api.elsevier.com/content/article/PII:S2949747724000174?httpAccept=text/plain>
 12. [doi:10.1002/cphc.202300570](https://doi.org/10.1002/cphc.202300570)
 Title
 Computational Energy Spectra of the H₂O@C₇₀ Endofullerene
 Authors
 Orlando Carrillo-Bohórquez; Álvaro Valdés; Rita Prosmi
 DOI
[doi:10.1002/cphc.202300570](https://doi.org/10.1002/cphc.202300570)
 Type
 Journal article
 Published in
 ChemPhysChem
 Published by
 Wiley
 ISSN
[1439-4235](https://doi.org/10.1002/cphc.202300570); [1439-7641](https://doi.org/10.1002/cphc.202300570)
 13. [doi:10.1002/cphc.202300317](https://doi.org/10.1002/cphc.202300317)
 Title
 High-level *ab initio* evidence of bipyramidal Cu₅ clusters as fluxional Jahn-Teller molecules
 Authors
 Alexander O. Mitrushchenkov; María Pilar de Lara-Castells
 DOI
[doi:10.1002/cphc.202300317](https://doi.org/10.1002/cphc.202300317)
 Type
 Journal article
 Published in
 ChemPhysChem
 Published by
 Wiley
 ISSN
[1439-4235](https://doi.org/10.1002/cphc.202300317); [1439-7641](https://doi.org/10.1002/cphc.202300317)
 14. [doi:10.1016/j.colsurfa.2024.134723](https://doi.org/10.1016/j.colsurfa.2024.134723)
 Title
 Systematic study of chromonic liquid crystal-based complex emulsions and their application in the preparation of silica nanomaterials
 Authors
 Adrià Pérez-Calm; Yury V. Kolen'ko; Laura M. Salonen; Hugo Busson; Jordi Esquena; Carlos Rodríguez-Abreu
 DOI
[doi:10.1016/j.colsurfa.2024.134723](https://doi.org/10.1016/j.colsurfa.2024.134723)
 Type
 Journal article
 Published in
 Colloids and Surfaces A: Physicochemical and Engineering Aspects
 Published by
 Elsevier BV
 ISSN
[0927-7757](https://doi.org/10.1016/j.colsurfa.2024.134723)
 Links
<https://api.elsevier.com/content/article/PII:S092775724015875?httpAccept=text/xml>;
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15. [doi:10.1016/j.colsurfa.2024.133658](https://doi.org/10.1016/j.colsurfa.2024.133658)

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DOI

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Published by

ISSN

Links

Impact of tannic acid on iron oxide nanoclusters synthesized by a polyol solvothermal method

Joana Vaz-Ramos; Théo Lucante; Jean-Marc Greneche; Cédric Leuvrey; [Vasiliki Papaefthymiou](#); Spyridon Zafeiratos; Anne Carton; Dominique Bégin; Stéphane Le Calvé; [Sylvie Bégin-Colin](#)

[doi:10.1016/j.colsurfa.2024.133658](https://doi.org/10.1016/j.colsurfa.2024.133658)

Journal article

Colloids and Surfaces A: Physicochemical and Engineering Aspects

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[0927-7757](#)

<https://api.elsevier.com/content/article/PII:S092775724005193?httpAccept=text/xml>;

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16. [doi:10.1038/s42004-023-01068-0](https://doi.org/10.1038/s42004-023-01068-0)

Title

Authors

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Published by

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Dynamic behaviour of platinum and copper dopants in gold nanoclusters supported on ceria catalysts

Nicole Müller; [Rareş Banu](#); Adea Loxha; [Florian Schrenk](#); Lorenz Lindenthal; Christoph Rameshan; Ernst Pittenauer; [Jordi Llorca](#); Janis Timoshenko; Carlo Marini; [Noelia Barrabés](#)

[doi:10.1038/s42004-023-01068-0](https://doi.org/10.1038/s42004-023-01068-0)

Journal article

Communications Chemistry

Springer Science and Business Media LLC

[2399-3669](#)

<https://www.nature.com/articles/s42004-023-01068-0.pdf>;

<https://www.nature.com/articles/s42004-023-01068-0>

17. [doi:10.1038/s42005-023-01513-5](https://doi.org/10.1038/s42005-023-01513-5)

Title

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Links

Bright continuously tunable vacuum ultraviolet source for ultrafast spectroscopy

[Lucie Jurkovičová](#); Ltaief Ben Ltaief; [Andreas Hult Roos](#); Ondřej Hort; Ondřej Finke; Martin Albrecht; Ziaul Hoque; [Eva Klimešová](#); Akgash Sundaralingam; Roman Antipenkov; Annika Grenfell; Alexandr Špaček; Wojciech Szuba; [Maria Krikunova](#); [Marcel Mudrich](#); [Jaroslav Nejdli](#); [Jakob Andreasson](#)

[doi:10.1038/s42005-023-01513-5](https://doi.org/10.1038/s42005-023-01513-5)

Journal article

Communications Physics

Springer Science and Business Media LLC

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<https://www.nature.com/articles/s42005-023-01513-5.pdf>;

<https://www.nature.com/articles/s42005-023-01513-5>

18. [doi:10.1016/j.comptc.2024.114587](https://doi.org/10.1016/j.comptc.2024.114587)

Title

Isomeric forms of 1,4-dioxane in a microsolvation environment

Authors

Fatime Mine Balci; Nevin Uras-Aytemiz

DOI

[doi:10.1016/j.comptc.2024.114587](https://doi.org/10.1016/j.comptc.2024.114587)

Type

Journal article

Published in

Computational and Theoretical Chemistry

Published by

Elsevier BV

ISSN

[2210-271X](https://doi.org/10.1016/j.comptc.2024.114587)

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19. [doi:10.1016/j.cpc.2024.109210](https://doi.org/10.1016/j.cpc.2024.109210)

Title

ZZPolyCalc: An open-source code with fragment caching for determination of Zhang-Zhang polynomials of carbon nanostructures

Authors

Rafał Podeszwa; Henryk A. Witek; Chien-Pin Chou

DOI

[doi:10.1016/j.cpc.2024.109210](https://doi.org/10.1016/j.cpc.2024.109210)

Type

Journal article

Published in

Computer Physics Communications

Published by

Elsevier BV

ISSN

[0010-4655](https://doi.org/10.1016/j.cpc.2024.109210)

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<https://api.elsevier.com/content/article/PII:S0010465524001334?httpAccept=text/xml>;
<https://api.elsevier.com/content/article/PII:S0010465524001334?httpAccept=text/plain>

20. [doi:10.1039/D4DT00116H](https://doi.org/10.1039/D4DT00116H)

Title

Probing structural and dynamic properties of MAPbCl₃ hybrid perovskite using Mn²⁺ EPR

Authors

Gediminas Usevičius; Justinas Turčak; Yuxuan

Zhang; Andrea Eggeling; Žyginta Einorytė;

Michael Allan Hope; Šarūnas Svirskas; Daniel

Klose; Vidmantas Kalendra; Kestutis Aidas;

Gunnar Jeschke; Jūras Banys; Mantas Šimėnas

[doi:10.1039/D4DT00116H](https://doi.org/10.1039/D4DT00116H)

DOI

Journal article

Type

Dalton Transactions

Published in

Royal Society of Chemistry (RSC)

Published by

[1477-9226](https://doi.org/10.1039/D4DT00116H); [1477-9234](https://doi.org/10.1039/D4DT00116H)

ISSNs

Link

<http://pubs.rsc.org/en/content/articlepdf/2024/DT/D4DT00116H>

21. [doi:10.1039/D4DT00400K](https://doi.org/10.1039/D4DT00400K)

Title

The role of intermolecular interactions in [Fe(X-salEen)₂]ClO₄ spin crossover complexes

Authors

Marcos A. Bento; Tiago Gomes; Frederico F.

