CATCOSY 2026

Facing challenges on the characterization of subnanometric metal and metal oxide (photo-/electro-)catalysts

2nd International Workshop CATCOSY

https://cost-cosy.eu/activity/catcosy-2026/

Symposium within 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/]

in-person Meeting – July 2nd-3rd 2026, Pisa, Italy
at: Hotel Repubblica Marinara (https://hotelrepubblicamarinara.it/)

Organizers: Alessandro Fortunelli, María Pilar de Lara-Castells, Stefan Vajda
alessandro.fortunelli@cnr.it, pilar.delara.castells@csic.es, stefan.vajda@jh-inst.cas.cz
Local Organizers: Alessandro Fortunelli & Thantip Roongcharoen (CNR-ICCOM)
alessandro.fortunelli@cnr.it & thantip.roongcharoen@cnr.it
AF & TR thank Alessio Pacifici-Pace for technical support.

Context

Following the success and building on the experience of the 1st International Workshop CATCOSY 2024 (https://cost-cosy.eu/activity/workshop-facing-challenges/), we planned this 2nd International Workshop CATCOSY 2026 as a transversal workshop led primarily by WG3 members, but also of interest for WG1 and WG2 members of the COSY COST Action (https://cost-cosy.eu/). As in CATCOSY 2024, we will primarily address subnanometer-to-nanometer transition metal and metal-oxide (photo-/electro-)catalysts, and the understanding of their unique structure/relationship properties. We have convened some of the top expertise within the COSY network on the experimental synthesis and characterization via microscopy and spectroscopy techniques, and on advanced theoretical modeling of these fascinating systems. The topics will be related to the most critical catalytic processes facing modern society: achieving a neutral carbon cycle, via small molecule activation in both reduction of inert species (CH_4, CO_2, …) and degradation of noxious compounds in e.g. wastewater treatment, as well as for hydrogen production. The ultimate goal is to design highly performant, long-lived, selective, affordable, and sustainable (photo-/electro-)catalytic materials via a detailed atomistic understanding and predictive modeling of their structure and dynamics, achieved through the investigation of realistic as well as ideal, prototypical systems. Themes such as cluster/support interactions, cluster-cluster interactions, photo-induced activation and reactivity, various forms of IR, UV-vis and X-ray spectroscopies, fluxional behavior also due to Jahn-Teller and pseudo-Jahn-Teller distortions, non-adiabatic effects, charge state, and the experimental monitoring and theoretical description of all these phenomena will be targeted in the Workshop.

The program features 16 invited and contributed 30-minute lectures, and 15-minute hot topic presentations by young researchers of the COST Action, motivating representation of YRIs and ITCs, and attendance, poster presentations and flash poster presentations. The workshop will include a round table and final general discussion, as a platform for deeper discussions and exchange of ideas among participants.

Join us for two days of insightful presentations and stimulating discussions!

Alessandro Fortunelli, María Pilar de Lara-Castells, Stefan Vajda, & Thantip Roongcharoen

Acknowledgements

We gratefully thank the support of the COST Action CA21101, supported by COST (European Cooperation in Science and Technology). Disclaimer: All opinions are of the authors and cannot be attributed to COST.

Important Practical Information

The conference room is located in the basement of the Hotel Repubblica Marinara (https://hotelrepubblicamarinara.it/home/contatti/, info@hotelrm.it, Tel: +39 050 3870100, Fax: +39 050 3870200).

COST requirements for reimbursed participants

Participants reimbursed by COST should have *received and accepted* beforehand an invitation on the e-COST platform (https://e-services.cost.eu/). For each day of in-person attendance, they should also holographically sign an attendance form that will be posted on a table next to the entrance of the conference room.

Instructions for presentations

Invited talks have a total of 30 minutes for their presentation: 25' plus 5' discussion.
Hot Topic Talks have a total of 15 minutes for their presentation: 12' plus 3' discussion.
Hot Topic presenters feel free to *also bring your contribution as a Poster*.
Poster: size 90 cm x 60 cm (let us know if you need a different format), please prepare 2 slides for a 2' flash presentation (only Posters, not Hot Topic Talks).
The last slot on July 2nd will be a flash presentation of posters. This will be immediately followed by a poster session, held on July 2nd from 18:00 till 20:00 PM. Please note that *free light alcoholic and non-alcoholic beverages will be served during the poster session*.

Meals

All coffee-breaks are free.
Lunches are fixed [Menus (water and coffee included): July 2nd: Caprese di bufala DOP; Tagliata di pollo rucola e grana con patate al forno; July 3rd: Piccola Parmigiana di melanzane; Paccheri freschi alla primavera di verdure] and have a cost of 20 € each. Ideally, they should have been pre.booked at the gforms forms.gle/b7JWRmSEhhEmLpec7 and/or forms.gle/2ua9b5aeR1ssW7zT6: if you have reserved lunches, then please *contact the Hotel Reception to buy your lunch coupon(s) beforehand*.
For dinners at the Hotel Restaurant, we have negotiated a discount of 10% on the regular cost for CATCOSY2026 participants.

Program, participants, and final Round Table

A detailed program, and a list of attending and registered participants, with contributions, follow. Please note that we will have a very intense first day and morning of the second day. In the afternoon of the second day we have planned a "Round Table and General Discussion": the idea is to *discuss one by one the contributions of the participants still present*, especially perspectives and possible collaborations.

WiFi

The two available networks are: *devitaliahotspot* (in the hotel rooms) and *eventi* (in the workshop conference room). The Hotel will provide passwords on-site.

Tourism

Pisa is a well-known touristic site, and the Hotel is located not far from the city center. Please contact the Reception for more information.

Weather

Forecasts indicate highs around 35℃, and – what is worse – lows around 23-24℃, thus the usual recommendations of avoiding outdoor activities in the hottest hours and drinking a lot of water…!

	PROGRAM				
	Thursday July 2nd				
	Session 1 - 2 h CATALYSIS				
09:00	Carbon capture and utilization (CCU) strategies: from CO2 hydrogenation on unconventional catalysts to integrated CCU	Laurent	Piccolo	30'	IL
09:30	Catalysis by Supported (Sub)Nanometer Clusters: Size, Composition and Support Effects	Stefan	Vajda	30'	IL
10:00	Heterogeneous Platinum Catalysts for Hydrogen Production via Aqueous-Phase Reforming: Influence of Metal Nanoparticle Size and Support	Claudio	Evangelisti	30'	IL
10:30	High-Throughput and Conformal Funnels in NanoCatalytic Processes	Alessandro	Fortunelli	30'	IL
11:00	coffee-break 30'			30'	
	Session 2 - 1.5 h MICROSCOPY				
11:30	Contributions of Advanced Transmission Electron Microscopy techniques to Understand Catalysis: from Clusters to Reactors	Juan Carlos	Hernández Garrido	30'	IL
12:00	Sub-nanometer photo-induced dynamics probed by fast electrons	Yoshie	Murooka	30'	IL
12:30	Advanced Electron Microscopy of Clusters Grown Inside Superfluid Helium Droplets	Wolfgang	Ernst	30'	IL
13:00	lunch 1.5 h			90'	
	Session 3 - 2 h CARBONACEOUS				
14:30	Embedding Models for Complex Systems: from Solvation to Plasmonic Nanostructured Materials	Chiara	Cappelli	30'	IL
15:00	Design of Low-Iridium Containing Ir–Ru–W Nanocomposite for Acidic Oxygen Evolution Reaction: a cooperation between ErreDue and ICCOM-CNR, Pisa	Carolina	Castello	15'	HT
15:15	Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ-Graphyne	Massimiliano	Bartolomei	30'	IL
15:45	Sub-nm titanium dioxide clusters: efficient photocatalysts for clean SOx conversion under visible light irradiation	Shaimaa	Habib	15'	HT
16:00	Hydrogen dissociation reaction catalyzed by Rhodium clusters supported on Fullerene	Estefania	German	15'	HT
16:15	The Water Splitting reaction: single Fe-atoms catalyst supported on Fullerenes	Johanna Yasmin	Sandoval Menjivar	15'	HT
16:30	coffee-break 30'			30'	
	Session 4 - 1 h SUBNANOSYSTEMS				
17:00	From Clusters to Atoms: Spontaneous Room-Temperature Fragmentation of Early Transition Metal Nanoclusters on Fe_3O_4(001)	Gabriele	Coltrioli	15'	HT
17:15	Model catalytic studies on iron oxide and nitride 2D nanoislands	Weronika	Andrzejewska	15'	HT
17:30	Polymerization Catalysis by Quantum-confined Ag Clusters	Xinran	Lu	15'	HT
17:45	4 flash poster presentation			15'	
	Photocatalytic Degradation of Chlorophenols with Metallophthalocyanine/g-C_3N_4 Composites	Çağla	Akkol		P
	Structure-Property Relationships in Graphene Oxide - Magnetite Hybrid Nanomaterials	Aynura	Karimova		P
	Design of a New Magnetic Bio-Nanocomposite and Multivariate Optimization of Cd(II) Preconcentration from Environmental Samples	Aslıhan	Yilmaz Çamoğlu		P
	Solvent Extraction of Cu with D2EHPA: Screening of Factors by Box–Behnken Design	Louichaoui	Tassadit		P
	Session 5 - 2 h POSTER SESSION				
18:00	POSTER SESSION			120'	
20:00	dinner				

