
# CONFERENCE ORGANIZERS

**Štefan Vajda** – Conference Chair
(J. Heyrovský Institute of Physical Chemistry, Czech Republic)

**Alessandro Fortunelli** (CNR-ICCOM, Pisa, Italy)

**Armin Kleibert** (PSI Villigen, Switzerland)

# LOCAL ORGANIZING COMMITTEE

Klaudie Soukupová – conference secretary

Naděžda Žilková

Mykhailo Vaidulych

Stanislav Valtera


**Technical Program as of May 24, 2023 – Please keep checking back for updates**

## Sunday, June 18

| | | |
|---|---|---|
| *14:00* | *Registration, putting up posters* | |
| **SuPM** | **Chair: Stefan Vajda** | |
| 16:45 | | Alessandro Fortunelli, Armin Kleibert & Stefan Vajda<br>Welcome by the Organizers |
| 16:50 | | **Martin Hof**<br>Word by the Director of HIPC |
| 17:00-17:25 | IL | **Beatriz Roldán Cuenya**<br>*Conference opening lecture*<br>From single atoms to clusters and nanoparticle catalysts in energy conversion |
| 17:25-17:50 | IL | **Atsushi Nakajima**<br>Molecularly controlled support effect on catalytic activity of Metal Subnanoclusters |
| 17:50-18:15 | IL | **Alessandro Fortunelli**<br>Computational modeling of catalytic processes for hydrogen production |
| 18:15-18:25 | | Discussion of the session |
| *18:30* | *Reception* | |


## Monday, June 19 – morning session

| **MoAM1** | **Chair: Ulrich Heiz** | |
|---|---|---|
| 8:30-8:40 | | Introduction by the Chair |
| 8:40-9:05 | IL | **Robert Schlögl**<br>The optimal size of catalytic nanoparticles |
| 9:05-9:30 | IL | **Cafer Yavuz**<br>NiMoCat: Coke and sintering resistant nanocatalyst for reforming hydrocarbons with $CO_2$ to make zero carbon fuels |
| 9:30-9:45 | HT<br>P15 | **Olga Lushchikova**<br>$CO_2$ activation by Cu clusters in superfluid helium nano-droplets |
| 9:45-10:00 | IHT | **Grant Johnson**<br>Atomically precise clusters in advanced energy applications |
| 10:00-10:10 | | Discussion of the session |
| *10:10-10:40* | | *Coffee Break* |

| **MoAM2** | **Chair: Scott Anderson** | |
|---|---|---|
| 10:40-10:50 | | Introduction by the Chair |
| 10:50-11:05 | HT<br>P21 | **Jan Balajka**<br>The atomic structure of reconstructed $Al_2O_3(0001)$ surface |
| 11:05-11:20 | IHT | **Zdenek Dohnálek**<br>Dynamics of single Rh atoms in $Fe_3O_4(001)$ surfaces under reaction conditions |
| 11:20-11:35 | IHT | **Christian Durante**<br>EC-STM exploration of Pt-Au nano-clusters nucleation and growth under the effect of Pt-N complexes and implications on the reactivity for Oxygen Reduction Reaction |
| 11:35-11:50 | HT<br>P14 | **Seok-Jin Kim**<br>Engineering catalyst support for improved ammonia decomposition |
| 11:50 -12:00 | | Discussion of the session |
| *12:00-13:30* | | *Lunch* |


## Monday, June 19 – afternoon session

| **MoPM1** | **Chair: Emil Roduner** | |
|---|---|---|
| 13:30-13:40 | | Introduction by the Chair |
| 13:40-14:05 | IL | **Armin Kleibert**<br>Towards optical control of magnetism at the nanoscale |
| 14:05-14:30 | IL | **Xiangzhong Chen**<br>Piezoelectric and magnetoelectric catalysis: emerging fields yet to be explored |
| 14:30-14:45 | HT P23 | **Kateryna Biliak**<br>Reactive-sputter-based synthesis of group IV transition metal nitride nanoparticles |
| 14:45-15:00 | HT P06 | **El yakout El koraychy**<br>Role of misfit strain on the growth of core@shell architectures of lattice mismatched nanoalloys: the case of AuCu |
| 15:00-15:10 | | Discussion of the session |
| *15:10-15:40* | | *Coffee Break* |

