3rd WORKING GROUP 4 MEETING 21/02/2025

Molecules confined in helium nanodroplets - recent progress and new ideas for research and collaborations in the 3rd grant period

13:00			Zoom link is open, please show up, have a chat, test your presentation
13:25	Marcel, Maria	Mudrich, Krikunova	Welcome
13:30	Rupert	Jagode	Fingerprint of Droplet Shape and Vortex at the Electronic Band Origin of Phthalocyanine in Superfluid Helium Droplets
14:00	Matthias	Veternik	Exploring Minute-Scale Storage of Helium Nanodroplets inside a Multireflectron
14:30	Lewis	Turnbull	Utilising helium nanodroplets to investigate metastable dimers formed between ethylene glycol and water
14:45	Leonie	Werner	Non-radiative dynamics of molecules dissolved in He droplets probed by time-resolved photoelectron spectroscopy
15:00	Coffee break and round table discussion		
15:30	Emil	Hansen	Adiabatic alignment of alkali dimers on the surface of helium droplets
16:00	Keshav	Sishodia	XUV fluorescence as a probe of the relaxation dynamics of resonantly excited He nanodroplets
16:30	Linos	Hecht	Two-Color X-ray Coherent Diffractive Imaging of Helium Nanodroplets

The 3rd FemCOSY Virtual Meeting will focus on presenting the initial findings from the gender imbalance survey, discussing the potential need for an additional survey, and planning a scientific publication on the topic. This event will feature insightful lectures from invited speakers and a discussion panel aimed at promoting gender balance initiatives in the scientific community.

Cluster Meeting 2025

June 22 - 27, 2025
J. Heyrovský Institute, Prague, Czech Republic

Welcome to Cluster Meeting 2025

The **Cluster Meeting 2025** is a topical international conference with main focus on catalysis, reactivity, characterization, imaging and modeling of primarily size-selected clusters, both free and supported. Selected hot topics from related areas of cluster science are included and special sessions on future perspectives are devoted to emerging theoretical and experimental approaches. The scientific program includes invited lectures, hot-topic and contributed talks as well as flash presentations and posters, which offers plenty of time for discussions. The goal of the conference is to promote scientific exchange and interdisciplinary collaborations so as to accelerate progress in this exciting field of nanoscience.

Cluster Meeting 2025 comes after two meeting of this conference series, the Cluster Meeting 2021 and

Important Dates

January 31, 2025
Abstract submission is OPEN

Read more

News

Please check back later for update.