	PROGRAM				
	Friday July 3rd				
	Session 6 - 2 h PARTICLES & HOMOGENEOUS				
09:00	Selectivity and adsorption mechanism of Magnetic Iron Oxide and Graphene-based Nanoadsorbents in the Removal of Polyaromatic Pollutants in Water	Sylvie	Begin-Colin	30'	IL
09:30	A general theory for designing multishell chiral clusters	Riccardo	Ferrando	30'	IL
10:00	Exploring the use of Ag pentamers as catalytic antioxidant sub-nanoenzymes	M. Arturo	Lopez-Quintela	30'	IL
10:30	Accurate Simulations of Water and Aqueous Solutions through Machine-Learning Interatomic Potentials	Giuseppe	Brancato	30'	IL
11:00	coffee-break 30'			30'	
	Session 7 - 1.5/2 h ELECTRONIC STRUCTURE & REACTIVITY				
11:30	Subnanometric Transition-Metal Clusters. Jahn-Teller Distortions, Non-adiabatic Effects, and Ab Initio Benchmarking OF DFT for IR/Raman Spectra	María Pilar	de Lara-Castells	30'	IL
12:00	Icy-Grain Catalysis in Space: A Route toward Molecular Complexity	Cristina	Puzzarini	30'	IL
12:30	Shedding IR light on gas-phase metal clusters: insights into structures and reactions	André	Fielicke	30'	IL
13:00	lunch 2 h			120'	
	Session 8 - 1.5 h ROUND TABLE & GENERAL DISCUSSION				
15:00	ROUND TABLE & GENERAL DISCUSSION			90'	
16:30	final coffee-break 30'			30'	
17:00	end of the Workshop				

List of participants attending in person

akkolcagla@gmail.com	Çağla Akkol	Karadeniz Technical University, Turkey
weronika.andrzejewska@amu.edu.pl	Weronika Andrzejewska	Adam Mickiewicz University in Poznań, Poland
giovanni.barcaro@cnr.it	Giovanni Barcaro	CNR-IPCF, Italy
maxbart@iff.csic.es	Massimiliano Bartolomei	IFF-CSIC, Spain
sylvie.begin@unistra.fr	Sylvie Begin-Colin	CNRS&University of Strasbourg, France
giuseppe.brancato@sns.it	Giuseppe Brancato	Scuola Normale Superiore, Italy
chiara.cappelli@sns.it	Chiara Cappelli	Scuola Normale Superiore, Italy
carolinacastello@erreduegas.it	Carolina Castello	Erredue S.P.A., Italy
francesca.cicogna@cnr.it	Francesca Cicogna	CNR-ICCOM, Italy
serena.coiai@cnr.it	Serena Coiai	CNR-ICCOM, Italy
gabriele.coltrioli@phd.units.it	Gabriele Coltrioli	University of Trieste, Italy
pilar.delara.castells@csic.es	María Pilar de Lara-Castells	IFF-CSIC, Spain
wolfgang.ernst@tugraz.at	Wolfgang Ernst	Graz University of Technology. Austria
claudio.evangelisti@cnr.it	Claudio Evangelisti	ICCOM-CNR, Italy
riccardo.ferrando@unige.it	Riccardo Ferrando	University of Genoa, Italy
alfonso.ferretti@sns.it	Alfonso Ferretti	Scuola Normale Superiore, Italy
fielicke@fhi-berlin.mpg.de	André Fielicke	FHI-MPG, Germany
alessandro.fortunelli@cnr.it	Alessandro Fortunelli	CNR-ICCOM, Italy
Dr.MarioGallRguez@gmail.com	Mario Gallego Rodríguez	ITQ-CSIC, Spain
estefania.german@uva.es	Estefania German	Universidad de Valladolid, Spain
tommaso.giovannini@uniroma2.it	Tommaso Giovannini	University of Rome Tor Vergata, Italy
pablo.grobasillobre@sns.it	Pablo Grobas Illobre	Scuola Normale Superiore, Italy
shaimaa.habib@sci.dmu.edu.eg	Shaimaa Habib	Faculty of science Damanhour University, Egypt
jcarlos.hernandez@gm.uca.es	Juan Carlos Hernández Garrido	Universidad de Cádiz, Spain
aynurakarimova@bsu.edu.az	Aynura Karimova	Baku State University, Azerbaijan
malopez.quintela@usc.es	M. Arturo Lopez-Quintela	University of Santiago de Compostela, Spain
xinran.lu@usc.es	Xinran Lu	University of Santiago de Compostela, Spain
norma.mallegni@cnr.it	Norma Mallegni	CNR, ICCOM, Italy
y.murooka@liverpool.ac.uk	Yoshie Murooka	University of Liverpool, UK
elisa.passaglia@cnr.it	Elisa Passaglia	ICCOM-CNR, Italy
laurent.piccolo@ircelyon.univ-lyon1.fr	Laurent Piccolo	IRCELYON, France
emanuela.pitzalis@cnr.it	Emanuela Pitzalis	ICCOM CNR, Italy
cristina.puzzarini@unibo.it	Cristina Puzzarini	University of Bologna, Italy
thantip.roong1994@gmail.com	Thantip Roongcharoen	CNR-ICCOM, Italy
johannayasmin.sandoval@estudiantes.uva.es	Johanna Yasmin Sandoval Menjivar	University of Valladolid, Spain
sumesh4sai@gmail.com	Sumesh Sasidharan	Aix Marseille Univeristy, France
louichaouitassadit@gmail.com	Louichaoui Tassadit	University of Biskra, Algeria
stefan.vajda@jh-inst.cas.cz	Stefan Vajda	Czech Academy of Sciences, Czechia
kimyager.aslihanyilmaz@gmail.com	Aslıhan Yilmaz Çamoğlu	Karadeniz Technical University, Turkey

List of registered participants (alphabetic order by last name)

Last Name	First Name	Affiliation	Indirizzo email
Abbas	Akbar	University Of Chinese Academy Of Sciences	akbarabbas543@gmail.com
Abghoui	Younes	University Of Iceland	younes@hi.is
Akkol	Çağla	Karadeniz Technical University	akkolcagla@gmail.com
Ali	Basharat	Pavol Jozef Safarik University	basharat.ali@student.upjs.sk
Alshayeb	Abdulrahman	Sakarya University, Türkiye	abdul.alshayeb@ogr.sakarya.edu.tr
Andrzejewska	Weronika	Adam Mickiewicz University	weronika.andrzejewska@amu.edu.pl
Ashraf	Muhammad Faisal	Institute Of Experimental Physics Sas	ashraf@saske.sk
Barcaro	Giovanni	Cnr-Ipcf	giovanni.barcaro@cnr.it
Bartolomei	Massimiliano	Instituto De Física Fundamental - Csic	maxbart@iff.csic.es
Bayar Muluk	Nuray	Kirikkale University	nuray.bayar@yahoo.com
Begin	Sylvie	Université De Strasbourg	sylvie.begin@unistra.fr
Berisha	Avni	University Of Prishtina	avni.berisha@uni-pr.edu
Bondi	Riccardo	Erredue Spa	riccardobondi@erreduegas.it
Brancato	Giuseppe	Scuola Normale Superiore	giuseppe.brancato@sns.it
Cabuk	Mehmet	Mersin University	mehmetcabuk@mersin.edu.tr
Cappelli	Chiara	Scuola Normale Superiore	chiara.cappelli@sns.it
Castello	Carolina	Erredue SPA, Italy	carolinacastello@erreduegas.it
Cicogna	Francesca	Cnr Iccom Ss Pisa	francesca.cicogna@cnr.it
Coiai	Serena	Cnr Iccom Ss Pisa	serena.coiai@cnr.it
Coltrioli	Gabriele	University Of Trieste	gabriele.coltrioli@phd.units.it
De Lara-Castells	María Pilar	Iff-Csic	pilar.delara.castells@csic.es
Demiroglu	Ilker	Assistant Professor	ilkerdemiroglu@eskisehir.edu.tr
Eren	Seçil	Sinop University /Physics Department	secileren.ph@gmail.com
Ernst	Wolfgang	Graz University Of Technology	wolfgang.ernst@tugraz.at
Evangelisti	Claudio	Iccom-Cnr	claudio.evangelisti@cnr.it
Ferrando	Riccardo	University Of Genoa	riccardo.ferrando@unige.it
Ferretti	Alfonso	Scuola Normale Superiore Di Pisa	alfonso.ferretti@sns.it
Fielicke	André	Fritz-Haber-Institut, Berlin	fielicke@fhi-berlin.mpg.de
Fortunelli	Alessandro	Cnr-Iccom, Pisa, Italy	alessandro.fortunelli@cnr.it
Gahramanli	Lala	Nano Research Laboratory	gahraman.lala@gmail.com
Gallego Rodríguez	Mario	CSIC, Spain	Dr.MarioGallRguez@gmail.com
German	Estefania	Universidad De Valladolid	estefania.german@uva.es
Giovannini	Tommaso	University Of Rome Tor Vergata	giovannini.tommaso@gmail.com
Grobas Illobre	Pablo	Scuola Normale Superiore	pablo.grobasillobre@sns.it
Habib	Shaimaa	Damanhour University	shaimaa.habib@sci.dmu.edu.eg
Hernández Garrido	Juan Carlos	Universidad De Cádiz	jcarlos.hernandez@gm.uca.es
Horrillo Güemes	Carmen Horrillo Güemes	Itefi-Csic	carmen.horrillo.guemes@csic.es
Jamal	Muhammad Wajdan		wajdanjamal25@gmail.com
Karaca	Ertugrul	Sakarya University	ertugrulkaraca@sakarya.edu.tr
Karimova	Aynura	Baku State University	aynurakarimova@bsu.edu.az
Kavak	Hamide	Cukurova Univsersity	hkavak@cu.edu.tr
Kumar	Vipin	Technical University Of Darmstadt	vipinkumar0247@gmail.com
Lopez-Quintela	M. Arturo	University Of Santiago De Compostela, Spain	malopez.quintela@usc.es
Lu	Xinran	University Of Santiago De Compostela, Spain	xinran.lu@usc.es
Mallegni	Norma	Cnr, Iccom	norma.mallegni@cnr.it
Martin Encinar	Luis	University Of Valladolid	luis.martin.encinar@uva.es
Murooka	Yoshie	The University Of Liverpool	y.murooka@liverpool.ac.uk
Passaglia	Elisa	Iccom-Cnr Pisa	elisa.passaglia@cnr.it
Paz	Guadalupe Paz	Inifta, Universidad Nacional De La Plata	guadalupepaz@inifta.unlp.edu.ar
Piccolo	Laurent	Ircelyon, France	laurent.piccolo@ircelyon.univ-lyon1.fr
Pitzalis	Emanuela	Iccom Cnr	emanuela.pitzalis@cnr.it
Puzzarini	Cristina	University Of Bologna	cristina.puzzarini@unibo.it
Qadeer	Abdul	Scuola Normale Superiore Di Pisa	abdul.qadeer@sns.it
Roongcharoen	Thantip	Cnr-Iccom	thantip.roong1994@gmail.com
Sandoval Menjivar	Johanna Yasmin	University Of Valladolid	johannayasmin.sandoval@estudiantes.uva.es
Sasidharan	Sumesh	Aix Marseille University	sumesh4sai@gmail.com
Serdaroğlu	Vildan	Karadeniz Technical University	vildanserdaroglu@ktu.edu.tr
Sher	Farooq	Nottingham Trent University	Farooq.Sher@ntu.ac.uk
Tassadit	Louichaoui	University of Biskra, Alegria	louichaoui.tassadit@gmail.com
Vajda	Stefan	J Heyrovsky Institute Of Physical Chemistry	stefan.vajda@jh-inst.cas.cz
Yılmaz	Murat	Osmaniye Korkut Ata University	muratyilmaz@osmaniye.edu.tr
Yılmaz Çamoğlu	Aslıhan	Kardeniz Technical University	kimyager.aslihanyilmaz@gmail.com
Özbek	Nurhayat	Karadeniz Technical University	nrhytozbek@gmail.com