Martins; Adrià Gil; Liliana P. Ferreira; Sónia

Barroso; Clara S. B. Gomes; Yann Garcia; Paulo

N. Martinho

[doi:10.1039/D4DT00400K](https://doi.org/10.1039/D4DT00400K)

DOI

Journal article

Type

Dalton Transactions

Published in

Royal Society of Chemistry (RSC)

Published by

[1477-9226](https://doi.org/10.1039/D4DT00400K); [1477-9234](https://doi.org/10.1039/D4DT00400K)

ISSNs

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| Link | http://pubs.rsc.org/en/content/articlepdf/2024/DT/D4DT00400K |
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| 22. doi:10.1051/epn/2022401 | |
| Title | A subnanometric material reveals new quantum-chemical insights into surface polarons |
| Authors | María Pilar de Lara-Castells; Salvador Miret-Artés |
| DOI | doi:10.1051/epn/2022401 |
| Type | Journal article |
| Published in | Europhysics News |
| Published by | EDP Sciences |
| ISSNs | 0531-7479 ; 1432-1092 |
| Link | https://www.europhysicsnews.org/10.1051/epn/2022401/pdf |
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| 23. doi:10.1039/D3FD00052D | |
| Title | Hunting for interstellar molecules: rotational spectra of reactive species |
| Authors | Cristina Puzzarini ; Silvia Alessandrini ; Luca Bizzocchi ; Mattia Melosso |
| DOI | doi:10.1039/D3FD00052D |
| Type | Journal article |
| Published in | Faraday Discussions |
| Published by | Royal Society of Chemistry (RSC) |
| ISSNs | 1359-6640 ; 1364-5498 |
| Link | http://pubs.rsc.org/en/content/articlepdf/2023/FD/D3FD00052D |
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| 24. doi:10.3389/fspas.2023.1128896 | |
| Title | Protonation of apolar species: From Cl ₂ H ⁺ to (E)-NCCHCHCNH ⁺ through computational investigations |
| Authors | Silvia Alessandrini; Luca Bizzocchi; Mattia Melosso; Cristina Puzzarini |
| DOI | doi:10.3389/fspas.2023.1128896 |
| Type | Journal article |
| Published in | Frontiers in Astronomy and Space Sciences |
| Published by | Frontiers Media SA |
| ISSN | 2296-987X |
| Link | https://www.frontiersin.org/articles/10.3389/fspas.2023.1128896/full |
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| 25. doi:10.3389/fspas.2023.1211784 | |
| Title | From the laboratory to the interstellar medium: a strategy to search for exotic molecules in space |
| Authors | Cristina Puzzarini; Silvia Alessandrini; Luca Bizzocchi; Mattia Melosso; Víctor M. Rivilla |
| DOI | doi:10.3389/fspas.2023.1211784 |
| Type | Journal article |
| Published in | Frontiers in Astronomy and Space Sciences |
| Published by | Frontiers Media SA |
| ISSN | 2296-987X |
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| 26. doi:10.3389/fphy.2023.1236987 | |
| Title | Interpretation and prediction of optical properties: novel fluorescent dyes as a test case |

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| <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSN</p> <p>Link</p> | <p>Xinxing Li; Xiuping Yin; Yue-Ling Bai; Malgorzata Biczysko</p> <p>doi:10.3389/fphy.2023.1236987</p> <p>Journal article</p> <p>Frontiers in Physics</p> <p>Frontiers Media SA</p> <p>2296-424X</p> <p>https://www.frontiersin.org/articles/10.3389/fphy.2023.1236987/full</p> |
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| <p>27. doi:10.3389/fchem.2022.983281</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSN</p> <p>Link</p> | <p>MD simulations explain the excess molar enthalpies in pseudo-binary mixtures of a choline chloride-based deep eutectic solvent with water or methanol</p> <p>Leon de Villiers Engelbrecht; Xiaoyan Ji; Carlo Maria Carbonaro; Aatto Laaksonen; Francesca Mocchi</p> <p>doi:10.3389/fchem.2022.983281</p> <p>Journal article</p> <p>Frontiers in Chemistry</p> <p>Frontiers Media SA</p> <p>2296-2646</p> <p>https://www.frontiersin.org/articles/10.3389/fchem.2022.983281/full</p> |
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| <p>28. doi:10.1063/5.0146680</p> <p>Title</p> <p>Author</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Family of Gaussian wavepacket dynamics methods from the perspective of a nonlinear Schrödinger equation</p> <p>Jiří J. L. Vaníček</p> <p>doi:10.1063/5.0146680</p> <p>Journal article</p> <p>The Journal of Chemical Physics</p> <p>AIP Publishing</p> <p>0021-9606; 1089-7690</p> <p>https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/5.0146680/18032127/014114_1_5.0146680.pdf</p> |
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| <p>29. doi:10.1080/07391102.2024.2329307</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Mechanistic insights into interactions between ionizable lipid nanodroplets and biomembranes</p> <p>Petra Čechová; Markéta Paloncýová; Martin Šrejber; Michal Otyepka</p> <p>doi:10.1080/07391102.2024.2329307</p> <p>Journal article</p> <p>Journal of Biomolecular Structure and Dynamics</p> <p>Informa UK Limited</p> <p>0739-1102; 1538-0254</p> <p>https://www.tandfonline.com/doi/pdf/10.1080/07391102.2024.2329307</p> |
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| <p>30. doi:10.1021/acs.jctc.3c00914</p> <p>Title</p> <p>Authors</p> <p>DOI</p> | <p>Unusual Dynamics and Vibrational Fingerprints of van der Waals Dimers Formed by Linear Molecules and Rare-Gas Atoms</p> <p>Roland Tóbiás; Irén Simkó; Attila G. Császár</p> <p>doi:10.1021/acs.jctc.3c00914</p> |
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| Type | Journal article |
| Published in | Journal of Chemical Theory and Computation |
| Published by | American Chemical Society (ACS) |
| ISSNs | 1549-9618 ; 1549-9626 |
| Link | https://pubs.acs.org/doi/pdf/10.1021/acs.jctc.3c00914 |
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31. [doi:10.1016/j.jcis.2024.07.067](https://doi.org/10.1016/j.jcis.2024.07.067)
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| Title | Harnessing photocatalytic activity of mesoporous graphitic carbon nitride decorated by copper single-atom catalysts for oxidative dehydrogenation of N-heterocycles |
| Authors | Rahul P. Gaikwad ; Indrajeet R. Warkad; Dinesh S. Chaudhari; Shan Jiang; Jeffrey T. Miller ; Hien N. Pham; Abhaya Datye ; Manoj B. Gawande |
| DOI | doi:10.1016/j.jcis.2024.07.067 |
| Type | Journal article |
| Published in | Journal of Colloid and Interface Science |
| Published by | Elsevier BV |
| ISSN | 0021-9797 |
| Links | https://api.elsevier.com/content/article/PII:S002197972401573X?httpAccept=text/xml ;
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32. [doi:10.1002/jcc.27110](https://doi.org/10.1002/jcc.27110)
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| Title | Confining CO ₂ inside sl clathrate hydrates: The impact of the CO ₂ –water interaction on quantized dynamics |
| Authors | Álvaro Valdés; Adriana Cabrera-Ramírez; Rita Prosmitti |
| DOI | doi:10.1002/jcc.27110 |
| Type | Journal article |
| Published in | Journal of Computational Chemistry |
| Published by | Wiley |
| ISSNs | 0192-8651 ; 1096-987X |
| Link | https://onlinelibrary.wiley.com/doi/pdf/10.1002/jcc.27110 |
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33. [doi:10.1039/D3TC01419C](https://doi.org/10.1039/D3TC01419C)
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| Title | The role of the degree of polymerization in the chiroptical properties of dynamic asymmetric poly(diphenylacetylene)s |
| Authors | Juan José Tarrío; Berta Fernández ; Emilio Quiñoá ; Félix Freire |
| DOI | doi:10.1039/D3TC01419C |
| Type | Journal article |
| Published in | Journal of Materials Chemistry C |
| Published by | Royal Society of Chemistry (RSC) |
| ISSNs | 2050-7526 ; 2050-7534 |
| Link | http://pubs.rsc.org/en/content/articlepdf/2023/TC/D3TC01419C |
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34. [doi:10.1016/j.jmgm.2023.108562](https://doi.org/10.1016/j.jmgm.2023.108562)
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| Title | Quantum computations in heavy noble-gas hydride cations: Reference energies and new spectroscopic data |
| Authors | María Judit Montes de Oca-Estévez; Rita Prosmitti |