Organizers

Štefan Vajda – Conference Chair

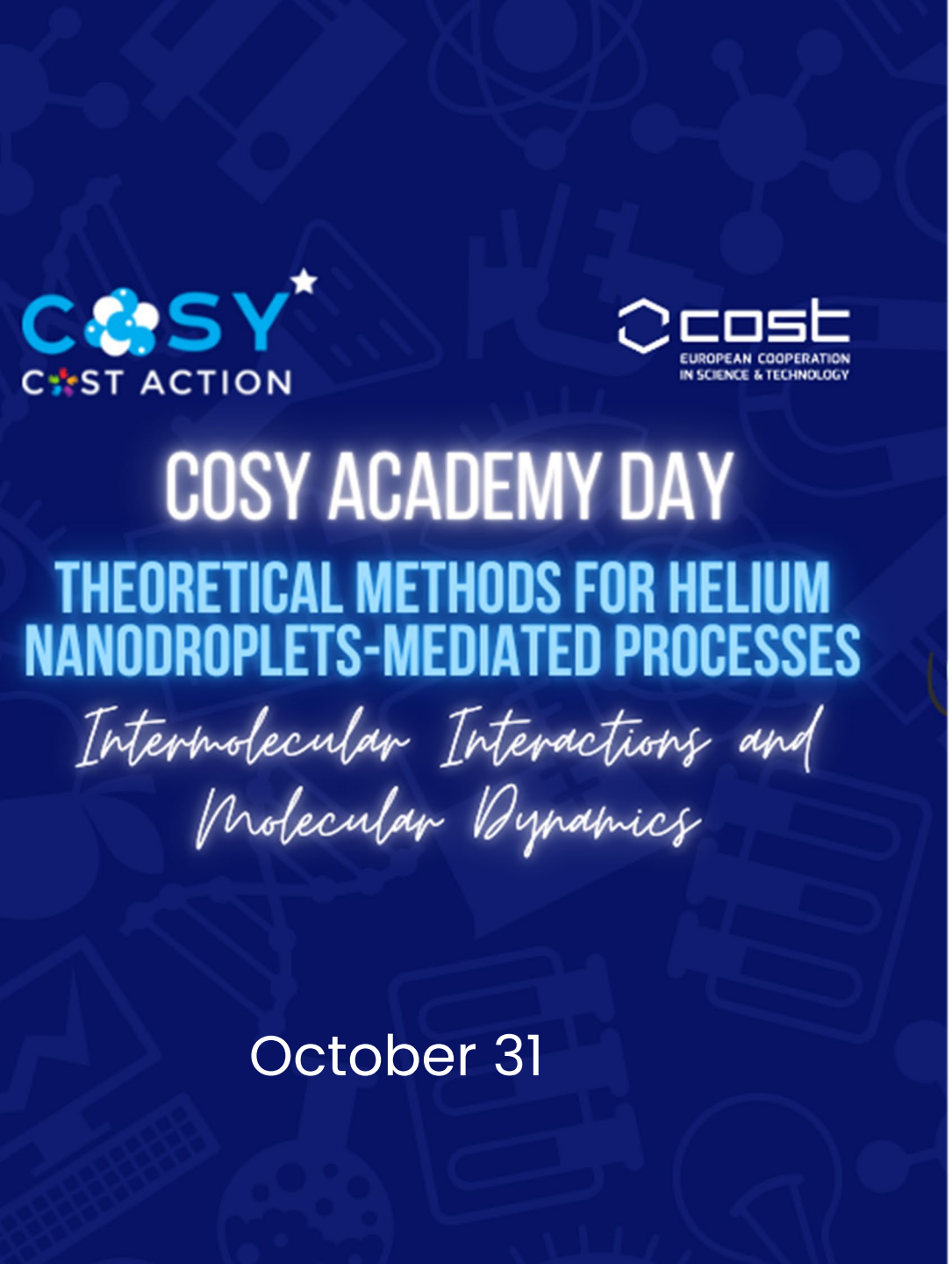
COSY
COST ACTION

cost
EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

3rd GENERAL MEETING OF THE "COSY" COST ACTION

Bologna, Italy

July 9 - July 11



The 1st event of COSY Academy will bring together expertise from WG1, WG2, and WG4, focusing on systems that are also relevant to WG3 and WG5. The main topics will include the characterization of charged metal clusters synthesized within helium nanodroplets and the IR spectra of small molecules interacting with polycyclic aromatic hydrocarbons (PAHs).

During the event, trainees will gain hands-on experience with Symmetry Adapted Perturbation Theory (SAPT) in two versions: Hartree-Fock-based and Density Functional Theory-based. They will also learn how to carry out ab-initio molecular dynamics simulations.

The program will include practical sessions led by early-stage researchers (YRIs) as trainers, fostering interactive learning and collaboration. Additionally, two lectures by international experts will provide theoretical and experimental overviews of the field:

- **A theoretical overview by the Chair of the Action**
- **An experimental overview by a recognized researcher in the field**

https://cost-cosy.eu/activity/1st-cosy-academy-day/

Symposium on Isolation of Transient Species in Superfluid Helium Droplets

at the 2025 International Chemical Congress of Pacific Basin Societies (PACIFICHEM) on Waikiki Beach

Honolulu, Hawaii, USA

December 15 - 20, 2025

Organizers

Dr. Susumu Kuma
RIKEN, Japan

Prof. Takamasa Momose
University of British Columbia, Canada

Prof. Andrey Vilesov
University of Southern California, USA

Zane Golpariani
University of Southern California, USA

International Conference on Quantum Fluid Clusters

This is the Website of the conference series

International Conference on Quantum Fluid Clusters

Next conference:

May 31 - June 4, 2026

Place:

University Center Obergurgl

Organizers:

Paul Scheier
Elisabeth Gruber

QFC Training School:

May 27 - May 30, 2026

Place:

University Center Obergurgl

Short Term Scientific Mission (STSM) grants

5 - 90 days, < €2500

Out of 29 STSM's in 2nd grant period → 5 for WG4

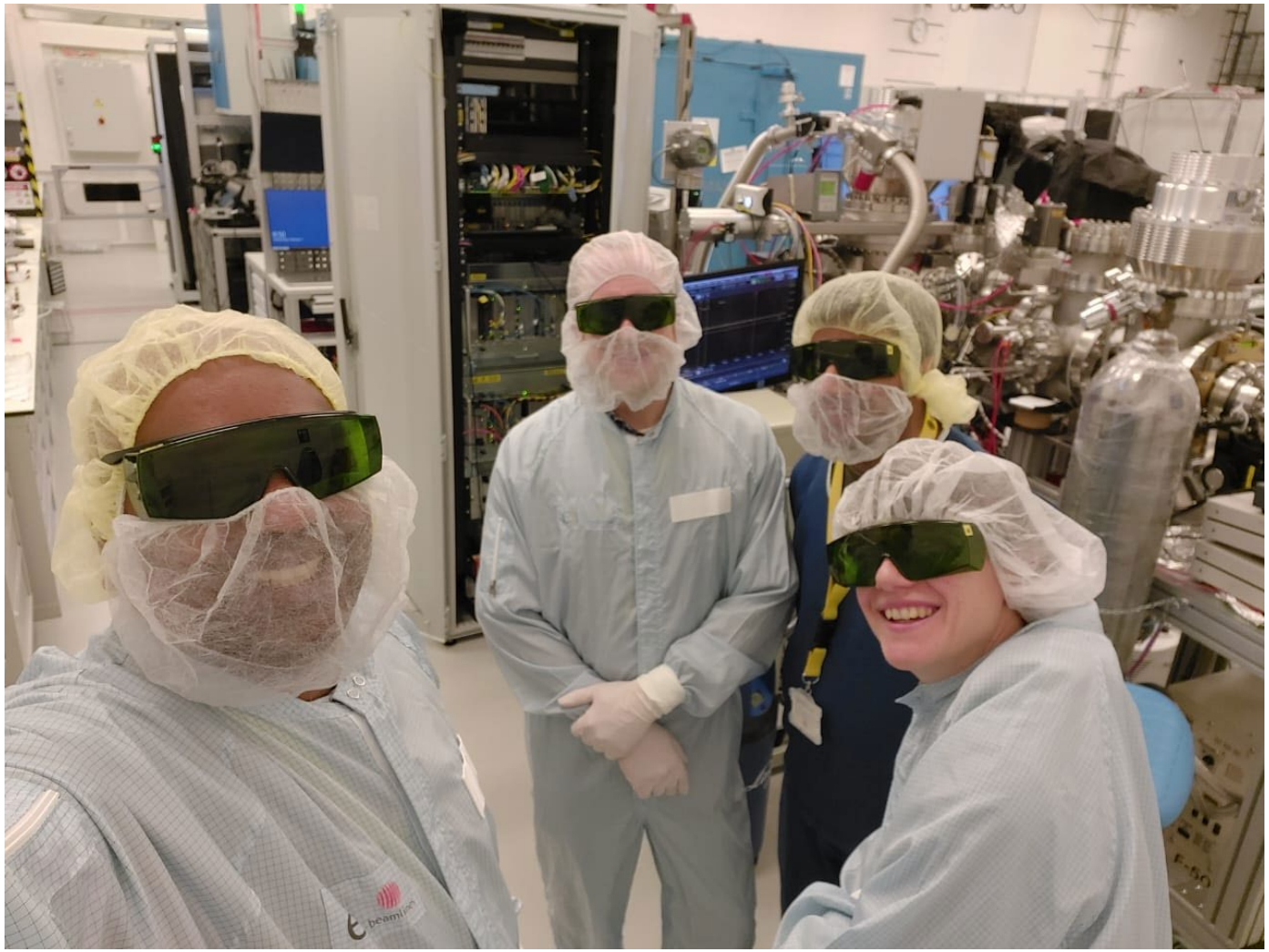
What Are STSMs?

Short Term Scientific Missions (STSMs) are exchange visits aimed at supporting researchers' individual mobility, strengthening existing networks and fostering collaboration. STSMs are intended especially, but not solely, for young researchers. An STSM should specifically contribute to the scientific objectives of the COST Action "SharingAndCaring", while enabling those partaking in the missions to establish new partnerships, learn new techniques, gain access to specific data, instruments and / or methods not available in their own institutions / organisations.