the complete list of submitted abstract follows (alphabetic order by last name)

Younes Abghoui

University of Iceland

younes@hi.is

Comparing Hydrogen Fuel Cells and Lithium-Ion Batteries for Sustainable Electric Vehicles

This work presents a comparative assessment of two leading energy storage technologies for electric vehicles (EVs): hydrogen fuel cells (HFCs) and lithium-ion batteries (LIBs). As demand for sustainable mobility increases, understanding the technological capabilities, limitations, and system-level implications of these technologies is essential for informed deployment across different transport applications.

Key performance metrics; including energy density, efficiency, charging/refueling characteristics, and environmental impact are examined to highlight the relative strengths and constraints of HFCs and LIBs. The analysis shows how LIBs currently dominate passenger EVs due to mature infrastructure and high efficiency, while HFCs offer advantages for long-range, heavy-duty, and fast-refueling applications where batteries face practical limitations.

Beyond device performance, the poster discusses infrastructure requirements, resource availability, and economic considerations that influence large-scale adoption. Recent technological developments and emerging trends are considered to evaluate how future advances may reshape the role of batteries and hydrogen in sustainable transportation.

In addition, innovative surface modification approach for cathode materials for the hydrogen evolution reaction (HER) is presented, highlighting novel material candidates with promising catalytic properties. These findings point toward opportunities for improving hydrogen production efficiency and support further investigation toward scalable and commercially relevant hydrogen technologies.

Çağla Akkol

Karadeniz Technical University

akkolcagla@gmail.com

The performance of phthalocyanine-based catalysts for photocatalytic degradation of chlorophenols

Photocatalysis is one of the promising techniques used in the degradation reactions of organic pollutants and is gaining increasing attention. Nowadays, using economical and environmentally friendly solvents, especially water, is of great importance in terms of green chemistry [1]. Chlorophenols are organic pollutants with high toxicity and environmental persistence, formed by the attachment of one or more chlorine atoms to a phenol ring. Chlorophenols, which enter aquatic environments through industrial wastewater, can remain in the environment for a long time due to their resistance to natural degradation.

In recent years, MPCs have attracted significant attention in catalysis due to the high catalytic activity of MPc that can be associated with central metal ions [2]. Cobalt and copper phthalocyanine (CoPc and CuPc), as transition metal complex catalysts with M-N4 active center, are among the most promising catalysts for this task due to their high activity and selectivity in oxidation processes[3]. Graphitic carbon nitride (g-C_3N_4) is a metal-free, chemically stable semiconductor with a suitable band gap that enables visible-light-driven photocatalysis. Owing to its low cost and facile synthesis, it has attracted significant attention for applications such as water splitting, CO_2 reduction, and environmental using photocatalytic processes [4]. In the study The photocatalytic performances of metallophthalocyanines/graphitic carbon nitride composites will be systematically investigated for the degradation of chlorinated phenolic pollutants, namely 2-chlorophenol, 2,3-dichlorophenol, and 2,3,6-trichlorophenol, under visible-light irradiation.DOI: 10.1016/j.inoche.2026.116457

Çağla Akkol

Karadeniz Technical University

akkolcagla@gmail.com

Photocatalytic Degradation of Chlorophenols with Metallophthalocyanine/g-C_3N_4 Composites

The degradation of chlorophenols is crucial to remove toxic, persistent, and bioaccumulative pollutants from the environment, protect ecosystems and human health, and enable sustainable pollution management through bioremediation and green chemistry. In this study, 2(3), 9(10), 16(17), 23(24)-Tetrakis-[ethyl (E)-3-[4-(phenoxy)phenyl]acrylate phthalocyaninato copper (II) (EpCA-CuPc) and 2(3), 9(10), 16(17), 23(24)-Tetrakis-[ethyl (E)-3-[4-(phenoxy)phenyl]acrylate phthalocyaninato cobalt (II) (EpCA-CoPc) were synthesized and characterized with different spectral techniques (FT-IR, UV–Vis and Mass) to undergo π-π interaction with graphitic carbon nitride to produce an effective catalyst. Two effective catalysts' structure were identified with FT-IR, SEM, XRD and BET then, their photocatalytic performances, recycling works in 2-chlorophenol, 2,3-dichlorophenol, and 2,3,6-trimethyl phenol degradation were examined. The optimum catalyst loading for the MPc/g-C_3N_4 composites was determined as 0.5 g/L, providing the highest photocatalytic efficiency. The EpCA-CoPc/g-C_3N_4 catalyst achieved 93.2% product selectivity and 85.8% conversion in the oxidation of 2-chlorophenol, while the EpCA-CuPc/g-C_3N_4 catalyst achieved approximately 87% removal. The conversion order of the pollutants was 2-CP > 2,3-DCP > 2,3,6-TCP, with benzoquinone derivatives identified as the major oxidation products. In recycling tests, both catalysts retained more than 50% of their activity after five cycles; EpCA-CoPc/g-C_3N_4 reached 65% conversion after the 4th cycle, and EpCA-CuPc/g-C_3N_4 reached 63% after the 3rd cycle.(Inorganic Chemistry Communications, 116457, 2026)

Basharat Ali

Pavol Jozef Safarik University - Centre of Low Temperature Physics, Faculty of Science - Slovakia (SK)

basharat.ali@student.upjs.sk

Tuning cerium(III) magnetism by confinement: intercalation of a dinuclear aqua-chlorido complex in synthetic saponite

The intercalation of cerium(III) chloride heptahydrate into synthetic saponite (Sap) was investigated by direct ion exchange, affording a Ce-Sap hybrid material whose structural, thermal and magnetic properties were compared with those of the parent hydrate. Single-crystal analysis of CeCl3·7H2O reveals dimeric aqua-chlorido complex cations, [Ce2(H_2O)14Cl2]4+, charge-balanced by chloride anions, highlighting a distinct structural motif relative to mononuclear lanthanide chloride hydrates. Powder X-ray diffraction and thermogravimetric analysis confirm successful intercalation and indicate reduced thermal stability of Ce-Sap, consistent with partial dehydration and confinement of hydrated Ce(III) species within the clay interlayers. The study of static magnetic properties confirmed magnetic coupling within {Ce2} dimers in CeCl3·7H2O, presumably of antiferromagnetic origin. The two lowest excited doublets induced by single-ion anisotropy are proposed to contribute to the decrease of the effective magnetic moment in CeCl3·7H2O upon cooling. The investigation of the dynamic response confirmed a narrow distribution of the relaxation times for both studied systems. Magnetic relaxation in CeCl3·7H2O is characterized by crossover from temperature-independent behavior governed by cross-relaxation and a thermally activated process of Orbach type with the energy gap Δ/kB= 51.5 K. The obtained value agrees reasonably with the energy of the first excited doublet of 82.6 K, as well as that of the lowest local vibrational mode of 72 K obtained by simulation of molecular dynamics. In contrast, the intercalated material Ce-Sap lacks cross-relaxation, consistent with a substantial structural reorganization upon intercalation; the dominant interlayer species are tentatively assigned as highly hydrated [Ce(H2O)9]3+ (or closely related hydration states). The remaining thermally activated relaxation in Ce-Sap is tentatively attributed to a pronounced phonon-bottleneck effect enabled by weak coupling of the hydrated Ce(III) centers to the host lattice.

