COSY WG3 Young Scientists Forum 2025 (YSF2025)
Experimental and Computational Approaches for Studying Multicomponent Confined Systems

4th Symposium of the Working Group 3
"Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale" of the COST Action CA21101 "CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY)"
[https://www.cost.eu/actions/CA21101/]

Virtual Meeting – December 17th 2025

Organizers: Alessandro Fortunelli, Lyudmila Moskaleva, WG3 leaders
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Context

We are pleased to announce the Young Scientists Forum 2025 (YSF2025) organized by Working Group 3 of the COST Action “COSY” (Confined Molecular Systems). This year’s theme, “Experimental and Computational Approaches for Studying Multicomponent Confined Systems,” addresses once more the exciting perspectives and challenges in current research on confined clusters and nanoparticles.

Who Can Attend:

- All WG3 as well as all COSY members are invited to attend

Who Should Present:

- For this event, presentations will be limited to Early Career Scientists (PhD students, postdocs, Young Researchers, within the first 10 years of their research activity, since graduation)

Format: In line with previous WG3 online events, the Forum will be held online in a Faraday Discussions format, which will allow attendees to discuss their research in collaborative environment. The Faraday Discussion format foresees that some materials of the presentations are available ahead of the discussion (such as DOIs or slides or videos), then allowing for their very short presentation by the presenters and reserving a much longer time for the ensuing discussions and questions from the other participants (grounded on the previously available materials). In YSF2025 two types of contributions are expected:

- Talks: 5 minutes presentations followed by 15 minutes discussion
- Brief Presentations: Flash presentations of 2 minutes followed by 8 minutes discussion

Call for Contributions: We invite Early Career Scientists to present their research. To foster discussion and knowledge sharing, presenters are requested to indicate the DOI(s) of the articles corresponding to their contributions, allowing attendees to read them in advance. If material is unpublished, please share some material such as ArXivs or preliminary reports or videos of previous presentations or directly your slides.

Following the success of our three previous WG3 symposia held in this format, incluing the YSF2024 held in an identical spirit last year, we are excited to continue this engaging and interactive approach for the YSF2025.

Join us for a day of insightful presentations and stimulating discussions!

Alessandro Fortunelli, Lyudmila Moskaleva, Petra Čechová, and Markéta Paloncyova

Acknowledgements

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Essential Program

09:00 – 09:05 Registration and Forewords

09:05 – 10:25 Session 1 – Metal nanoparticles
Chair: Alessandro Fortunelli
Presenters: Abidi (L), Andrzejewska (L), Alimonti (S), Nardi (S), Zinzani (S), Finger Basso (S)

10:25 – 10:40 Coffee Break (15 minutes)

10:40 – 11:50 Session 2 – Catalysis and Graphene Derivatives
Chair: Lyudmila Moskaleva
Presenters: Gleeson (L), Sodomaco (L), Sandoval Menjivar (S), Roongcharoen (S), Shi (S)

11:50 – 12:20 Quick Lunch Break (30 minutes)

12:20 – 13:40 Session 3 – Organic molecules and systems I
Chair: Markéta Paloncýová
Presenters: Sipavičius (L), Nedělníková (L), Ferretti (S), Abu el Rub (S), Garcia Alfonso (S), Murnikova (S)

13:40 – 13:55 Coffee Break (15 minutes)

13:55 – 15:05 Session 4 – Organic molecules and systems II
Chair: Petra Čechová
Presenters: Nicoli (L), Lupi (L), Chadalíková (S), Santos (S), Field-Theodore (S)

15:05 – 15:15 Closing Remarks

Program Table

09:00-09:05		**Registration and Forewords**
Session 1		Chair: Alessandro Fortunelli
09:05-09:25	Nawras Abidi	How to dope the basal plane of 2H-MoS2 to boost the hydrogen evolution reaction?
09:25-09:45	Weronika Andrzejewska	Iron nitrides on copper and their transformations in air and solution.
09:45-09:55	Davide Alimonti	Machine Learning Potentials for Metallic Nanoparticles from small datasets
09:55-10:05	Gilberto Nardi	Sintering of copper nanoparticles with a novel machine learning potential
10:05-10:15	Sofia Zinzani	Morphological stability of Au-metal nanosatellites
10:15-10:25	Leticia Finger Basso	Gold Decoration To Improve Rh-Nanoalloys for CO-Adsorption
10:25-10:40		Break
Session 2		Chair: Lyudmila Moskaleva
10:40-11:00	Ronan Gleeson	Accurate XPS calculations of graphene based materials
11:00-11:20	Sveva Sodomaco	From Raman to Infrared: An Atomistic QM/Classical Framework for Surface-Enhanced Spectroscopies
11:20-11:30	Johanna Yasmin Sandoval Menjivar	Building single atom and single cluster TM catalyst on GDY and BGDY layers
11:30-11:40	Thantip Roongcharoen	Conformal Sampling of Catalytic Processes applied to Carbon Dioxide Hydrogenation reaction on Cu and Ni catalysts
11:40-11:50	Junjie Shi	Synergy of Oxygen and Water in Ceria-Catalyzed Direct Conversion of Methane to Methanol under Continuous Flow
11:50-12:20		Break
Session 3		Chair: Markéta Paloncýová
12:20-12:40	Einaras Sipavičus	Intermolecular organization in aqueous mixtures of choline lysinate studied via NMR and molecular dynamics/quantum mechanics
12:40-13:00	Andrea Nedělník-ová	How theory could unlock the perfect graphene form for tomorrow's brain implants
13:00-13:10	Alfonso Ferretti	Calibrating DFT-D to high-level QM and distilling it into MLIPs for water and aqueous $MgCl_2$, delivering accurate water properties and ion-hydration dynamics from clusters to ice
13:10-13:20	Anamarija Abu el Rub	Metal nanoparticles funcionalized by amino acids: Experimental and computational insights
13:20-13:30	Ernesto Garcia Alfonso	Molecular Dynamics of Thiolate (Glutathione:AcCy) - Protected Au25 Nanoclusters for Photodynamic Therapy
13:30-13:40	Zyginta Murnikova	Study of Enhanced Solubility of Glibenclamide in Aqueous Ionic Liquid Solutions
13:40-13:55		Break
Session 4		Chair: Petra Čechová

13:55-14:15	Alessandro Nicoli	Ultra-large docking virtual screening of understudied GPCRs
14:15-14:35	Jacopo Lupi	Ammonia Formation in Glycine Pyrolysis via Novel Ionic-Pair Mechanisms
14:35-14:45	Adéla Chadalíková	Ammonia Formation in Glycine Pyrolysis via Novel Ionic-Pair Mechanisms
14:45-14:55	Joana Santos	Computational Design of Nature-Inspired Adsorbents Models for Pesticide Removal
14:55-15:05	Terri Field-Theodore	Interstellar insights into glycolonitrile formation
15:05-15:15		Closing Remarks