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| <p>DOI
Type
Published in
Published by
ISSN
Links</p> | <p>doi:10.1016/j.jmfm.2023.108562
Journal article
Journal of Molecular Graphics and Modelling
Elsevier BV
1093-3263
https://api.elsevier.com/content/article/PII:S1093326323001602?httpAccept=text/xml;
https://api.elsevier.com/content/article/PII:S1093326323001602?httpAccept=text/plain</p> |
| <p>35. doi:10.1016/j.molliq.2023.122828
Title

Authors

DOI
Type
Published in
Published by
ISSN
Links</p> | <p>Conformational flexibility of spermidine³⁺ interacting with DNA double helix
Sergiy Perepelytsya; Tudor Vasiliu; Aatto Laaksonen; Leon De Villiers Engelbrecht; Giuseppe Brancato; Francesca Mocci
doi:10.1016/j.molliq.2023.122828
Journal article
Journal of Molecular Liquids
Elsevier BV
0167-7322
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https://api.elsevier.com/content/article/PII:S016773223016331?httpAccept=text/plain</p> |
| <p>36. doi:10.1016/j.jms.2023.111834
Title

Authors

DOI
Type
Published in
Published by
ISSN
Links</p> | <p>Joint survey of the experimental high-resolution spectra of H₁₆O₃₇Cl and H₁₆O₃₅Cl with a reanalysis of the 2v₂ band
Gábor Ecseri; Irén Simkó; Tibor Furtenbacher; Balázs Rácsai; Luciano Fusina; Gianfranco Di Lonardo; Kirk A. Peterson; Attila G. Császár
doi:10.1016/j.jms.2023.111834
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B Ardini; F Richter; L Uboldi; P Cinquegrana; M Danailov; A Demidovich; S D Ganeshamandiram; S Hartweg; G Kurdi; F Landmesser; M Michelbach; A Ngai; I Nikolov; N Rendler; F Stienkemeier; D Uhl; L Bruder; G Cerullo; C Manzoni
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<https://iopscience.iop.org/article/10.1088/1361-6455/ad2e2d>;

<https://iopscience.iop.org/article/10.1088/1361-6455/ad2e2d/pdf>

Intra-strand phosphate-mediated pathways in microsolvated double-stranded DNA

[Georgia Polycarpou](#); [Spiros S Skourtis](#)

[doi:10.1088/1361-648X/ad559d](https://doi.org/10.1088/1361-648X/ad559d)

Journal article

Journal of Physics: Condensed Matter

IOP Publishing

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39. [doi:10.1016/j.jqsrt.2023.108644](https://doi.org/10.1016/j.jqsrt.2023.108644)

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Optimization of the femtosecond laser impulse for excitation and the Spin-Orbit mediated dissociation in the NaRb Dimer

J. Kozicki; [P. Jasik](#); T. Kilich; J.E. Sienkiewicz

[doi:10.1016/j.jqsrt.2023.108644](https://doi.org/10.1016/j.jqsrt.2023.108644)

Journal article

Journal of Quantitative Spectroscopy and Radiative Transfer

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40. [doi:10.1021/jacs.3c12470](https://doi.org/10.1021/jacs.3c12470)

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Peeking into the Femtosecond Hot-Carrier Dynamics Reveals Unexpected Mechanisms in Plasmonic Photocatalysis

Giulia Dall'Osto; Margherita Marsili; [Mirko Vanzan](#); [Daniele Toffoli](#); [Mauro Stener](#); [Stefano Corni](#); [Emanuele Coccia](#)

[doi:10.1021/jacs.3c12470](https://doi.org/10.1021/jacs.3c12470)

Journal article

Journal of the American Chemical Society

American Chemical Society (ACS)

[0002-7863; 1520-5126](https://doi.org/10.1021/jacs.3c12470)

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41. [doi:10.1021/jacs.3c06157](https://doi.org/10.1021/jacs.3c06157)

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Mechanistic Basis for Red Light Switching of Azonium Ions

[Miroslav Medved'](#); [Mariangela Di Donato](#); [Wybren Jan Buma](#); [Adèle D. Laurent](#); [Lucien Lameijer](#); Tomáš Hrivnák; Ivan Romanov; Susannah Tran; [Ben L. Feringa](#); [Wiktor Szymanski](#); [G. Andrew Woolley](#)

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Polarons in Two-Dimensional Material under UV
Light Irradiation
Giorgio Zoppellaro; Miroslav Medved ; Vítězslav Hrubý ; Radek Zbořil ; Michal Otyepka ; Petr Lazar
doi:10.1021/jacs.3c13296
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DOI
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spectra of $^{16}\text{O}^{12}\text{C}^{18}\text{O}$
Dunia Alatoom ; Mohammad Taha I. Ibrahim ;
Tibor Furtenbacher ; Attila G. Császár ; M.
Alghizzawi; Sergei N. Yurchenko ; Ala'a A. A. Azzam ; Jonathan Tennyson
doi:10.1002/jcc.27453
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Published in
Published by
ISSNs
Link | MARVEL analysis of high-resolution rovibrational
spectra of $^{13}\text{C}^{16}\text{O}_2$
Mohammad Taha I. Ibrahim; Dunia Alatoom;
Tibor Furtenbacher; Attila G. Császár; Sergei N.
Yurchenko; Ala'a A. A. Azzam; Jonathan
Tennyson
doi:10.1002/jcc.27266
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Authors

DOI
Type | Dichroism of plasmonic chiral nanoalloys by
rational design
Pierpaolo D'Antoni; Daniele Toffoli ; Giovanna
Fronzoni; Mauro Stener ; Luca Sementa ;
Alessandro Fortunelli
doi:10.1002/jcc.27359
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Wiley
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Title

States of Pt/CeO₂ catalysts for CO oxidation below room temperature

Authors

Elena M. Slavinskaya; Andrey I. Stadnichenko; Jon E. Quinlivan Domínguez; Olga A. Stonkus; [Mykhailo Vorokhta](#); [Břetislav Šmíd](#); Pablo Castro-Latorre; [Albert Bruix](#); Konstantin M. Neyman; Andrei I. Boronin

DOI

[doi:10.1016/j.jcat.2023.03.004](#)

Type

Journal article

Published in

Journal of Catalysis

Published by

Elsevier BV

ISSN

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47. [doi:10.1063/10.0024969](#)

Title

Unusual bending patterns of spermidine³⁺ bound to DNA double helix

Authors

[Sergiy Perepelytsya](#); [Tudor Vasiliu](#); [Aatto Laaksonen](#); Leon De Villiers Engelbrecht; [Francesca Mocchi](#)

DOI

[doi:10.1063/10.0024969](#)

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Journal article

Published in

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Published by

AIP Publishing

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[1063-777X](#); [1090-6517](#)

Link

https://pubs.aip.org/aip/ltp/article-pdf/50/3/204/19860562/204_1_10.0024969.pdf

48. [doi:10.3390/ma16062233](#)

Title

Speciation of Hexavalent Chromium in Aqueous Solutions Using a Magnetic Silica-Coated Amino-Modified Glycidyl Methacrylate Polymer Nanocomposite

Authors

[Ljiljana Suručić](#); Goran Janjić; Bojana Marković; [Tamara Tadić](#); Zorica Vuković; [Aleksandra Nastasović](#); [Antonije Onjia](#)

DOI

[doi:10.3390/ma16062233](#)