Basharat Ali

Pavol Jozef Safarik University - Centre of Low Temperature Physics, Faculty of Science - Slovakia (SK)

basharat.ali@student.upjs.sk

Synergistically Engineered Cr_2O_3/WO_3 Heterostructures for Bifunctional Water Splitting and Energy Storage Applications

Herein we report the synthesis of Cr2O3@WO3 and WO3 nanostructures using a solvothermal method, which just needs mild conditions. The response of the Cr2O3@WO3-based nanocomposite is much higher than that of pristine Cr2O3 and WO3-based nanostructures. The nanocomposites of Cr2O3@WO3 exhibited better electrocatalytic activity, at a current density of 10 mAcm−2 in alkaline media, with low overpotentials of 128.9 and 382mV for hydrogen and oxygen evolution processes (HER and OER), respectively. Moreover, this material exhibits excellent kinetics, a high electrochemically active surface area, low charge transfer resistance, and great long term stability for 12 hours. By using galvanostatic charge-discharge (GCD), electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV), the supercapacitive characteristics of these nanoparticles were examined. At a current density of 0.8 A/g, the Cr2O3@WO3 nanocomposite achieved a specific capacitance of 1470 F/g. The supercapacitor made of Cr2O3@WO3 shows an impressive 76.92 % capacitance retention after 5000th cycles. In an alkaline environment, Cr2O3@WO3 has a power density of 160 W/kg and an energy density of 32.7 Wh/kg. The reason for the response is considered to be that a heterostructure is formed between Cr2O3 (a P-type semiconductor) and WO3 (an N-type semiconductor).

Abdulrahman Alshayeb

Sakarya University, Türkiye

abdul.alshayeb@ogr.sakarya.edu.tr

Ab Initio Investigation of the Elastic and Mechanical Properties of Cr_3Rh: A Density Functional Theory Study

Chromium-based compounds are of significant interest in condensed matter physics due to their diverse electronic and structural properties. However, the elastic behavior of the Cr3Rh system remains largely unexplored from a theoretical perspective. In this work, we present a comprehensive first-principles study of the structural and elastic properties of Cr3Rh using Density Functional Theory (DFT) as implemented in the Quantum ESPRESSO package.

To ensure an obtimal physical description, we investigate the influence of Spin-Orbit Coupling (SOC) compared to Non-Spin-Orbit Coupling (NSOC) calculations on the mechanical stability and elastic constants Cij. We report the calculated bulk modulus, shear modulus, and Young's modulus, providing insight into the material's stiffness and brittle-versus-ductile transition. Our preliminary results aim to provide the first theoretical benchmark for the elastic landscape of Cr3Rh offering a foundation for future experimental verification and potential applications in specialized alloy design.

Weronika Andrzejewska

NanoBioMedical Centre, Adam Mickiewicz University in Poznań, Poland

weronika.andrzejewska@amu.edu.pl

Interaction of O_2 with ultrathin iron nitride islands on Cu(001) and Cu(111)

Iron nitrides constitute an interesting group of materials with superior magnetic properties. They also exhibit catalytic activity in several industrially-relevant reactions or appear as intermediate phases, e.g. during ammonia (NH3) oxidation over iron oxides. However, the mechanisms underlying the chemistry of different iron nitride surfaces are, to a wide extent, unexplored. We have studied the interaction of molecular oxygen (O2) with ultrathin iron nitride islands epitaxially grown on Cu(001) and Cu(111) single-crystal substrates. The obtained scanning tunneling microscopy and spectroscopy (STM/STS), low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) results reveal the differences in the structure of the islands on both supports and provide information on the oxygen adsorption on the studied iron nitride surfaces. Notably, quadrupole mass spectroscopy (QMS) data prove that reaction of dissociated O atoms with the lattice N atoms in iron nitride leads to the formation of nitric oxide (NO) – one of common products of NH3 oxidation.

Acknowledgments

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Massimiliano Bartolomei

Instituto de Física Fundamental - CSIC (Madrid, Spain)

maxbart@iff.csic.es

Carbon Dioxide Preferential Adsorption and Conversion on Sodium Decorated γ-Graphyne

Addressing carbon dioxide (CO2) emissions represents a major challenge for modern society and the development of innovative and efficient technologies for CO2 capture and conversion is paramount. Carbon materials are promising candidates for this purpose due to their versatility and sustainability. Here, we theoretically demonstrate that gamma-graphyne two-dimensional carbon layers hosting sodium (Na) atoms upon its subnanometric pores show a significant and selective adsorption of CO2 with respect to other representative post-combustion gas species. In particular, this occurs for a high density of Na decoration over the carbon surface and in such cases CO2 is adsorbed as an activated anionic species. Importantly, in this activated form CO2 becomes very reactive and can be easily converted into sodium formate via a highly exothermic process. These findings suggest that Na-decorated gamma-graphynes represent very promising adsorbing platforms based on earth-abundant elements to be used for the efficient CO2 capture and in-situ conversion into added-value products.

Sylvie Begin

ICPEES UMR 7515 CNRS Université de Strasbourg

sylvie.begin@unistra.fr

Selectivity and adsorption mechanism of Magnetic Iron Oxide and Graphene-based Nanoadsorbents in the Removal of Polyaromatic Pollutants in Water

The widespread presence of polycyclic aromatic hydrocarbons (PAHs) in water has driven the development/urgent need of advanced nanomaterial-based adsorption strategies for water decontamination. Here, few-layer graphene/tannic acid/iron oxide nanocomposites (FLG@TA@RSN), as well as bare iron oxide raspberry-shaped nanostructures (RSN) and tannic acid-functionalized RSN (RSN@TA), were synthesized for the removal of a mixture of 15 fluorescent priority polycyclic aromatic hydrocarbons (PAHs) in water. The FLG@TA@RSN composite material exhibited the best overall adsorption performance, with removal efficiencies (RE) above 96% for the largest 8 of the 15 PAHs . Increasing the concentration of the composite from 500up to 1,000 mg/L enhanced the uptake of smaller PAHs, such as pyrene, fluoranthene, anthracene and phenanthrene. Interestingly, both RSN and RSN@TA also demonstrated significant adsorption of especially larger PAHs, particularly (RE>70%), showing that they also contribute highly to PAHs removal. Such a selectivity for PAHs such as benzo(a)anthracene and larger was observed for RSN and RSN@TA at any adsorbent concentration. Analysis of adsorption mechanisms showed that PAHs adsorption occurred primarily through π - π stacking with the composite, while Fe-OH - π interactions were identified for RSN and RSN@TA following an investigation of possible interactions mechanisms. These findings highlight the synergistic performance of the magnetic FLG@TA@RSN composites and reveal intrinsic adsorption capabilities and selective behavior of iron oxide-based nanomaterials, providing new insights into the adsorption mechanisms of the different developed adsorbents.

Avni Berisha

University of Prishtina

avni.berisha@uni-pr.edu

Cluster–Cluster Interactions in $Be_{12}O_{12}$ and $Mg_{12}O_{12}$ Subnanometric Oxide Clusters: Insights from Population Analysis, QTAIM, RDG, and DLPNO-CCSD(T) Energy Decomposition

Subnanometric oxide clusters, such as $Be_{12}O_{12}$ and $Mg_{12}O_{12}$, are attracting increasing attention as model systems for understanding catalytic behavior at the nanoscale. While their individual properties are relatively well explored, much less is known about what happens when these clusters interact with each other. In realistic catalytic environments, such interactions are unavoidable and can lead to subtle but important changes in electronic structure and reactivity. In this contribution, we take a closer look at how $Be_{12}O_{12}$ and $Mg_{12}O_{12}$ clusters influence one another when brought into contact. Using density functional theory (DFT), we examine how electron density redistributes at the cluster interface. Population analysis (Mulliken and Hirshfeld) helps us follow charge transfer, while QTAIM provides a detailed picture of bonding features. At the same time, RDG analysis allows us to visualize the noncovalent interactions that stabilize these cluster assemblies.