| **MoPM2** | **Chair: Grant Johnson** | |
|---|---|---|
| 15:40-15:50 | | Introduction by the Chair |
| 15:50-16:05 | HT P38 | **Ji Yujing**<br>Low-temperature oxidation of CO by Fe-C-Al sites generated on Fe-oxide/$Al_2O_3$ surface prepared by TR-CVD method |
| 16:05-16:20 | HT P10 | **Elisa Jimenez-Izal**<br>Pt:Ge ratio as a lever of activity and selectivity control of PtGe clusters |
| 16:20-16:35 | HT P34 | **Rares Banu**<br>Chiral gold nanoclusters as promising catalysts for asymmetric reactions |
| 16:35-16:50 | HT P17 | **Micha Polak**<br>Adsorption under nanoconfinement: Prediction of significantly enhanced surface-coverage and selectivity pertinent to gas storage and separation in porous materials |
| 16:50-17:05 | HT P49 | **Libor Novák**<br>MicroReactor for in situ SEM imaging of chemical processes |
| 17:05-17:15 | | Discussion of the session |

| **Poster I** | **Chair: Jan Hagen & Ludger Wöste** |
|---|---|
| 17:15-18:00 | Flash Presentations – Odd Poster Numbers |
| 18:00 – 21:00 | Poster Session I |

## Tuesday, June 20 – morning session

| TuAM1 | Chair: Zdenek Dohnálek | |
|---|---|---|
| 8:00-8:10 | | Introduction by the Chair |
| 8:10-8:35 | IL | **Eric Altman**<br>Growth, structure, reactivity and magnetic properties of single layer 2D transition metal silicates |
| 8:35-9:00 | IL | **Ulrike Diebold**<br>Surface structure, defects, and adsorption on a model (photo-)catalyst material: $In_2O_3$(111) |
| 9:00-9:25 | IL | **Jeroen van Bokhoven**<br>Nano-sized particles under pressure |
| 9:25-9:50 | IL | **Paolo Milani**<br>Building reliable devices with unreliable components: supersonic cluster beam fabrication of neuromorphic data processing systems |
| 9:50-10:00 | | Discussion of the session |
| *10:00-10:30* | | *Coffee Break* |

| TuAM2 | Chair: Mauro Stener | |
|---|---|---|
| 10:30-10:40 | | Introduction by the Chair |
| 10:40-11:05 | IL | **Francesca Baletto**<br>Nanofaceting and catalysis |
| 11:05-11:30 | IL | **David Wales**<br>Energy landscapes: From molecules and nanodevices to machine learning |
| 11:30-11:45 | HT P08 | **Chris Heard**<br>Accelerated modelling of supported Pt clusters via reactive machine learning potentials |
| 11:45-12:10 | IL | **Timo Jacob**<br>On the role of surface oxides on Pt-based catalysts |
| 12:10-12:20 | | Discussion of the session |
| *12:20-13:30* | | *Lunch* |

## Tuesday, June 20 – afternoon session

| **TuPM1** | **Chair: Armin Kleibert** | |
|---|---|---|
| 13:30-13:40 | | Introduction by the Chair |
| 13:40-14:05 | IL | **Pascal Andreazza**<br>Ageing of out-of-equilibrium Ag-Pt nanoalloys in temperature and under gas exposure |
| 14:05-14:30 | IL | **Anatoly Frenkel**<br>Monomers, dimers and trimers: characterization and control of catalytic ensembles |
| 14:30-14:55 | IL | **Janis Timoshenko**<br>Tracking the evolution of copper clusters, nanoparticles and nanocubes by time- resolved X-ray absorption spectroscopy and machine learning |
| 14:55-15:10 | HT<br>P47 | **Liana Socaciu-Siebert**<br>NAP-XPS instrumentation and applications: Quo Vadis? |
| 15:10-15:25 | IHT | **Thorsten Bernhardt**<br>Isolated calcium manganese oxide clusters:<br>Bioinspired model systems for sustainable catalytic water splitting |
| 15:25-15:35 | | Discussion of the session |
| *15:35-16:00* | | *Coffee Break* |

