COSY WG3 S-2

Control at the Nanoscale – Manipulating Structure and Properties of Nanoscale Clusters – Recent Experimental and Theoretical Advances and Future Challenges

2nd 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 – November 27th 2023
https://cost-cosy.eu/activity/second-virtual-meeting-of-the-cosy-wg3/
https://www.linkedin.com/events/7125535662048489474/

Organized within the "COSY" COST Action (https://cost-cosy.eu/)
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The Symposium will be held on Zoom, please download Zoom in advance
Alessandro Fortunelli is inviting you to a Zoom meeting.
Topic: COSY WG3 S-2 symposium on "Control at the Nanoscale"
Date: 27 Nov 2023 08:30 AM – 05:30 PM Rome, Italy
To access Zoom, please copy&paste link in a browser a few ' in advance and then register with first/last name and email (we keep track for COST report)
https://us06web.zoom.us/j/82827390493
ID riunione: 828 2739 0493

Context

Following the 1st Virtual Symposium of the Working Group #3 (WG3) held last year on December 19th 2022, we decided to organized a similar one in this 2nd GP of the "COSY" Action: the **COSY WG3 S-2 SYMPOSIUM** "**Control at the Nanoscale - Manipulating Structure and Properties of Nanoscale Clusters. Recent Experimental and Theoretical Advances and Future Challenges**".

We recall that the goal of this COSY meeting, as of the Action itself, is to promote as much as possible scientific exchanges and triggering collaborations, and that WG3 sees a wide spread of expertise, systems, and topics, and a sheer impressive breadth of research topics, varying over confined systems (clusters) at different size régimes (10-5 nm, 1-5 nm, subnano) and material classes (metal or metal-oxide clusters/nanoparticles, deposited and on which substrate vs. colloidal and in which environment). The theme we have selected this year is: "Control at the Nanoscale", and its objective is to address the major challenge of research on confined nanosystems, i.e., to control "uncontrollable" matter (at both experimental and theoretical levels). We believe this theme is of general interest and broad enough to accommodate different perspectives, let's see how COSY members will interpret it!

To maximize discussions, also this year we decided to hold presentations in a "Faraday Discussions mode". Formally, we distinguish between "oral" and poster" presentations, which however differ only in the amount of time assigned:

longer ("oral") presentations (L) have 5' time to succintly describe their work (about 5-6 slides), followed by an open discussion and Q&A of about 15' time (open to all other attendants, both presenters and not)

shorter ("poster") presentations (S) will also have oral flash presentations of 2-3' time (about 2-3 slides), followed by an open discussion and Q&A of about 7-8' time

It is therefore **important for the good success of the meeting that attendees read in advance the DOIs/Links for each of the contributions**, **both oral and poster**: in the same way as in the Faraday Discussions series, participants will thus have the chance to know in advance the topic and the content of presentations, triggering discussions and interactions to maximum. Registration form: https://forms.gle/p9bvTfaYwgiYxJCK7.

We look forward to the meeting and we really hope that this unusual approach will be successful!

Acknowledgements
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Essential Program – November 27th 2023

08:50 – 09:10 Registration and Forewords

09:10 – 10:40 "Session 1 – Small Clusters" – **Chairs:** Fortunelli & Roongcharoen
Presenters: Lopez-Quintela (L), Carrol (L), Krupka (S), Sanader-Maršić (S), Quintana-González (S), Shi (S)

10:40 – 10:50 Short Break

10:50 – 12:20 "Session 2 – Larger Clusters and Particles" – **Chairs:** Moskaleva & Carroll
Presenters: Melani (L), Barrabés (L), Banu (S), Bruix (S), Laverdure (S), Roongcharoen (S), Fortunelli/Kadam (S)

12:20 – 13:20 Lunch Break

13:20 – 14:50 "Session 3 – Complex Processes under Confinement" – **Chairs:** Giovannini & Šekutor
Presenters: Mudric (L), Rupprechter (L), Zinzani (S), Marques (S), Santos (S), Ólafsson (S), Lushchikova (S)

14:50 – 15:00 Short Break

15:00 – 16:30 "Session 4 - Optical Properties" – **Chairs:** López & Melani
Presenters: Vanzan (L), Giovannini (L), Stener (S), Striccoli (S-1), Striccoli (S-2), Naumkin (S), Belo (S)

16:30 – 17:00 "Session 5 - Discussion on podcast and TFGs" – **Chairs:** Fortunelli & Moskaleva

Program with Titles of Presentations and DOIs/Links

08:50 – 09:10 Registration and Forewords

09:10 – 10:40 "Session 1 – Small Clusters" – **Chairs:** Fortunelli & Roongcharoen
M. Arturo Lopez-Quintela (L), 2D-polymerization on bulk inert surfaces using Ag5 and Cu5 clusters as extrinsic catalysts, Manuscript under review in Nature Chemistry, for the topic, see e.g. https://link.springer.com/referenceworkentry/10.1007/978-94-017-9780-1_55
Lenard Carroll (L), Carbon vacancy-assisted stabilization of individual Cu5 clusters on graphene. Insights from ab initio molecular dynamics, https://doi.org/10.1039/D2CP05843J
Katarzyna Krupka (S), A comprehensive study of intermolecular interactions between metal atomic quantum clusters (AQCs) and aromatic hydrocarbons, https://doi.org/10.1002/cphc.202300317, https://doi.org/10.1016/j.jcis.2021.12.186
Željka Sanader Maršić (S), Insights into the Impact of Gold Nanoclusters Au10SG10 on Human Microglia, https://doi.org/10.1021/acschemneuro.1c00621
Juan José Quintana González (S), Au@MoS2 structures: effect of shelling and defects engineering on the hydrogen production activity, https://doi.org/10.1016/j.ijhydene.2023.10.044
Junjie Shi (S), Gold clusters supported by ceria-praseodymia mixed oxides: Asymmetric oxygen vacancies induced high-performance water gas shift, https://doi.org/10.1016/j.apcatb.2021.120789