To go a step further, we apply the local energy decomposition (LED) approach within the DLPNO-CCSD(T) framework, which enables us to break down the interaction into physically meaningful contributions such as electrostatics, exchange, dispersion, and correlation.

By combining these complementary tools, we aim to build a clear and intuitive atomistic picture of cluster–cluster interactions and their consequences for electronic structure. Ultimately, this understanding can help guide the design of more efficient and cooperative catalyst systems based on interacting subnanometric clusters.

Giuseppe Brancato

Scuola Normale Superiore

giuseppe.brancato@sns.it

Accurate Simulations of Water and Aqueous Solutions through Machine-Learning Interatomic Potentials

Dispersion-corrected density functional theory (DFT-D) is widely employed to model large molecular systems at an affordable computational cost and to develop machine-learning interatomic potentials (MLIPs), enabling reliable molecular dynamics (MD) simulations of condensed-phase systems. Yet, given a molecular system, the choice of a specific DFT-D model that can achieve the necessary accuracy over an extended range of physicochemical properties and conditions is generally not trivial. Here, we report an effective computational strategy for enhancing the accuracy of standard DFT-D models toward high-level quantum mechanical data and for developing MLIPs preserving the same high fidelity. Taking water as a paradigmatic example, we derive a novel MLIP and demonstrate that its use allows us to accurately predict a wide range of properties in diverse forms, from small clusters to bulk liquid and ice, such as radial distribution functions, fusion/vaporization enthalpies, diffusion constants, and density isobars, capturing remarkably well its peculiar and anomalous behavior, often elusive even to standard first-principle MD simulations. Furthermore, we show how the same computational strategy can be readily extended to treat aqueous solutions: we develop a MLIP and use it to predict the metal ion hydration structure and the water exchange dynamics exhibiting a significantly improved agreement with experiments with respect to both standard DFT-D and classical force fields.

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Mehmet Cabuk

Mersin University

mehmetcabuk@mersin.edu.tr

Electrorheological Behavior of Magnetic and Conducting Co-Ferrite/ Chitosan Biocomposite Particles

Electrorheological fluids, magnetic nanoparticles, biocomposites

Chiara Cappelli

Scuola Normale Superiore

chiara.cappelli@sns.it

Embedding Models for Complex Systems: from Solvation to Plasmonic Nanostructured Materials

Fully atomistic multiscale approaches have demonstrated considerable success in modeling complex systems in the condensed phase. A particularly effective strategy, especially employed for solvated systems, involves focusing on a specific portion described at the Quantum Mechanical (QM) level, while treating the remaining portion classically using tailored Molecular Mechanics (MM) force-fields. Extending such methodologies to complex plasmonic nanostructured materials poses additional challenges because resonance with external probing fields must be considered.

I will focus on recent contributions to the development of fully atomistic multiscale approaches for complex systems, showcasing pilot applications that underscore the potential of these methods.

Carolina Castello

Erredue spa

carolinacastello@erreduegas.it

Design of Low-Iridium Containing Ir–Ru–W Nanocomposite for Acidic Oxygen Evolution Reaction: a cooperation between ErreDue and ICCOM-CNR, Pisa

Iridium oxide-based electrocatalysts are widely considered as the most practical anodic catalysts for proton exchange membrane water electrolysis (PEMWE) due to their high activity as well as their exceptional stability in the acidic oxygen evolution reaction (OER). However, their use on a large scale is limited by the high cost and limited reserves of iridium metal. Herein, we present a IrRuW-based mixed oxide material containing a relatively modest iridium content of 23 atom % with respect to the total metal amount. The morphological, structural, and textural properties of the freshly prepared material were investigated by X-ray diffraction (XRD), N2 physisorption, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS) techniques. The material, tested in rotating disk electrode (RDE) half-cell experiments, exhibited improved OER electrocatalytic performance in HClO4 0.1 M (i.e., −80 mV potential at 10 mA/cm2) compared to IrO2 and IrRuOx, respectively, used as benchmark catalysts. The electrocatalytic performances of the trimetallic system were then studied in a lab-scale and up-scaled industrial PEMWE cell setup, confirming its applicability in real flow-cell setups: a stable 2.05 V for over 500 h of utilization at 0.8 A/cm2 was registered. XRD, TEM, and inductively coupled plasma-optical emission spectroscopy (ICP-OES) analysis of the postcatalysis IrRuWOx and IrRuOx systems, respectively, pointed out the beneficial effect of the presence of tungsten on the final structural stability/durability of the material, together with no Ru leaching for the trimetallic system.

Gabriele Coltrioli

University of Trieste

gabriele.coltrioli@phd.units.it

From Clusters to Atoms: Spontaneous Room-Temperature Fragmentation of Early Transition Metal Nanoclusters on $Fe_3O_4(001)$

The stability of supported nanoclusters is a central challenge in the quest to designing durable heterogeneous catalysts. While degradation is typically attributed to thermally driven sintering, we report an alternative pathway: the spontaneous non-thermal fragmentation of size-selected early transition metal nanoclusters on reconstructed $Fe_3O_4(001)$. By combining High Resolution X-ray Photoelectron Spectroscopy with Density Functional Theory, we show how the clusters dissociate into atomic species at room temperature with no exposure to reactive gases. This behavior arises from the interplay between the metal-oxygen bonding and the surface reconstruction, which together overcome the intrinsic metal-metal cohesion.

The fragmentation tendency follows the trend Ta > W > Mo, in direct correlation with metal oxophilicity and adsorption energies. Further oxidation enhances fragmentation, particularly for larger clusters, ultimately yielding highly dispersed metal species. These results identify adsorption-induced fragmentation as a fundamental expression of metal-support interactions, introducing a non-thermal route to the generation of high-density single-atom sites from nanocluster precursors, offering a new paradigm for the design of next-generation catalysts.

María Pilar de Lara-Castells

IFF-CSIC

pilar.delara.castells@csic.es

Subnanometric Transition-Metal Clusters. Jahn-Teller Distortions, Non-adiabatic Effects, and Ab Initio Benchmarking OF DFT for IR/Raman Spectra

Recent advances in the synthesis and characterization of atomically precise, monodisperse metal clusters (AMCs), composed of only one to ten atoms, are providing unprecedented insight into the physical and chemical nature of matter. Their quantized, "molecule-like" electronic structure imparts unusual stability and properties that differ markedly from those of both nanoparticles and bulk materials. When incorporated into materials that interact with environmental molecules and sunlight, AMCs can exhibit enhanced (photo)catalytic activity, alongside distinctive electronic and optical properties [1,2,8].

In this lecture, state-of-the-art ab initio modeling of both free and surface-supported AMCs will be presented, drawing on an overview of recent studies [1–13]. Particular emphasis will be placed on *ab initio* evidence supporting the description of AMCs as fluxional Jahn–Teller systems [1,5,11,12], the influence of AMC–support interactions on associated conical intersections [7], and the role of non-adiabatic effects in their reactivity in O2-rich environments. Finally, recent progress in the *ab initio* benchmarking of density functional theory (DFT) methods for predicting IR and Raman spectra of AMCs will be highlighted, including the effects of anharmonicity and bimetallic intermixing [12,13].

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Ilker Demiroglu

Eskişehir Teknik Üniversitesi

ilkerdemiroglu@eskisehir.edu.tr

Machine-Learning Interatomic Potentials for O_2- and CO-Functionalized Au–Rh Nanoparticles

Bimetallic Au–Rh nanoparticles are promising catalysts for oxidation and (de)hydrogenation reactions, yet first-principles simulations at realistic sizes and temperatures are computationally prohibitive. Here, we develop machine-learning interatomic potentials for O_2- and CO-functionalized Au–Rh nanoparticles that retain near density-functional theory (DFT) accuracy while enabling large-scale, finite-temperature simulations.

The models are trained on ab initio molecular dynamics data spanning multiple temperatures, particle sizes, and morphologies (pure, core–shell, Janus, and ordered alloys). The dataset is carefully filtered and balanced to ensure diverse and physically meaningful atomic configurations. Validation against DFT shows high accuracy for both energies and forces across all systems, with no evidence of overfitting to specific structures.

Finite-temperature analysis using radial distribution functions reveals that alloyed nanoparticles—especially core–shell and Janus morphologies—better preserve short-range order upon heating compared to ordered alloys and monometallic counterparts, indicating enhanced thermal robustness.

The developed potentials enable the investigation of catalytic phenomena beyond the reach of direct electronic-structure methods, including coverage-dependent stability, adsorbate-induced restructuring, competitive adsorption, and morphology evolution under realistic conditions.

Seçil Eren

Sinop University /physics department

secileren.ph@gmail.com

Synthesis and Spectroscopic Characterization of Mixed-Ligand Metal Complexes and Quinolone Derivatives

This study focuses on the experimental synthesis of new transition metal complexes using quinolone-based ligands. The structural properties and coordination environments of these mixed-ligand complexes are investigated through detailed spectroscopic techniques, including FT-IR and UV–Vis. The study aims to evaluate the molecular stability of the synthesized metal systems and their potential catalytic or biological applications within the scope of WG2 activities.