| **TuPM2** | **Chair: Claude Henry** | |
|---|---|---|
| 16:00-16:10 | | Introduction by the Chair |
| 16:10-16:35 | IL | **Scott Anderson**<br>Size-selected catalysis and electrocatalysis: effects of cluster electronic structure and fluxionality on activity and stability under reaction conditions |
| 16:35-16:50 | HT<br>P03 | **Gunther Andersson**<br>Atomic layer deposited overlayers on metal clusters |
| 16:50-17:15 | IL | **Jan Macak**<br>Atomic layer deposition of noble metal nanoparticles for catalytic applications |
| 17:15-17:40 | IL | **Yu Lei**<br>Synthesis of well-defined heterogeneous catalysts using atomic layer deposition |
| 17:40-17:50 | | Discussion of the session |

*18:00* *Departure of the bus for the Conference Dinner (Social Evening)*


## Wednesday, June 21

| **WeAM1** | **Chair: María Pilar de Lara-Castells** | |
|---|---|---|
| 8:30-8:40 | | Introduction by the Chair |
| 8:40-9:05 | IL | **Mauro Stener**<br>Chirality in metal clusters: Computational approaches for plasmons, Circular Dichroism and ligand dynamics |
| 9:05-9:30 | IL | **Vlasta Bonačić-Koutecký**<br>Metallic quantum clusters and surrounding for catalysis and bioimaging |
| 9:30-9:45 | HT<br>P09 | **Petra Simoncic**<br>3D-electron diffraction: Revealing the growth mechanism of nanoparticles |
| 9:45-10:10 | IL | **Arturo López-Quintela**<br>Metal clusters of 5 atoms: Are they especially unique in catalysis? |
| 10:10-10:20 | | Discussion of the session |
| *10:20-10:45* | | *Coffee Break* |

| **WeAM2** | **Chair: Alessandro Fortunelli** | |
|---|---|---|
| 10:45-10:55 | | Introduction by the Chair |
| 10:55-11:20 | IL | **María Pilar de Lara-Castells**<br>Unsupported and graphene-supported atomic copper clusters and silver atoms: soft-deposition, stabilization, aggregation, and oxidation |
| 11:20-11:45 | IL | **Gareth Parkinson**<br>Probing the fundamentals of hydroformylation on Single-atom catalysts |
| 11:45-12:10 | IL | **Richard Palmer**<br>Nanoclusters in the real world: Insights into deposited clusters from aberration-corrected electron microscopy |
| 12:10-12:25 | HT<br>P52 | **Noelia Barrabés**<br>Bimetallic active sites designed with atomic precision using metal nanoclusters: structural evolution and reactivity by operando spectroscopy |
| 12:25-12:35 | | Discussion of the session |
| *12:35-14:00* | | *Lunch* |

| **WePM1** | |
|---|---|
| *14:30* | *Departure of the bus to NanoCat Labs Excursion/Free Afternoon* |


## Thursday, June 22 – morning session

| **ThAM1** | **Chair: Jan Macak** | |
|---|---|---|
| 8:30-8:40 | | Introduction by the Chair |
| 8:40-9:05 | IL | **Claudio Evangelisti**<br>From metal vapor to supported nanoparticles: Recent advances on Platinum-based heterogeneous catalysts obtained by metal vapor synthesis approach |
| 9:05-9:30 | IL | **Young Dok Kim**<br>Photocatalysts for environmental remediation: Studies from rutile $TiO_2$ to $TiO_2$/cement composite |
| 9:30-9:45 | HT<br>P04 | **Moritz Eder**<br>Clusters and size effects in hydrogen evolution from alcohols on $TiO_2$(110) |
| 9:45-9:55 | | Discussion of the session |
| *10:00-10:30* | | *Coffee Break* |