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Fine Tuning the Intermolecular Interactions of Water Clusters Using the Dispersion-Corrected Density Functional Theory

Authors

[Alfonso Ferretti](#); Laura Canal; Robert A. Sorodoc;

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doi:10.3390/molecules28093834
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https://www.mdpi.com/1420-3049/28/9/3834/pdf</p> |
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Title

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DOI
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Published in
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Link</p> | <p>Toward Accurate yet Effective Computations of Rotational Spectroscopy Parameters for Biomolecule Building Blocks
Vincenzo Barone; Silvia Di Grande; Cristina Puzzarini
doi:10.3390/molecules28020913
Journal article
Molecules
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1420-3049
https://www.mdpi.com/1420-3049/28/2/913/pdf</p> |
| <p>51. doi:10.3390/molecules28031430
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Authors
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Published in
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Link</p> | <p>Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates
Justyna Krupa; Maria Wierzejewska; Jan Lundell
doi:10.3390/molecules28031430
Journal article
Molecules
MDPI AG
1420-3049
https://www.mdpi.com/1420-3049/28/3/1430/pdf</p> |
| <p>52. doi:10.3390/molecules28073226
Title

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DOI
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Published in
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ISSN
Link</p> | <p>Computational Protocol for the Identification of Candidates for Radioastronomical Detection and Its Application to the C₃H₃NO Family of Isomers
Silvia Alessandrini; Mattia Melosso; V́ctor M. Rivilla; Luca Bizzocchi; Cristina Puzzarini
doi:10.3390/molecules28073226
Journal article
Molecules
MDPI AG
1420-3049
https://www.mdpi.com/1420-3049/28/7/3226/pdf</p> |
| <p>53. doi:10.3390/molecules28155646
Title

Authors

DOI
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Aggelos Avramopoulos; Heribert Reis; Demeter Tzeli; Robert Zaleřny; Manthos G. Papadopoulos
doi:10.3390/molecules28155646
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54. [doi:10.3390/molecules28237893](https://doi.org/10.3390/molecules28237893)

Title

Confining He Atoms in Diverse Ice-Phases:
Examining the Stability of He Hydrate Crystals
through DFT Approaches

Authors

[Raquel Yanes-Rodríguez](#); [Rita Prosimiti](#)

DOI

[doi:10.3390/molecules28237893](https://doi.org/10.3390/molecules28237893)

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Published by

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ISSN

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<https://www.mdpi.com/1420-3049/28/23/7893/pdf>

55. [doi:10.1093/mnras/stad2253](https://doi.org/10.1093/mnras/stad2253)

Title

Gas-phase formation route for *trans*-HC(O)SH
and its isomers under interstellar conditions: a
state-of-the-art quantum-chemical study

Authors

Hexu Ye; [Silvia Alessandrini](#); [Cristina Puzzarini](#)

DOI

[doi:10.1093/mnras/stad2253](https://doi.org/10.1093/mnras/stad2253)

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Published in

Monthly Notices of the Royal Astronomical
Society

Published by

Oxford University Press (OUP)

ISSNs

[0035-8711](#); [1365-2966](#)

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56. [doi:10.1093/mnras/stad3140](https://doi.org/10.1093/mnras/stad3140)

Title

Collisional excitation of PO⁺ by *para*-H₂: potential
energy surface, scattering calculations, and
astrophysical applications

Authors

[F Tonolo](#); [L Bizzocchi](#); [V M Rivilla](#); [F Lique](#); [M Melosso](#); [C Puzzarini](#)

DOI

[doi:10.1093/mnras/stad3140](https://doi.org/10.1093/mnras/stad3140)

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Published by

Oxford University Press (OUP)

ISSNs

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57. [doi:10.1039/D3NR03295G](https://doi.org/10.1039/D3NR03295G)

Title

Electron energy loss and angular asymmetry
induced by elastic scattering in superfluid helium
nanodroplets

Authors

[Jakob D. Asmussen](#); [Keshav Sishodia](#); Björn
Bastian; Abdul R. Abid; [Ltaief Ben Ltaief](#); [Henrik B. Pedersen](#); Subhendu De; Cristian Medina;
Nitish Pal; [Robert Richter](#); Thomas Fennel;
Sivarama Krishnan; [Marcel Mudrich](#)

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[doi:10.1039/D3NR03295G](https://doi.org/10.1039/D3NR03295G)

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[2040-3364](#); [2040-3372](#)
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58. [doi:10.1039/D3NR04067D](#)

Title

Atomistic mechanisms underlying plastic flow at ultralow yield stress in ductile carbon aerogels
Giorgio Conter; [Kailu Xiao](#); [Xianqian Wu](#); William A. Goddard; [Alessandro Fortunelli](#)
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59. [doi:10.1039/D3NR06189B](#)

Title

Tuning electronic levels in photoactive hydroxylated titania nanosystems: combining the ligand dipole effect and quantum confinement
[Miguel Recio-Poo](#); [Ángel Morales-García](#); [Francesc Illas](#); [Stefan T. Bromley](#)
[doi:10.1039/D3NR06189B](#)

Authors

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60. [doi:10.1038/s41929-024-01180-x](#)

Title

Embedded oxide clusters stabilize sub-2 nm Pt nanoparticles for highly durable fuel cells
[Bosi Peng](#); [Zeyan Liu](#); Luca Sementa; Qingying Jia; [Qiang Sun](#); [Carlo U. Segre](#); Ershuai Liu; Mingjie Xu; [Yu-Han Tsai](#); [Xingxu Yan](#); Zipeng Zhao; [Jin Huang](#); Xiaoqing Pan; [Xiangfeng Duan](#); [Alessandro Fortunelli](#); [Yu Huang](#)
[doi:10.1038/s41929-024-01180-x](#)

Authors

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Title

Mechanistic studies of a lipase unveil effect of pH on hydrolysis products of small PET modules
[Katarzyna Świderek](#); [Susana Velasco-Lozano](#); Miquel À. Galmés; [Ion Olazabal](#); [Haritz Sardon](#); [Fernando López-Gallego](#); [Vicent Moliner](#)
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| Published by | Springer Science and Business Media LLC |
| ISSN | 2041-1723 |
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| Authors | Aby Cheruvathoor Poulose ; Miroslav Medved ; Vasudeva Rao Bakuru; Akashdeep Sharma; Deepika Singh; Suresh Babu Kalidindi ; Hugo Bares ; Michal Otyepka ; Kolleboyina Jayaramulu; Aristides Bakandritsos ; Radek Zbořil
doi:10.1038/s41467-023-36602-0 |
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| Type | Journal article |
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| Published by | Springer Science and Business Media LLC |
| ISSN | 2041-1723 |
| Links | https://www.nature.com/articles/s41467-023-36602-0.pdf ;
https://www.nature.com/articles/s41467-023-36602-0 |
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| Authors | C Medina; A Ø Lægdsmand; L Ben Ltaief ; Z Hoque; A H Roos ; L Jurkovičová ; O Hort; O Finke; M Albrecht; J Nejd; F Stienkemeier ; J Andreasson; E Klimešová ; M Krikunova; A Heidenreich ; M Mudrich
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| Authors | Eduard V. Monaico ; Elena I. Monaico ; Veaceslav V. Ursaki ; Ion M. Tiginyanu
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| Published by | Royal Society of Chemistry (RSC) |
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| Title | Meta-stability through intermolecular interactions protecting the identity of atomic metal clusters: <i>ab initio</i> evidences in $(\text{Cu}_5\text{--Cu}_5)_n$ ($n < 3$) cases |
| Authors | Berta Fernández ; María Pilar de Lara-Castells |
| DOI | doi:10.1039/D2CP03537E |
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| Published in | Physical Chemistry Chemical Physics |
| Published by | Royal Society of Chemistry (RSC) |
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| Authors | Otoniel Denis-Alpizar ; Alexandre Zanchet ; Thierry Stoecklin |
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| Type | Journal article |
| Published in | Physical Chemistry Chemical Physics |
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| 69. doi:10.1039/D3CP00096F | |
| Title | Aggregation patterns of curcumin and piperine mixtures in different polar media |