Wolfgang Ernst

Technische Universität Graz

wolfgang.ernst@tugraz.at

Advanced Electron Microscopy of Clusters Grown Inside Superfluid Helium Droplets

Superfluid helium nanodroplets act as ultracold, nanoscale “cryostats” that enable the synthesis of exceptionally pure metallic, bimetallic, and hybrid nanoparticles with precise control over size and architecture. This review highlights how advanced electron

microscopy—particularly aberration-corrected scanning transmission electron microscopy combined with spectroscopy—reveals the structure, composition, and three-dimensional morphology of these particles at near-atomic resolution.

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Claudio Evangelisti

ICCOM-CNR

claudio.evangelisti@cnr.it

Heterogeneous Platinum Catalysts for Hydrogen Production via Aqueous-Phase Reforming: Influence of Metal Nanoparticle Size and Support

The global drive toward clean and sustainable energy systems has intensified interest in hydrogen as a versatile, carbon neutral energy carrier and a viable alternative to fossil fuels. Although catalytic steam reforming of fossil fuels remains the dominant route for hydrogen production, its significant environmental drawbacks have spurred the search for greener and more sustainable alternatives. In this context, aqueous phase reforming (APR) of biomass derived compounds has emerged as a promising strategy for hydrogen generation, owing to its relatively mild operating conditions and its potential for carbon neutral operation.

In this work, we report the synthesis of Pt clusters (average diameter d = 0.35 nm), size controlled Pt nanoparticles (d = 1.5 and 2.5 nm), prepared via the metal vapor synthesis (MVS) method, as well as Pt single atom catalysts (SACs) supported on high surface area carbon materials, including both commercially available and nitrogen doped carbons. The catalytic performance of these materials was investigated in the APR of biomass derived oxygenated compounds, namely ethylene glycol and glycolic acid, as well as methanol, toward hydrogen production. Particular attention will be devoted to elucidating the relationship between the morphological and structural features of the supported Pt species and their catalytic behavior in terms of activity, selectivity, and long term stability.

Riccardo Ferrando

University of Genoa

riccardo.ferrando@unige.it

A general theory for designing multishell chiral clusters

Here we show a general method to construct icosahedral clusters made of shells containing different atomic species [1]. Cluster structures are mapped into paths in the close-packed two dimensional lattice. In this way, both chiral and achiral structures mnaturally emerge. The theory is applied to a variety of binary, ternary and quaternary systems for both transition and alkali metal clusters.

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André Fielicke

Fritz-Haber-Institut, Berlin

fielicke@fhi-berlin.mpg.de

Shedding IR light on gas-phase metal clusters: insights into structures and reactions

Transition metal clusters are frequently used as model systems for low coordinated sites of extended surfaces and their study can provide valuable insights into the mechanisms of surface reactions. In many cases, however, there is still a lack of information on their structures and the relationship between structure and chemical behaviour. Using vibrational spectroscopy of gas-phase clusters one can obtain information about the clusters' structure or the behaviour of adsorbed species. The latter provides valuable insights into the binding geometry, the activation of bonds within the ligands or reactions occurring on the clusters' surface. Cluster size specific data can be obtained using infrared multiple photon dissociation spectroscopy. To cover the required spectral range from the far to the mid-IR our experiments make use of IR free electron lasers. The talk will sketch our endeavours to obtain structural information for neutral gold clusters up to Au20 and present new data for the activation of H2 by cationic cobalt clusters, pointing to the existence of stable molecular Cox+-H2 complexes as intermediates of metal-hydrid formation.

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Alessandro Fortunelli

CNR-ICCOM

alessandro.fortunelli@cnr.it

High-Throughput and Conformal Funnels in NanoCatalytic Processes

I will discuss general principles, challenges, and recent advances in theoretical and computational modeling of heterogeneous nano-catalysts as confined systems. Starting from the dramatically urgent societal need of novel, more active, more selective, cheaper, and sustainable catalysts for all of the critical mass-scale catalytic processes used in chemical industry, I will discuss the opportunities offered by confinement and nano-structuration, the challenges presented to approaches aiming at efficient and practical high-throughput catalysts screening, and some recent advances [1,2,3,4,5] that promise to provide a possible solution to this important problem.

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Lala Gahramanli

Nano Research Laboratory

gahraman.lala@gmail.com

Plasmonic–Semiconductor–Graphene Hybrid Nanostructures for Enhanced Photocatalytic Degradation of Organic Pollutants

This work focuses on the design and investigation of advanced plasmonic–semiconductor hybrid nanostructures based on 2D/1D graphene/Ag–Ag_2S systems for photocatalytic environmental applications. The materials were synthesized and characterized using XRD, SEM, FTIR, and UV–Vis spectroscopy to establish structure–property relationships. The hybrid system demonstrates enhanced photocatalytic performance in methylene blue degradation, achieving up to ~89.55% efficiency under acidic conditions due to synergistic effects between graphene conductivity, Ag plasmonic response, and Ag_2S semiconductor behavior .

The improved activity is attributed to efficient charge separation at the heterojunction interface, plasmon-induced hot electron generation, and rapid electron transport through graphene layers. The study highlights the importance of interfacial engineering, charge carrier dynamics, and multi-phase band structure in designing highly efficient and sustainable photocatalysts. These findings are directly relevant to key catalytic challenges such as wastewater treatment and energy-related small molecule activation, aligning with the CATCOSY workshop themes on atomistic understanding and predictive modeling of catalytic systems.

Mario Gallego Rodríguez

Universitat Politècnica de València

Dr.MarioGallRquez@gmail.com

Selective Oxidation of Methane into Methanol with Molecular O2 using Cun Nanoclusters within CHA Models: A Computational Study

Sub-nanometer metal clusters composed by just a few atoms exhibit electronic, optical, and catalytic properties different from those of larger nanoparticles and bulk metals, which are associated to the accessibility of their low coordinated atoms and to a molecular-like electronic structure with discrete energy levels and localized orbitals. The catalytic properties of metal clusters depend strongly on their size and shape and can be altered by interactions with protecting ligands or when they are stabilized on inorganic supports. Understanding the nature and extent of these modifications is key to potentially achieve a fine tuning of their catalytic performance [1-3].

Former theoretical work [4] in our group demonstrated that isolated copper nanoclusters possess the ability to activate methane through an homolytic path involving relatively low activation energy barriers for all the individual elementary steps on Cu5 and Cu7 nanoclusters. Nevertheless, the formation of a highly stable CH3 group coordinated to Cun in a bidentate mode represents a great limitation, since it leads to really high activation barriers for the methanol formation step. Furthermore, our investigation on the reactivity towards O2 dissociation of Cu5 and Cu7 clusters confined within the cavities of the CHA zeolite and the successive dissociation of multiple O2 molecules [5] shed light on the great resistance against deep oxidation and opened the possibility of encountering multiple spin surface pathways that can potentially diminish the activation barriers of the target reaction.

In order to verify whether the general trends previously reported are followed in the methane-to-methanol process (MTM) catalyzed by copper clusters confined within a CHA zeolite, two different clusters were considered, Cu5-2D, and Cu7, stabilized within the cages of CHA models containing two framework Al atoms. The adsorption and activation of methane, the formation of desired methanol and undesired byproduct species, and the desorption of methanol were investigated using dispersion-corrected DFT calculations.

The results confirm energy barriers similar to those reported in the literature with no water molecules assisting the process

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Estefania German

Universidad de Valladolid

estefania.german@uva.es

Hydrogen dissociation reaction catalyzed by Rhodium clusters supported on Fullerene

A current area of research focuses on hydrogen adsorption and storage in metal-doped carbon materials. Using density functional theory, we have studied molecular and dissociative adsorption of H2 on neutral and cationic RhnC60 complexes with n = 1-8. The Rh atoms form compact clusters on the surface of the fullerene. Dissociative chemisorption of one H2 molecule is more stable than molecular adsorption except on n = 3 and 4 charged RhnC60. When RhnC60 is ionized, the electronic charge deficit remains localized in the rhodium cluster. The molecular and dissociative adsorption features on cationic RhnC60+ and neutral RhnC60 complexes are in general similar, but some differences can be highlighted. Molecular and dissociative H2 adsorption on neutral Rh2C60 are competitive; in fact, molecular adsorption is slightly more stable. Another difference is that the dissociative adsorption energies on some of the neutral RhnC60 complexes are substantially larger than the dissociative adsorption energies on the corresponding RhnC60+ cationic complexes by amounts between 0.2 and 0.6 eV. Activation barriers for dissociation of the adsorbed H2 molecule strongly depend on the charge state and cluster size. These barriers help to interpret the adsorption state (molecular or dissociated) of experimentally produced hydrogenated RhnC60+ complexes.

Shaimaa Habib

Physisc department Faculty of science Damanhour University Egypt

shaimaa.habib@sci.dmu.edu.eg

Sub-nm titanium dioxide clusters: efficient photocatalysts for clean SOx conversion under visible light irradiation

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Juan Carlos Hernández Garrido

Universidad de Cádiz

jcarlos.hernandez@qm.uca.es

Contributions of Advanced Transmission Electron Microscopy techniques to Understand Catalysis: from Clusters to Reactors.