| **ThAM2** | **Chair: Noelia Barrabés** | |
|---|---|---|
| 10:30-10:40 | | Introduction by the Chair |
| 10:40-11:05 | IL | **Marc Willinger**<br>On the many faces of strong metal-support interactions |
| 11:05-11:25 | HT<br>P48 | **Hannes Frey**<br>Visualizing platinum-induced hydrogen spillover on iron oxide in real-time and space using quantitative techniques |
| 11:25-11:50 | IL | **Yoshie Murooka**<br>A new Relativistic Ultrafast Electron Diffraction and Imaging (RUEDI) National Facility for nanomaterials and catalysis in the U.K. |
| 11:50-12:05 | IHT | **Stephan Bartling**<br>NAP-XPS study of Mo/HZSM-5 under methane dehydroaromatization conditions |
| 12:05-12:15 | | Discussion of the session |
| *12:15-13:30* | | *Lunch* |

## Thursday, June 22 – afternoon session

| **ThPM1** | **Chair: Thorsten Bernhardt** | |
|---|---|---|
| 13:30-13:40 | | Introduction by the Chair |
| 13:40-14:05 | IL | **Julia Stähler**<br>Ultrafast Quasiparticle Dynamics and the role of screening at complex interfaces |
| 14:05-14:20 | HT<br>P19 | **Mihai Vaida**<br>Monitoring the electronic properties and non-metal to metal transition of supported cluster with femtosecond extreme ultraviolet laser pulses |
| 14:20-14:35 | IHT | **Scott Sayres**<br>Ultrafast dynamics of strongly correlated metal oxide clusters |
| 14:35-14:50 | HT<br>P13 | **Eva Klimešová**<br>Ultrafast dynamics in clusters and nanodroplets at ELI Beamlines |
| 14:50-15:00 | | Discussion of the session |
| *15:00-15:30* | | *Coffee Break* |

| **ThPM2** | **Chair: Alessandro Baraldi** | |
|---|---|---|
| 15:30-15:40 | | Introduction by the Chair |
| 15:40-16:05 | IL | **Martin Kalbáč**<br>From graphene functionalization to functional devices |
| 16:05-16:20 | HT<br>P35 | **Johanna Sandoval Menjivar**<br>Cobalt functionalization of carbon-based materials for hydrogen storage. |
| 16:20-16:35 | HT<br>P29 | **Deborah Perco**<br>The highest oxidation state observed in graphene-supported sub-nanometer iron oxide clusters |
| 16:35-16:50 | HT<br>P25 | **Federico Loi**<br>Oxidation of size-selected $Ag_n$ clusters on graphene: a combined experimental and theoretical XPS study |
| 16:50-17:00 | | Discussion of the session |

| **Poster II** | **Chair: Scott Sayres & Marc Willinger** |
|---|---|
| 17:15-18:00 | Flash Presentations – Even Poster Numbers |
| 18:00-21:00 | Poster Session II |

## Friday, June 23

| FriAM1 | Chair: Chris Heard | |
|---|---|---|
| 8:30-8:40 | | Introduction by the Chair |
| 8:40-9:05 | IL | **Andrey Shukurov**<br>Reactive-sputter-based synthesis of group IV transition metal nitride nanoparticles |
| 9:05-9:30 | IL | **Roman Bulánek**<br>Metal clusters encapsulated within zeolite support: Synthesis and catalytic applications |
| 9:30-9:45 | HT<br>P16 | **Luis Molina**<br>DFT simulations of structure and chemical reactivity of small Pt clusters doped with Zr |
| 9:45-10:00 | HT<br>P37 | **Nicholas Smith**<br>Applying the divide-and-conquer paradigm to cluster global optimisation |
| 10:00-10:10 | | Discussion of the session |
| *10:15-10:45* | | *Coffee Break* |