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| <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>J. R. C. Santos; P. E. Abreu; J. M. C. Marques
doi:10.1039/D3CP00096F</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP00096F</p> |
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| <p>70. doi:10.1039/D2CP02169B</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Aggregation and support effects in the oxidation of fluxional atomic metal clusters. The paradigmatic Cu₅ case</p> <p>Jaime Garrido-Aldea; María Pilar de Lara-Castells
doi:10.1039/D2CP02169B</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2022/CP/D2CP02169B</p> |
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| <p>71. doi:10.1039/D3CP90063K</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Stability and properties of new-generation metal and metal-oxide clusters down to subnanometer scale</p> <p>María Pilar de Lara-Castells; Cristina Puzzarini; Vlasta Bonačić-Koutecký; M. Arturo López-Quintela; Stefan Vajda
doi:10.1039/D3CP90063K</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP90063K</p> |
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| <p>72. doi:10.1039/D4CP00789A</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Combined experimental and computational study of the photoabsorption of the monodoped and nondoped nanoclusters Au₂₄Pt(SR)₁₈, Ag₂₄Pt(SR)₁₈, and Ag₂₅(SR)₁₈</p> <p>Pierpaolo D'Antoni; Luca Sementa; Sara Bonacchi; Mattia Reato; Flavio Maran; Alessandro Fortunelli; Mauro Stener
doi:10.1039/D4CP00789A</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP00789A</p> |
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| <p>73. doi:10.1039/D3CP02720A</p> <p>Title</p> | <p>Towards the generation of potential energy surfaces of weakly bound medium-sized molecular systems: the case of benzonitrile–He complex</p> |
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| <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Eya Derbali; Yosra Ajili; Bilel Mehnen; Piotr S. Żuchowski; Dariusz Kędziera; Muneerah Mogren Al-Mogren; Nejmi-Edine Jaidane; Majdi Hochlaf
 doi:10.1039/D3CP02720A
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP02720A</p> |
| <p>74. doi:10.1039/D4CP01147C</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Bond breaking and making in mixed clusters of fullerene and coronene molecules induced by keV-ion impact</p> <p>Naemi Florin; Alicja Domaracka; Patrick Rousseau; Michael Gatchell; Henning Zettergren
 doi:10.1039/D4CP01147C
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP01147C</p> |
| <p>75. doi:10.1039/D3CP02367B</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Nanostructured supramolecular networks from self-assembled diamondoid molecules under ultracold conditions</p> <p>Marija Alešković; Florian Küstner; Roman Messner; Florian Lackner; Wolfgang E. Ernst; Marina Šekutor
 doi:10.1039/D3CP02367B
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP02367B</p> |
| <p>76. doi:10.1039/D3CP05071H</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Simulating high-pressure surface reactions with molecular beams</p> <p>Amjad Al Taleb; Frederik Schiller; Denis V. Vyalikh; José María Pérez; Sabine V. Auras; Daniel Farías; J. Enrique Ortega
 doi:10.1039/D3CP05071H
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2024/CP/D3CP05071H</p> |
| <p>77. doi:10.1039/D3CP02412A</p> <p>Title</p> | <p>Decoding the infrared spectra changes upon formation of molecular complexes: the case of halogen bonding in pyridine–perfluorohaloarene</p> |

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| <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>complexes</p> <p>Alex Iglesias-Reguant; Heribert Reis; Miroslav Medved'; Borys Ośmiałowski; Robert Zaleśny; Josep M. Luis
doi:10.1039/D3CP02412A</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP02412A</p> |
| <p>78. doi:10.1039/D3CP00489A</p> <p>Title</p> <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Diamondoid ether clusters in helium nanodroplets</p> <p>Jasna Alić; Roman Messner; Marija Alešković; Florian Küstner; Mirta Rubčić; Florian Lackner; Wolfgang E. Ernst; Marina Šekutor
doi:10.1039/D3CP00489A</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP00489A</p> |
| <p>79. doi:10.1039/D2CP03524C</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Catalytic activity of 1D chains of gold oxide on a stepped gold surface from density functional theory</p> <p>Shikun Li; Okikiola Olaniyan; Lenard L. Carroll; Marcus Bäumer; Lyudmila V. Moskalova
doi:10.1039/D2CP03524C</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2022/CP/D2CP03524C</p> |
| <p>80. doi:10.1039/D3CP02879H</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Secondary ionization of pyrimidine nucleobases and their microhydrated derivatives in helium nanodroplets</p> <p>Jakob D. Asmussen; Abdul R. Abid; Akgash Sundaralingam; Björn Bastian; Keshav Sishodia; Subhendu De; Ltaief Ben Ltaief; Sivarama Krishnan; Henrik B. Pedersen; Marcel Mudrich
doi:10.1039/D3CP02879H</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP02879H</p> |
| <p>81. doi:10.1039/D4CP00465E</p> <p>Title</p> | <p>Doubly charged dimers and trimers of heavy noble gases</p> |

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| <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Gabriel Schöpfer; Stefan Bergmeister; Milan Ončák; Janessa Stromberg; Masoomah Mahmoodi-Darian; Paul Scheier; Olof Echt; Elisabeth Gruber
doi:10.1039/D4CP00465E</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP00465E</p> |
| <p>82. doi:10.1039/D3CP01835K</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>On the $^{12}\text{C}_2\text{H}_2$ near-infrared spectrum: absolute transition frequencies and an improved spectroscopic network at the kHz accuracy level</p> <p>Antonio Castrillo; Eugenio Fasci; Tibor Furtenbacher; Vittorio D'Agostino; Muhammad A. Khan; Stefania Gravina; Livio Gianfrani; Attila G. Császár
doi:10.1039/D3CP01835K</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP01835K</p> |
| <p>83. doi:10.1039/d3cp00489a</p> <p>Title</p> <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Diamondoid ether clusters in helium nanodroplets</p> <p>Jasna Alić; Roman Messner; Marija Alešković; Florian Küstner; Mirta Rubčić; Florian Lackner; Wolfgang E. Ernst; Marina Šekutor
doi:10.1039/d3cp00489a</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP00489A</p> |
| <p>84. doi:10.1039/D4CP02406K</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Raman optical activity study of deuterated sugars: deuterium labelling as a tool for structural analysis</p> <p>Tohru Taniguchi; Davidson Obinna Agbo; Qin Yang; Josef Kapitán; Tao Wu; Shuki Oyama; Shuji Akai; Yoshinari Sawama; Petr Bouř
doi:10.1039/D4CP02406K</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP02406K</p> |
| <p>85. doi:10.1039/D2CP04569A</p> <p>Title</p> | <p>Structure and formation of copper cluster ions in</p> |

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| <p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>multiply charged He nanodroplets
O. V. Lushchikova; M. Gatchell; J. Reichegger; S. Kollotzek; F. Zappa; M. Mahmoodi-Darian; P. Scheier
doi:10.1039/D2CP04569A
Journal article
Physical Chemistry Chemical Physics
Royal Society of Chemistry (RSC)
1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D2CP04569A</p> |
| <p>86. doi:10.1039/D3CP05865D</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>A kernel-based machine learning potential and quantum vibrational state analysis of the cationic Ar hydride (Ar_2H^+)
María Judit Montes de Oca-Estévez; Álvaro Valdés; Rita Prosimi
doi:10.1039/D3CP05865D
Journal article
Physical Chemistry Chemical Physics
Royal Society of Chemistry (RSC)
1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2024/CP/D3CP05865D</p> |
| <p>87. doi:10.1039/D3CP03452F</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Solvation of cationic copper clusters in molecular hydrogen
O. V. Lushchikova; J. Reichegger; S. Kollotzek; F. Zappa; M. Mahmoodi-Darian; M. Bartolomei; J. Campos-Martínez; T. González-Lezana; F. Pirani; P. Scheier
doi:10.1039/D3CP03452F
Journal article
Physical Chemistry Chemical Physics
Royal Society of Chemistry (RSC)
1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP03452F</p> |
| <p>88. doi:10.1039/D3CP03984F</p> <p>Title</p>