The rational design of heterogeneous catalysts demands a profound understanding of their structure, composition, and dynamics across multiple length scales. Advanced Transmission and Scanning Transmission Electron Microscopy (TEM/STEM) techniques have become indispensable tools in this endeavour, offering unique capabilities to bridge atomic and macroscopic scales with nanometric resolution.

In this talk, we present how a suite of advanced (S)TEM-based methodologies — including aberration-corrected HAADF-STEM imaging, analytical EELS/EDX spectroscopy, quantitative 3D electron tomography, and in-situ/operando electron microscopy under controlled gas atmospheres — can be combined to address key open questions in heterogeneous catalysis. Selected case studies will illustrate this multi-technique approach. Special attention will be paid to the characterization of subnanometric metal clusters and single-atom species, where the sensitivity of aberration-corrected STEM to atomic number allows their direct visualization and structural determination on complex supports, and where subtle changes in coordination and oxidation state govern catalytic performance. Finally, the talk will address how these approaches can be extended toward the understanding of catalytic processes at larger scales, connecting atomic-level insights with macroscopic reactor performance.

The results discussed underline the critical role of advanced electron microscopy as a cornerstone characterization platform in the development of next-generation, sustainable catalytic materials for energy and environmental applications.

Aynura Karimova

Baku State University

aynurakarimova@bsu.edu.az

Structure-Property Relationships in Graphene Oxide - Magnetite Hybrid Nanomaterials

Graphene oxide (GO)–Fe_3O_4 hybrid nanomaterials represent a multifunctional platform combining the high surface area and π-conjugated structure of GO with the magnetic properties of Fe_3O_4 nanoparticles. In this study, we investigate the structure–property relationships governing drug loading efficiency in GO–Fe_3O_4 hybrid systems, with particular emphasis on interfacial interactions at the nanoscale.

The hybrid nanostructures were synthesized via a co-precipitation method followed by surface functionalization with chitosan and graphene oxide. Structural characterization using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and transmission electron microscopy (TEM) confirmed the successful formation of Fe_3O_4 nanoparticles and their effective immobilization onto GO sheets, resulting in improved dispersion and reduced aggregation compared to chitosan-coated systems.

Drug loading efficiency was quantitatively evaluated using UV–Vis spectroscopy based on the Beer–Lambert law. The results revealed a significant enhancement in loading efficiency for GO-containing systems (81%) compared to chitosan-coated nanoparticles (53%). This improvement is attributed to the synergistic effect of GO, which provides additional active sites for adsorption through π–π stacking interactions, hydrogen bonding, and electrostatic interactions with drug molecules.

These findings highlight the critical role of nanoscale interfacial interactions in determining the functional performance of hybrid nanomaterials and provide insights into the rational design of advanced nanostructures with tunable properties. https://doi.org/10.3389/fnano.2025.1634225

Hamide Kavak

Cukurova University

hkavak@cu.edu.tr

Development of functional metal oxides thin films for various applications

Metal oxide semiconductors have attracted significant interest owing to their unique physical and chemical properties. When integrated with various nanostructures, they hold great promise for a wide range of applications. These materials have demonstrated substantial success in diverse optoelectronic devices, including solar cells, lasers, light-emitting diodes (LEDs), and photodetectors.

Zinc oxide (ZnO) and cuprous oxide (Cu2O) thin films are environmentally friendly and low-cost semiconductors and have various optoelectronic applications. ZnO and Cu2O thin films can be deposited under normal laboratory conditions via low-cost and simple chemical methods. However, the main concerns of the low-cost methods are the growth of pure films and efficient interface between the films. In this study, the one-step spin coating method was employed to prepare ZnO thin films. The electrodeposition of Cu2O thin film was achieved via developed a simple two electrodes cell. The structural, morphological, optical and electrical properties of metal oxide layers were determined. ZnO is intrinsically n-type and it is still challenging to obtain stable p-type conductivity, which can be achieved by tailoring the doping rate. The properties of ZnO thin films and their impacts on ZnO/Cu2O bilayer heterojunction efficiency were elaborated by means of current-voltage (I-V) characterizations. The results demonstrated satisfactory rectifying behavior, highlighting the potential of these heterostructures for future optoelectronic applications. These materials also used as an electron and hole transporting layer in the fabrication of solar cells.

Vipin Kumar

Technical University of Darmstadt, Germany

vipinkumar0247@gmail.com

Experimental and DFT analysis of antisite disorder and Griffiths phase in Dy2CoMnO6: structural, electronic, and magnetic insights

The intricate interaction of emergent degrees of freedom, ground state degeneracy, and competing magnetic interactions in oxide-based double perovskite frustrated magnets can give rise to exotic excitations and correlated quantum phenomena with promising technological applications. This study investigates the structural, magnetic, and electronic properties of Dy2CoMnO6 synthesized via solid-state reaction. Rietveld refinement of XRD data confirms a monoclinic P21/n structure, with Raman spectra revealing BO6 polyhedral dynamics. XPS analysis indicates mixed valence states of Co and Mn. Magnetic measurements show ferromagnetic ordering below Tc = 87 K due to Co2+ – Mn4+ superexchange, along with a Griffiths phase above Tc (TG = 91 K) and canted antiferromagnetic correlations at low temperature. A coercivity of 6.8 kOe at 10 K further supports FM behavior. Density functional theory (DFT) calculations validate the stability of Dy2CoMnO6 in the ferromagnetic phase, showing that the ferromagnetic state is energetically more favorable than the antiferromagnetic state. The direct band gap of Dy2CoMnO6 was found to be approximately 1.47 eV, while the indirect band gap was around 1.04 eV. Electronic band structure and density of states calculations predict band gaps of 1.60 eV and 3.20 eV for the minority and majority spin orientations, respectively, confirming the semiconductor nature of Dy2CoMnO6. These calculated values closely match the experimentally observed band gap.

M. Arturo Lopez-Quintela

University of Santiago de Compostela (Spain)

malopez.quintela@usc.es

Exploring the use of Ag pentamers as catalytic antioxidant sub-nanoenzymes

Xinran Lu

University of Santiago de Compostela (Spain)

xinran.lu@usc.es

Polymerization Catalysis by Quantum-confined Ag Clusters

In this work, we report the catalytic performance of Ag clusters (mainly Ag_5) in different polymerization reactions and investigate their activity deposited on surfaces and dispersed in solution. Due to quantum confinement, clusters with sizes below 1-2 nm exhibit properties different from bulk metal and nanoparticles, and their atomic-scale dimensions enable them to act as individual active sites in catalysis.

For the on suface-state catalysis, we deposited Ag clusters onto a semiconducting TiO2 surface by spin coating. The interactions between the clusters and the TiO2,investigated using different surface characterization techniques (AFM, XRD, and XPS), reveal an increased concentration of non-lattice oxygen at the surface upon cluster incorporation. These results indicate the strong potential of Ag clusters for the catalysis of 2D-polymerization, like the growth of graphene nanoribbons. Given the relatively few studies on the synthesis of graphene on semiconductors or insulators, the clusters can enhance the substrate reactivity and provide adatoms for the reaction, thereby establishing a novel catalytic system for nanographene synthesis on non-conducting surfaces. Furthermore, methylene blue degradation experiments demonstrate enhanced photocatalytic activity in the cluster-modified samples.

For the solution-phase reaction, we studied the catalytic activity of Ag clusters dispersed in hexanediol diacrylate (HDDA) for a new 3D-polymerization reaction with diglycidyl ether of bisphenol A (DGEBA). FTIR, NMR and DSC reveal that Ag clusters selectively activate ether and ester oxygen atoms in DGEBA, facilitating their reaction with the C=C bonds of HDDA, while preserving the epoxy groups. This behavior contrasts with conventional epoxy polymerization mechanisms. The resulting system enables a new curing strategy that retains epoxy functionality, allowing further crosslinking with traditional hardeners.

Overall, the use of clusters as polymerization catalysts provides new insights into routes toward multifunctional polymer synthesis, and further studies along these directions are ongoing.

(Unpublished work)

Luis Martin Encinar

University of Valladolid

luis.martin.encinar@uva.es

Machine Learning Interatomic Potentials for Hydrogen Catalysis on 2D Carbon-based materials

Carbon-based nanoporous and layered materials doped with transition metals (TM) are promising candidates for hydrogen storage platforms according to Density Functional Theory (DFT) studies.a,b However, modelling the adsorption/desorption of hydrogen under realistic conditions requires large-scale Ab Initio Molecular Dynamics (AIMD) simulations that are computationally prohibitive. In this context, universal Machine Learning Interatomic Potentials (uMLIPs) provide transferable and computationally efficient models capable of capturing DFT accuracy across large systems and long timescales.c

In this work, we tested different uMLIPs on TM–carbon platforms. In particular, we examined its performance on properties such as thermal stability, radial distribution function, adsorption energies and geometries of TM atoms/clusters, diffusion pathways and migration barriers, and vibrational properties. Our results showed that MACE-MH_OC20 and NequIP-OAM-XL models, despite not being specifically trained on our target TM-carbon platforms, agree with the main structural, energetic, and dynamical properties observed in DFT. Then, we fine-tuned both uMLIPs models using a large and diverse dataset that includes a wide range of TM clusters and carbon-based layers (including defective ones), mostly generated from AIMD simulations covering near- and out-of-equilibrium structures. Our aim is to train a model that can be reliably transferred for dynamic catalytic studies. Finally, extensive MD simulations of hydrogen adsorption and desorption will be performed to evaluate the hydrogen storage capacity of TM-carbon platforms under practical conditions.