Who can apply?

STSMs are open for PhDs, PostDocs, and advanced career researchers employed at institutions in countries participating in "SharingAndCaring", or at approved institutions. STSMs must be performed between COST countries - researchers cannot apply for an STSM within their own country.

Short Term Scientific Mission (STSM) grants



Katrin Erath-Dulitz (U Innsbruck) joined projects proposed by Sivarama Krishnan and Marcel Mudrich; host: Maria Krikunova and Jakob Andreasson at ELI Beamlines

Topics: Time-resolved Interatomic Coulombic Decay and nanoplasma ignition in pure and alkali-doped helium nanodroplets

Start and end date: 22/01/2023 to 03/02/2023

WORKING GROUP 4: 3rd grant period goals

Helium Nanodroplets in Science and Engineering

Emphasizing joint experimental-theory efforts in WG4 to:

1) **Resolve the structure of multiply-charged helium nanodroplets and embedded molecules**
2) **Explore relaxation processes in embedded molecules, with focus on light-harvesting complexes**
3) **Time-resolved studies of aggregated formation**
4) **Direct imaging of the structural dynamics of helium droplets and embedded aggregates**
5) **Nanoparticle deposition and stabilization**
6) **Spectroscopy of metal clusters and carbonaceous species of astrophysical relevance formed in helium nanodroplets**
7) **Spectrometric study of diamondoid derivatives**
8) **Synchrotron studies of radiation chemistry of microsolvated biomolecules**

https://cost-cosy.eu/objectives/third-grant-period-goals/

allowed us to obtain natural orbitals. An analysis of the Mulliken charges[27] was accomplished for both Cu_5 and Cu_5–Cu_5 clusters. Additionally, for the sake of comparison, Coupled Cluster Singles and Doubles (CCSD) calculations have been carried out as implemented in the GAUSSIAN 09 code.[28]

Initial optimizations of the coupled Cu_5–Cu_5 cluster geometries were performed at PBE and B3LYP levels,[29,30] using D4 Grimme's parameterization[31] to account for the dispersion correction. An excellent performance has been achieved with the predecessor PBE-D3(BJ) ansatz[32] in describing both supported and unsupported subnanometer silver[3,33] and copper[16,34] clusters. We used the atom-centered Def2-SVP[35] basis set for copper atoms. All dispersion-corrected DFT-based calculations have been performed with the ORCA suite of programs (version 5.0.1).[36–38]

We started our coupled Cu_5–Cu_5 cluster calculations with a bipyramidal arrangement for the Cu_5 sub-unit. In this way, we placed together two trigonal bypiramidal arrangements with the center of mass of one of them located in the origin of the coordinate system and the corresponding main symmetry axis along the *Z* axis. The position of the second Cu_5 molecule with respect to the first one was modified in a range of distances and orientations. For this, we varied the distance between the two centers of mass along each of the axes, making it equal to 4.0, 5.0 and 6.0 Å for *X*, 6.0 and 7.0 Å for *Y*, and 7.0 and 8.0 Å for displacements along the *Z*-axis. Regarding the angles we considered three rotations for each of the geometries, *i.e.* the first

Acknowledgements

We thank Lyudmila Moskaleva, Alexander O. Mitrushchenkov, and Alexander Zanchet for very useful discussions. This work has been partly supported by the Spanish Agencia Estatal de Investigación (AEI) under Grant No. PID2020-117605GB-I00. This publication is also based upon work of COST Action CA21101 "Confined molecular systems: from a new generation of materials to the stars" (COSY) supported by COST (European Cooperation in Science and Technology). We are also greatly thankful for the support of the EU Doctoral Network PHYMOL 101073474 (project call reference HORIZON-MSCA-2021-DN-01. One of the authors (B. F.) acknowledges Xunta de Galicia (grant number ED431C 2021/40) for further financial support. The CESGA supercomputer center (Spain) is acknowledged for having provided the computational resources. We also acknowledge support of the publication fee by the CSIC Open Access Publication Support Initiative through its Unit of Information Resources for Research (URICI).

Notes and references

1 M. P. de Lara-Castells, *J. Colloid Interface Sci.*, 2022, **612**, 737–759.

2 J. Juraj, A. Fortunelli and S. Vajda, *Phys. Chem. Chem. Phys.*, 2022, **24**, 12083–12115.