<p>Authors</p>

<p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Rotational spectra and semi-experimental structures of furonitrile and its water cluster
Mattia Melosso; Silvia Alessandrini; Lorenzo Spada; Alessio Melli; Xiujuan Wang; Yang Zheng; Chunguo Duan; Jiayi Li; Weiping Du; Qian Gou; Luca Bizzocchi; Luca Dore; Vincenzo Barone; Cristina Puzzarini
doi:10.1039/D3CP03984F
Journal article
Physical Chemistry Chemical Physics
Royal Society of Chemistry (RSC)
1463-9076; 1463-9084
http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP03984F</p> |
| <p>89. doi:10.1039/D4CP01797H</p> | |

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| <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Spectroscopic investigation of size-dependent CO₂ binding on cationic copper clusters: analysis of the CO₂ asymmetric stretch</p> <p>A. M. Reider; M. Szalay; J. Reichegger; J. Barabás; M. Schmidt; M. Kappe; T. Höltzl; P. Scheier; O. V. Lushchikova
doi:10.1039/D4CP01797H</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084</p> <p>http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP01797H</p> |
| <p>90. doi:10.1039/D2CP04076J</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Coordination effects on the binding of late 3d single metal species to cyanographene</p> <p>Róbert Průcha; Vítězslav Hrubý; Dagmar Zaoralová; Eva Otyepková; Veronika Šedajová; Jan Kolařík; Radek Zbořil; Miroslav Medved'; Michal Otyepka
doi:10.1039/D2CP04076J</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084</p> <p>http://pubs.rsc.org/en/content/articlepdf/2023/CP/D2CP04076J</p> |
| <p>91. doi:10.1039/D2CP05843J</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Carbon vacancy-assisted stabilization of individual Cu₅ clusters on graphene. Insights from <i>ab initio</i> molecular dynamics</p> <p>Lenard L. Carroll; Lyudmila V. Moskaleva; María Pilar de Lara-Castells
doi:10.1039/D2CP05843J</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084</p> <p>http://pubs.rsc.org/en/content/articlepdf/2023/CP/D2CP05843J</p> |
| <p>92. doi:10.1039/D3CP01460F</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>An <i>ab initio</i> study of the photodissociation of CH₂I and CH₂I⁺</p> <p>A. Bouallagui; A. Zanchet; L. Bañares; A. García-Vela
doi:10.1039/D3CP01460F</p> <p>Journal article</p> <p>Physical Chemistry Chemical Physics</p> <p>Royal Society of Chemistry (RSC)</p> <p>1463-9076; 1463-9084</p> <p>http://pubs.rsc.org/en/content/articlepdf/2023/CP/D3CP01460F</p> |
| <p>93. doi:10.1039/D2CP04295A</p> <p>Title</p> | <p>Selective adsorption of sulphur dioxide and</p> |

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| <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>hydrogen sulphide by metal–organic frameworks
 S. Grubišić; R. Dahmani; I. Djordjević; M. Sentić;
 M. Hochlaf
 doi:10.1039/D2CP04295A
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2023/CP/D2CP04295A</p> |
| <p>94. doi:10.1039/D4CP01736F</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Reactive collisions between electrons and BeH⁺ above dissociation threshold
 Emerance Djuissi; Jeoffrey Boffelli; Riyad Hassaine; Nicolina Pop; Vincenzo Laporta; Kalyan Chakrabarti; Mehdi Ayouz; Arnaud Bultel; János Zsolt Mezei; Ioan F. Schneider
 doi:10.1039/D4CP01736F
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP01736F</p> |
| <p>95. doi:10.1039/D2CP05082J</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Imaging the photodissociation dynamics of internally excited ethyl radicals from high Rydberg states
 Luis Rubio-Lago; David V. Chicharro; Sonia Marggi Poullain; Alexandre Zanchet; Greta Koumarianou; Pavle Glodic; Peter C. Samartzis; Alberto García-Vela; Luis Bañares
 doi:10.1039/D2CP05082J
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2023/CP/D2CP05082J</p> |
| <p>96. doi:10.1039/D4CP01711K</p> <p>Title</p> <p>Authors</p> <p>DOI</p> <p>Type</p> <p>Published in</p> <p>Published by</p> <p>ISSNs</p> <p>Link</p> | <p>Rate coefficients for the O + H₂ and O + D₂ reactions: how well ring polymer molecular dynamics accounts for tunnelling
 Marta Menéndez; Anzhela Veselinova; Alexandre Zanchet; Pablo G. Jambrina; F. Javier Aoiz
 doi:10.1039/D4CP01711K
 Journal article
 Physical Chemistry Chemical Physics
 Royal Society of Chemistry (RSC)
 1463-9076; 1463-9084
 http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP01711K</p> |
| <p>97. doi:10.1002/ssstr.202400147</p> <p>Title</p> | <p>An Ab Initio Journey toward the Molecular□Level</p> |

Author
DOI
Type
Published in
Published by
ISSNs
Link

Understanding and Predictability of
Subnanometric Metal Clusters
[María Pilar de Lara-Castells](#)
[doi:10.1002/ssstr.202400147](https://doi.org/10.1002/ssstr.202400147)
Journal article
Small Structures
Wiley
[2688-4062; 2688-4062](#)
<https://onlinelibrary.wiley.com/doi/pdf/10.1002/ssstr.202400147>

98.

Due to the limit of 100 publications in this form, the full list of COST Action CA21101 "COSY" publications is available at: <https://cost-cosy.eu/cosy-papers> (see, for a more detailed list: <https://cost-cosy.eu/articles>).

99. [doi:10.1039/D4RA05401F](https://doi.org/10.1039/D4RA05401F)

Title

A practical post-Hartree-Fock approach describing open-shell metal cluster-support interactions. Application to Cu₃ adsorption on benzene/coronene

Authors

[Katarzyna M. Krupka](#); [Agnieszka Krzemińska](#); [María Pilar de Lara-Castells](#)

DOI

[doi:10.1039/D4RA05401F](https://doi.org/10.1039/D4RA05401F)

Type

Journal article

Published in

RSC Advances

Published by

Royal Society of Chemistry (RSC)

ISSN

[2046-2069](#)

Link

<http://pubs.rsc.org/en/content/articlepdf/2024/RA/D4RA05401F>

100. [doi:10.1039/D4CP03271C](https://doi.org/10.1039/D4CP03271C)

Title

Support effects on conical intersections of Jahn–Teller fluxional metal clusters on the sub-nanoscale

Authors

[Katarzyna M. Krupka](#); [María Pilar de Lara-Castells](#)

DOI

[doi:10.1039/D4CP03271C](https://doi.org/10.1039/D4CP03271C)

Type

Journal article

Published in

Physical Chemistry Chemical Physics

Published by

Royal Society of Chemistry (RSC)

ISSNs

[1463-9076; 1463-9084](#)

Link

<http://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP03271C>

Proposals/ projects

The Action reported 5 project(s) and 6 proposal(s) resulting from the Action networking.