Yoshie Murooka

University of Liverpool

y.murooka@liverpool.ac.uk

Sub-nanometer photo-induced dynamics probed by fast electrons

Fast dynamics under irradiations at the sub-nanometer scale has been advanced over decades by using fast electron and digital detector. Ultrafast laser technology, in particular, has dramatically increased the temporal resolution of electron diffraction and microscopy over the past 20 years. Using femtosecond pulsed electron beams, for example, light-induced structural dynamics of nanoparticles [1] and surface structures, charge transfer at substrate surfaces, have been clarified in both reciprocal space and real space.

Recently, Scanning Transmission Electron Microscope imaging utilising Compressed Sensing (CS) has been developed [2]. This enables observation of beam-sensitive samples, can reduce acquisition time, and allows low dose observations. At the presentation, the author would like to discuss about our current status and new opportunities in sub-nanometer fast dynamics especially in a state-of-art transmission electron microscope. The author would like to acknowledge Prof. N.D. Browning (University of Liverpool) for the CS development.

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[2] 10.1016/j.ultramic.2021.113451

Guadalupe Paz Paz

INIFTA, Universidad Nacional de La Plata

guadalupepaz@inifta.unlp.edu.ar

Cu_5 Atomic Clusters for Mild Oxidation of Thiophenic Sulfur Compounds probed by in situ XANES spectroscopy.

Authors: Guadalupe Paz, Khalil Jori, Iria Rodriguez, David Buceta, Lisandro Giovanetti, Martin Mizrahi, Arturo Lopez Quintela and Félix G. Requejo.

Institution: INIFTA, Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (Argentina)

We investigate the catalytic performance of Cu5 atomic quantum clusters (AQCs) in the oxidative transformation of refractory sulfur compounds. Using S-XANES spectroscopy, we demonstrate that these sub-nanometer clusters promote the deep oxidation of thiophenic molecules to S6+ species under ambient conditions in aqueous media. The correlation between AQC concentration and the resulting fractions of S5+and S6+ intermediates is discussed. Additionally, in situ S-XANES evidence supports the efficacy of Cu5 clusters in emulsion-based systems, enabling efficient interfacial catalysis between aqueous and organic phases. These results highlight AQCs as a promising platform for developing advanced catalytic processes for the deep desulfurization of petroleum-derived feeds.

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Laurent Piccolo

IRCELYON

laurent.piccolo@ircelyon.univ-lyon1.fr

Carbon capture and utilization (CCU) strategies: from CO2 hydrogenation on unconventional catalysts to integrated CCU

Together with CCS (carbon capture and storage), CCU is regarded as an important transition pathway for limiting industrial emissions of CO2 and converting this greenhouse gas into valuable chemicals and fuels, such as methanol and carbon monoxide.

This presentation will provide an overview of current approaches to catalytic CO2 valorization – primarily thermal hydrogenation, but also electroreduction – along with the corresponding catalytic materials and reaction conditions that govern product selectivity and yield. A relatively recent and powerful strategy, integrated CCU, which involves cycling between CO2 adsorption and hydrogenation steps, will also be introduced.

The works of our group on ultradispersed metal-based catalysts will illustrate these concepts, including Re(Mo)/oxide systems for methanol synthesis and integrated methanation, Pt/carbides for the reverse water-gas shift reaction, and Co-N-C single-site catalysts for electroreduction.

Cristina Puzzarini

University of Bologna

cristina.puzzarini@unibo.it

Icy-Grain Catalysis in Space: A Route toward Molecular Complexity

Interstellar dust grains coated by molecular ices provide unique catalytic environments where chemical complexity can emerge under the extreme conditions of space. Acting simultaneously as concentrators of reactants, catalytic surfaces, and efficient energy sinks, icy mantles enable reactions that would otherwise be inefficient or inaccessible in the gas phase. Water-rich ice surfaces promote radical-radical and radical-molecule reactions by stabilizing intermediates, lowering activation barriers, and dissipating excess reaction energy. Recent computational studies have shown that the formation of molecules such as glycolamide, a structural isomer of glycine, can proceed efficiently on interstellar ice grains through surface-assisted reaction pathways involving key prebiotic intermediates. These findings support the view that icy grains are active chemical reactors driving molecular evolution from simple species toward increasing complexity. This contribution will discuss the catalytic role of interstellar ices, the molecular-level mechanisms underlying grain-surface chemistry, and the required computational strategy.

Johanna Yasmin Sandoval Menjivar

University of Valladolid

johannayasmin.sandoval@estudiantes.uva.es

The Water Splitting reaction: single Fe-atoms catalyst supported on Fullerenes

One of the methods studied for green hydrogen production is through the water splitting reaction. This process consists of two distinct stages, which are: the desorption of two hydrogen molecules and the desorption of molecular oxygen. For the water splitting a good catalyst is needed, leading to reaction steps with small energy barrier-jumps. We have investigated this reaction by performing calculations based on the DFT formalism. In this work, single Fe-atoms were used as catalysts with fullerene (C60) as support. Different mechanisms were studied for this reaction, which we will discuss step by step.

Farooq Sher

Nottingham Trent University

Farooq.Sher@ntu.ac.uk

Structure property relationships for the rational design of subnanometric metal and metal oxide catalysts in net zero processes

Subnanometric metal and metal oxide catalysts exhibit unique physicochemical properties that differ fundamentally from their nanoparticulate and bulk counterparts, offering new opportunities for high activity, selectivity, and stability in catalytic processes. This contribution focuses on understanding structure property relationships in these systems, with particular emphasis on atomistic features such as cluster size, electronic structure, metal support interactions, and dynamic restructuring under reaction conditions.

The work explores how these factors influence catalytic performance in key net zero processes, including CO2 conversion, small molecule activation, and sustainable hydrogen production. Advanced characterization techniques combined with theoretical insights are discussed to elucidate active sites and reaction pathways. The ultimate aim is to support the rational design of efficient, durable, and cost effective catalytic materials for sustainable chemical transformations.

Louichaoui Tassadit

University Mohamed Khider Biskra

louichaoui.tassadit@gmail.com

Solvent Extraction of Cu with D2EHPA: Screening of Factors by Box–Behnken Design

sovant extraction of metals

Stefan Vajda

J Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences

stefan.vajda@jh-inst.cas.cz

Catalysis by Supported (Sub)Nanometer Clusters: Size, Composition and Support Effects

The main part of the presentation will focus on oxidative reactions by size- and composition-selected atomic clusters, such as CO oxidation, dehydrogenation or partial oxidation reactions. As time allows, select examples of the use larger nanoparticles in these reactions will be highlighted.

Murat Yılmaz

Osmaniye Korkut Ata University (Türkiye)

muratyilmaz@osmaniye.edu.tr

Biomass-Derived Activated Carbon Materials for Environmental Remediation, CO2 Capture, and Energy Applications: Current Challenges and Future Perspectives

Biomass-derived activated carbons have emerged as sustainable and versatile materials for environmental and energy-related applications due to their tunable pore structure, high surface area, chemical stability, and low-cost production. Recent studies have demonstrated that agricultural and industrial biomass wastes, including tea waste, olive seeds, peanut shells, and similar lignocellulosic precursors, can be transformed into high-performance porous carbons through physical and chemical activation routes. This literature-oriented contribution summarizes recent advances in the synthesis, surface functionalization, and application of biomass-based activated carbons for wastewater treatment, CO2 adsorption, and electrochemical energy storage.

Special attention is given to the adsorption and catalytic interaction mechanisms involved in the removal of pharmaceuticals, dyes, and heavy metals from aqueous systems, as well as to the role of heteroatom doping and surface oxygen functionalities in enhancing adsorption efficiency and electrochemical performance. Furthermore, current trends involving carbon-supported nano/subnanometric metal or metal oxide species for photocatalytic and electrocatalytic environmental applications are critically discussed. The relationship between precursor composition, activation strategy, pore architecture, and material performance is highlighted to provide insight into the rational design of sustainable multifunctional carbon materials. Finally, major challenges and future research directions for integrating biomass-derived porous carbons into next-generation catalytic and energy systems are outlined.

Aslıhan Yılmaz Çamoğlu

Kardeniz Technical University

kimyager.aslihanyilmaz@gmail.com

Design of a New Magnetic Bio-Nanocomposite and Multivariate Optimization of Cd(II) Preconcentration from Environmental Samples

In this study, magnetic CoFe2O4 was synthesized via the coprecipitation method, and dead bacteria was loaded onto this magnetic nanoparticle. The obtained adsorbent as characterized by FTIR (Fig. 1), SEM-EDX and XRD techniques. Finally, the prepared adsorbent was utilized for the solid phase extraction of Cd(II) ions using the batch method before determination by FAAS. The central composite design (CCD) was used to investigate the most effective factors of pH, amount of adsorbent, desorption time, eluent concentration and their interactions. Furthermore, CCD is used to optimize the process and to obtain response surface graphics.