10:40 – 10:50 Short Break

10:50 – 12:20 "Session 2 – Larger Clusters and Particles" – **Chairs:** Moskaleva & Carroll
Giacomo Melani (L), First-principles simulations of catalytic reactions on metal surfaces with high-performance machine learning potentials, https://online.kitp.ucsb.edu/online/interfaces-c23/fortunelli/
Barrabés (L), Noelia Barrabes, Tuning catalytic active sites by monolayer protected metal nanoclusters at atomic level: core/ligands/support synergy and evolution under reaction conditions by operando spectroscopy, https://doi.org/10.1039/D2CP04498F, https://doi.org/10.1002/cctc.202200322, https://doi.org/10.1002/cctc.202200322, https://doi.org/10.1016/j.cattod.2022.02.014
Banu (S), Rares Banu, Reactivity and stability of thiolate protected chiral gold nanoclusters, https://doi.org/10.1021/acsnano.3c06568
Bruix (S), Albert Bruix, Combining global optimization and ab initio thermodynamics for the characterization of nanostructures under reaction conditions, https://doi.org/10.1063/5.0099927, https://doi.org/10.1038/s41929-019-0298-3
Laverdure (S), Laura Laverdure, Computational criteria for hydrogen evolution on Au25-based nanoclusters, https://doi.org/10.1021/acscatal.3c01065
Thantip Roongcharoen (S), Oxidation and de-alloying of PtMn particle models: a computational investigation, https://doi.org/10.1039/D2FD00107A
Alessandro Fortunelli/Shashikant Kadam (S), Support-oriented selectivity in the oxidative dehydrogenation of cyclohexane by CoFe2O4 nanoparticles, https://doi.org/10.1021/acscatal.3c02592

12:20 – 13:20 Lunch Break

13:20 – 14:50 "Session 3 – Complex Processes under Confinement" – **Chairs:** Giovannini & Šekutor
Marcel Mudrich (L), Helium nanodroplets as nano-cryo reactors for formation and spectroscopy of novel nanostructures, https://doi.org/10.1039/d3cp02879h
Günther Rupprechter (L), Directly observing the complexity of catalytic reactions on a nanoparticle by surface microscopy, https://doi.org/10.1038/s41467-023-43026-3
Sofia Zinzani (S), Effects of a surrounding environment during the coalescence of AuPd nanoparticles, https://doi.org/10.48550/arXiv.2307.14046
Jorge Marques (S), Aggregation of curcumin and piperine in a mixture of water and ethanol by molecular dynamics simulations, https://doi.org/10.1039/D3CP00096F

Joana Santos (S), Exploring the interaction of Imidacloprid with the Acetylcholine-Binding Protein by docking and molecular dynamics, https://drive.google.com/file/d/1-InobxDbiB_5f7a55J_wEg7hA-KAPCxZ/view?usp=drive_link
Sveinn Ólafsson (S), Progress in experimental characterisation of Rydberg matter of Hydrogen, https://doi.org/10.1088/1402-4896/ab1276
Olga Lushchikova (S), Solvation of Cun+/- with He and H2, https://doi.org/10.1039/D2CP04569A, https://doi.org/10.1039/D3CP03452F

14:50 – 15:00 Short Break

15:00 – 16:30 "Session 4 - Optical Properties" – **Chairs:** López & Melani
Mirko Vanzan (L), On the optical properties of Au-based nanoalloys, https://doi.org/10.1002/cphc.202200035
Tommaso Giovannini (L), Plasmonics of Bimetallic Nanoparticles: an Atomistic Classical Modeling, https://doi.org/10.3389/fphot.2023.1199598
Mauro Stener (S), A Resolution of Identity Technique to Speed up TDDFT with Hybrid Functionals: Implementation and Application to the Magic Cluster Series Au8n+4(SC6H5)4n+8 (n = 3–6), https://doi.org/10.1021/acs.jpca.3c05368
Marinella Striccoli (S-1), Semiconductor quantum dot dimers at sub-nanometer interparticle distance, https://doi.org/10.1007/s12274-020-2747-3
Marinella Striccoli (S-2), Dye derived carbon dots, https://doi.org/10.1021/acsnano.3c05566
Fedor Naumkin (S), Benzene complexes with main-group metal atoms: Structure/isomerization controlled aromaticity and IR spectra, https://doi.org/10.3390/molecules28165985
Dulce Belo (S), Single Component Molecular Metals, https://doi.org/10.1039/d1tc01407b, https://doi.org/10.1039/d0dt02931a

16:30 – 17:00 "Session 5 - Discussion on podcast and TFGs" – **Chairs:** Fortunelli & Moskaleva