Key details of the projects are shown below:

1. OPen-shell ELectronic SYStems - OPELSYS (National)
2. María de Maeztu Unit of Excellence - IQTC

- (National)
- 3. DNA under fire – Elucidating multiple and non-local ionization of the building blocks of DNA by X-ray irradiation
(National)
- 4. Singlet fission and ICD in tailored molecular complexes for boosting organic solar cells
(National)
- 5. Exploring vibrational intermolecular Coulombic decay in mixed water clusters
(National)

Other outputs / achievements

The following other outputs/ achievements contributing to the COST mission resulted from the Action:

1. Paul Scheier (Innsbruck), Felix Laimer (Innsbruck), Lorenz Kranabetter (Aarhus C), Fabio Zappa (Innsbruck), Michael Renzler (Innsbruck), Lukas Thiefenthaler (Innsbruck), Simon Albertini (Zurich), Paul Martini (Stockholm), Siegfried Kollotzek (Innsbruck)

UNIVERSITÄT INNSBRUCK (Innsbruck), USA - Patent Nr. 12,068,147, Size selected clusters and nanoparticles

Method for producing multiply-charged helium nanodroplets and charged dopant clusters and nanoparticles out of the helium nanodroplets, the method comprising: producing neutral helium nanodroplets in a cold head via expansion of a pressurized, pre-cooled, supersonic helium beam of high purity through a nozzle into high vacuum with a base pressure under operation preferably below 20 mPa, ionizing the helium nanodroplets by electron impact, wherein the electron impact leads to multiply-charged helium nanodroplets, doping the charged helium nanodroplets with dopant vapor in the pickup cell, wherein the doped nanodroplets form cluster ions with the initial charges acting as seeds, wherein the size of the nanoparticles can vary from a few atoms up to 105 atoms by arranging the size of the neutral helium nanodroplets, the charge of the helium nanodroplets and the density of dopant vapor in the pickup cell.

Impacts

The Action reported the following impact(s):

Description of the impact, i.e. what will change, and for whom, as a result of what the Action achieved	Type of impact	Timing of impact
The COSY-INTER, COSY-DYN, COSY-NANO, and COSY-ASTRO datasets, as well as machine learning resources, will accelerate scientific discoveries by enabling faster, more accurate modeling in fields like materials science, nanotechnology, and astrochemistry. They will foster cross-disciplinary insights, empower researchers with better predictive tools, and make advanced data analysis more accessible to a broader scientific community, ultimately enhancing research efficiency and collaboration across diverse domains.	Scientific / Technological	Foreseen by the end of the Action

Dissemination and exploitation of Action results

Dissemination and exploitation approach of the Action

The Action's dissemination and exploitation approach as well as all activities undertaken to ensure dissemination and exploitation of Action results and the outcomes of these activities are described below.

The COSY Action has prioritized the dissemination and exploitation of its activities within the scientific and academic communities. A dedicated Web Development Team maintains the COSY webpage, regularly updating it with information on events, publications, achievements, and ongoing efforts. To further enhance the visibility of the Action, a COSY Social Media Team was established, actively engaging audiences on LinkedIn, X (formerly Twitter) and Instagram. These efforts have significantly boosted engagement, with COSY's LinkedIn now boasting over 600 followers and increased visibility among European scientific communities, governmental institutions, and recognized scientific publishers. In addition to these efforts, COSY has organized events aimed at improving science communication skills, particularly for Early Career Investigators (ECIs). Notable initiatives include the "Listen-my-presentation" event, where ECIs receive feedback on their presentations, and a soft-skills training session held during the 2nd Training School. These sessions are designed to enhance communication skills and foster professional development. Additional events focused on science communication and outreach are planned for the 3rd Grant Period, further supporting COSY's mission to promote both scientific excellence and effective communication.

Dissemination

Dissemination meetings funded by the Action (possible only until 31st October 2021)

The Action did not fund any Dissemination Meetings

Other dissemination activities

The Action also undertook the following dissemination activities:

Activity	05.03.24 COST Infoday at CSIC. The Chair of the COST Action was invited to deliver a lecture about the creation of a COST proposal as well as the first steps as Main Proposer and Action Chair once the proposal is approved. The activity was public and announced in the social media: Programme: https://www.horizonteeuropa.es/jornada-informativa-sobre-el-programa-de-cooperacion-europea-en-ciencia-y-tecnologia-cost-1 Presentations: https://saco.csic.es/index.php/s/MSrRcHotock2mnS , Twitter: https://x.com/COSY_Action/status/1765423123359215993 ; https://x.com/Europeos_CSIC/status/1762162081229324607
Target	Potential applicants to COST Actions affiliated in all the CSIC centers in Spain.
Outcome	50 participants. Numerous questions from applicants to solve doubts before applying to COST Actions.
Link	https://www.horizonteeuropa.es/jornada-informativa-sobre-el-programa-de-cooperacion-europea-en-ciencia-y-tecnologia-cost-1

Activity	MACCS1: 1st Italian Chinese Swedish workshop on Modeling and Characterization of Complex Systems. The aim of the meeting is to understand and explain the behavior of complex systems of interest in the field of materials science, biotechnology, green chemistry through experiments combined with modeling at different scales.
Target	Scientists, researchers and students in the field of Physics, Chemistry and Chemical Engineering
Outcome	There were 50 attending people, 16 talks and 16 poster presentations. COSY members participating: F. Mocci, C.M. Carbonaro, C. Olla (University of Cagliari, Italy); Aatto Laaksonen (Stockholm University, Sweden); XiaoYan Ji, Leon Engelbrecht (Luleå University of Technology Luleå, Sweden); Narcis-Iulian Cibotariu ("Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania)
Link	https://convegna.unica.it/maccs1/

Activity	NanoLumCat Ostrava Workshop: Revealing the Future of Light Transformation. Experts in the fields of carbon dots and single atom photocatalysis were united to broaden the horizons of nanomaterial science with a focus on renewable energy applications. The workshop invites participants to dive deep into the exciting worlds of carbon dots and single atom-based photo(electro)catalysis.
Target	Scientists, researchers and students in the field of chemistry, physics and engineering interested in carbon nanomaterials for environmental, energy and photonic applications
Outcome	There were 50 people attending the meeting, 25 talks were presented. Some COSY members involved: F. Mocci, C. Olla, C.M. Carbonaro (University of Cagliari, Italy); Miroslav Medved' (Matej Bel University, Slovak Republic), Michal Otyepka, Markéta Paloncýová (Catrin, Palacký University Olomouc, Czech Republic). Within the workshop, several of the COSY members presented findings and discussed the pre-submission details of a manuscript based on a collaboration that started at the COSY General Meeting in Cadiz (2023).
Link	https://events.it4i.cz/event/220/

Activity	Interpreting how intermolecular interactions determine the properties of supramolecular helices and the corresponding materials
Target	Scientist, researchers and students in the field of chemistry, physics and materials science at World Congress of Advanced Materials (WCAM2023)
Outcome	A COSY member - Berta Fernández Rodríguez - presented an invited on-line talk to the international community of materials science
Link	https://www.bitcongress.com/wcam2023/Welcome.asp

Activity	TSRC Workshop on Intermolecular interactions: New challenges for ab initio theory.
Target	Scientists, researchers and students at TSRC Workshop on Intermolecular interactions: New challenges for ab initio theory.
Outcome	A COSY member - Berta Fernández Rodríguez - co-organized the Workshop and presented an invited talk - The FGC approach for correcting noncovalent interactions in SQM methods
Link	https://meetings.telluridscience.org/meetings/workshop-details?wid=1130

Activity	Three Examples of Efficient Evaluation of Intermolecular Interactions - 18th International Conference of Computational Methods in Sciences and Engineering
Target	Scientists, researchers and students in the field of chemistry, physics and engineering at the 18th International Conference of Computational Methods in Sciences and Engineering.
Outcome	A COSY member - Berta Fernández Rodríguez - presented an invited on-line talk.
Link	http://www.history.iccmse.org/archives/ICCMSE2022/www.iccmse.org/index.html

Activity	16th National Physical Chemistry Meeting of the Portuguese Society of Chemistry
Target	Portuguese researchers, doctoral candidates, students from the physical chemistry area
Outcome	Oral presentation: "Unveiling Pesticide Interactions: Insights from the Aplysia californica AChBP-Imidacloprid Complex" by COSY members Joana R. C. Santos, Paulo E. Abreu, Jorge M. C. Marques
Link	https://xvienqf.events.chemistry.pt/

Activity	16th National Physical Chemistry Meeting of the Portuguese Society of Chemistry
Target	Portuguese researchers, doctoral candidates and students from the physical chemistry area
Outcome	Poster presentation: "Energetics and structures of borophene nanoclusters" by COSY members - J.M.C. Marques, F. Zergani, M. Bartolomei, F. Pirani
Link	https://xvienqf.events.chemistry.pt/

Activity	2nd BioExcel Conference on Advances in Biomolecular Simulations in Brno, Czech Republic
Target	Biomolecular research community interested in an integrative modelling, free energy and drug design, workflows, automation and data integration.
Outcome	Poster presentation: "Molecular dynamics-driven selection of vectors for targeted delivery of doxorubicin" by G. Gocheva, S. Iliev, N. Markova, N. Ivanova, G. Madjarova, J. Petkova, A. Ivanova
Link	https://bioexcel.eu/events/2nd-bioexcel-conference-on-advances-in-biomolecular-simulations/

Activity	2nd PHYMOL Training School, St Catharine's College, Cambridge/Queen Mary University of London, UK
Target	PHYMOL MSCA DN Doctoral Candidates, Principal Investigators, Partners of the Network from the United States (Molssi)
Outcome	DC oral presentation: K.M. Krupka - A practical ab initio approach to open-shell metal cluster-support interactions
Link	https://phymol.eu/events

Activity	Organisation of the The 15th International Conference on Quantum Fluid Clusters
Target	All members of WG4 and other researchers working in the field of quantum fluid clusters
Outcome	Successful conference with 85 participants from quantum fluid clusters community all around the world
Link	https://conferences.au.dk/qfc2024

Activity	Organization of the TSRC Workshop on Intermolecular interactions: New challenges for ab initio theory
Target	WG1 members and the international theoretical chemistry and physics community, interested in intermolecular interactions and ab initio theory
Outcome	The organization of a successful international workshop with many experts in the field participating
Link	https://meetings.telluridescience.org/meetings/workshop-details?wid=1130

Activity	2nd PHYMOL Training School, St Catharine's College, Cambridge/Queen Mary University of London, UK
Target	PHYMOL MSCA DN Doctoral Candidates, Principal Investigators, Partners of the Network from the United States (Molssi)
Outcome	Organization of the successful training school - B. Fernandez, A.Misquitta, P.Zuchowski
Link	https://phymol.eu/events

Activity	1st PHYMOL Training School, Nicolaus Copernicus University in Torun, Poland
Target	PHYMOL MSCA DN Doctoral Candidates, Principal Investigators, Partners of the Network from the United States (Molssi)
Outcome	Organization of the successful training school - B. Fernandez, A.Misquitta, P.Zuchowski
Link	https://phymol.eu/events

Activity	PHYMOL MSCA Doctoral Network Kick-off Conference 2023, University of Luxembourg, Luxembourg
Target	PHYMOL MSCA DN Doctoral Candidates, Principal Investigators and Network Partner
Outcome	DC8 Introduction Talk - K.M.Krupka - Influence of Substituent Effects on Intra- and Intermolecular Hydrogen Bonding in Schiff Bases and Benzimidazole Derivatives: A Comprehensive Study, State-of-the art modelling of new quantum materials: unsupported and surface-supported atomic metal clusters
Link	https://phymol.github.io/

Activity	The Cluster Meeting 2023 - a topical international conference with main focus on catalysis, reactivity, characterization, imaging and modeling of primarily size-selected clusters, both free and supported.
Target	The international community of cluster and nanoscience - 108 participants from 18 countries
Outcome	Invited lecture and invited introduction to COST Action CA21101 "COSY"- María Pilar de Lara-Castells
Link	https://clustermeeting2023.eu/

Exploitation activities

The Action undertook the following activities to ensure exploitation (use, in particular in a commercial context) of the Action's achievements:

Activity	Regular updates on the COSY Action's webpage (https://cost-cosy.eu) provide essential information about activities, events, and research advancements of the Action
Target	COSY Action members, researchers, students, stakeholders like policymakers and industry partners, academic institutions, gender equality initiatives, and the general public, all interested in scientific developments and collaboration opportunities
Outcome	Regular updates increase visibility for collaborations, keep all the stakeholders informed, promote knowledge exchange, attract diverse participation, and strengthen the COSY Action's impact in the scientific community

Activity	Regular updates on LinkedIn, X (formerly Twitter), and Instagram enhance the COSY Action's online presence. LinkedIn focus on professional networking and content creating, while Instagram share visually engaging content related to scientific advancements. X provide quick updates and promote events, maximizing outreach. https://es.linkedin.com/company/cosy-cost-action-ca21101 https://x.com/COSY_Action https://www.instagram.com/cosy_cost_ca21101/
Target	The target audience includes researchers, industry professionals, and stakeholders on LinkedIn. Instagram appeal to a broader audience interested in science communication, including students and the general public. X attract followers looking for concise updates and timely announcements.
Outcome	Regular social media updates enhance visibility and engagement, facilitating networking among professionals, building a community interested in COSY Action's topics and ensuring dissemination of information.

Activity	A COSY Webinar Series is organized to present the latest findings and methodologies from the COSY Action and external guests from the COSY-related fields. https://cost-cosy.eu/activity/1st-webinar-of-the-cost-action-cosy/ https://cost-cosy.eu/activity/2nd-webinar-of-the-cost-action-cosy/
Target	The target audience includes established and early-stage researchers, students, and professionals interested in the COSY Action's research areas.
Outcome	The webinar series provides a platform for real-time interaction and scientific discussion, regardless of participants' stage of career and country of affiliation or mobility possibilities. Each webinar features expert speakers and includes an interactive Q&A segment, allowing participants to engage directly with the content.

Activity	An open discussion session was organized in a round-table format at the CATCOSY 2024 Meeting. https://cost-cosy.eu/activity/workshop-facing-challenges/
Target	The target audience included established and early-stage researchers, scientists, and stakeholders from both theoretical and experimental backgrounds, participating in the CATCOSY 2024 Meeting. This inclusive environment encouraged collaboration and networking.
Outcome	This session focused on facilitating dialogue between theoretical researchers and experimentalists, combining their expertise to generate new ideas within the COSY network and establish plans for maintaining the Action's network.

Activity	The 1st Listen to My Presentation Event provided a platform for early-career participants to present their research and receive constructive feedback from the COSY Science Communication Team. https://cost-cosy.eu/activity/the-1st-listen-to-my-presentation-event/
Target	The target audience included early-career COSY Action members, students, doctoral candidates and postdoctoral researchers seeking to improve their presentation skills.
Outcome	The event facilitated the exchange of opinions and constructive feedback, helping participants refine their research presentations. By fostering a supportive environment for dialogue and soft-skills development, it strengthened the COSY network and attracted external early-career scientists.

Activity	The COSY Podcast Series aims to disseminate COSY Action science to the general audience and science enthusiasts. The first episode has already been created by the Action Chair: https://researchpod.org/informatics-technology/cost-action-cosy-new-generation-materials .
Target	The target audience includes the general public, science enthusiasts, researchers, and students interested in the COSY Action's science fields. The popular format appeal to a wide range of listeners, including those new to the topics covered.
Outcome	The COSY Podcast Series enhances public understanding of the COSY Action's research and promotes the Action's milestones and progress. Plans are underway for each working group to produce their own episode, which is nearing completion. By featuring diverse voices from each group, the podcast will raise awareness and attract a broader audience to the Action's initiatives.

Action Expenditure

The table below shows the budget allocated to the Action for each Grant Period (funds allocated for the first meeting of the Action and any Final Action Dissemination are not included):

#	Grant Period	Start Date	End Date	Budget allocated to Action (EUR)
1	AGA-CA21101-1	1-11-2022	31-10-2023	156,231.09 (EUR)
2	AGA-CA21101-2	1-11-2023	31-10-2024	242,500.16 (EUR)
3	AGA-CA21101-3	1-11-2024	31-10-2025	215,000.55 (EUR)