| FriAM2 | Chair: Yoshie Murooka | |
|---|---|---|
| 10:45-10:55 | | Introduction by the Chair |
| 10:55-11:10 | HT<br>P12 | **Shashikant Kadam**<br>$CoFe_2O_4$/rGO nanohybrids as selective catalysts for oxidative dehydrogenation reactions: Role of dynamic nature of $O_h$ and $T_d$ sites |
| 11:10-11:25 | IHT | **Kevin Oldenburg**<br>Locally excited plasmon resonances of size-selected silver nanoparticles |
| 11:25-11:40 | HT<br>P05 | **Björn Bastian**<br>Plasmon resonance quenching of a single Au nanoparticle in the gas phase |
| 11:40-11:55 | HT<br>P02 | **Benajmin Demirdjian**<br>Plasmonic sensing to follow the reactivity on Pt nanoparticles and clusters |
| 11:55-12:10 | HT<br>P01 | **Abdul Rahman Abid**<br>Soft ionization of water cluster by resonant photoexcitation in doped helium nanodroplets at AMOLine ASTRID2 |
| 12:10-12:25 | HT<br>P31 | **Kristýna Pokorná**<br>Accuracy evaluation of reactive neural network potentials for Pt nanoparticles on hydroxylated silica |
| 12:25-12:35 | | Discussion of the session |
| *12:35* | | *Polls results announcements: Best Poster Awards* |
| *13:00* | | *Farewell* |


# POSTERS

**Monday Poster Session I preceded by Flash Talks – Odd poster numbers**

**Thursday Poster Session II preceded by Flash Talks – Even poster numbers**

**All posters on display Sunday afternoon – Friday morning, including those abstracts which were selected for Hot Topic talk**

P01 **Abdul Rahman Abid**
Soft ionization of water cluster by resonant photoexcitation in doped helium nanodroplets at AMOLine ASTRID2

P02 **Benjamin Demirdjian**
Plasmonic sensing to follow the reactivity on Pt nanoparticles and clusters.

P03 **Gunther Andersson**
Atomic layer deposited overlayers on metal clusters

P04 **Moritz Eder**
Clusters and size effects in hydrogen evolution from alcohols on $TiO_2$(110)

P05 **Björn Bastian**
Plasmon resonance quenching of a single Au nanoparticle in the gas phase

P06 **El yakout El koraychy**
Role of misfit strain on the growth of core@shell architectures of lattice mismatched nanoalloys: the case of AuCu

P07 **Joana R.C. Santos**
Aggregation of curcumin and piperine mixtures in different polar media investigated by Molecular Dynamics simulations

P08 **Christopher Heard**
Accelerated modelling of supported Pt clusters via reactive machine learning potentials

P09 **Petra Simoncic**
3D-electron diffraction: Revealing the growth mechanism of nanoparticles

P10 **Elisa Jimenez-Izal**
Pt:Ge ratio as a lever of activity and selectivity control of PtGe clusters

P11 **Papri Chakraborty**
Resolving structures of gas-phase fragments of atomically precise clusters through trapped ion mobility mass spectrometry

P12 **Shashikant Kadam**
$CoFe_2O4$/rGO nanohybrids as selective catalysts for oxidative dehydrogenation reactions: Role of dynamic nature of $O_h$ and $T_d$ sites

P13 **Eva Klimešová**
Ultrafast dynamics in clusters and nanodroplets at ELI Beamlines

P14 **Seok-Jin Kim**
Engineering catalyst support for improved ammonia decomposition

P15 **Olga Lushchikova**
$CO_2$ activation by Cu clusters in superfluid helium nano-droplets

P16 **Luis M. Molina**
DFT simulations of structure and chemical reactivity of small Pt clusters doped with Zr

P17 **Micha Polak**
Adsorption under nanoconfinement: Prediction of significantly enhanced surface-coverage and selectivity pertinent to gas storage and separation in porous materials

P19 **Mihai Vaida**
Monitoring the electronic properties and non-metal to metal transition of supported cluster with femtosecond extreme ultraviolet laser pulses

P20 **Joanna Olszówka**
Preparation and in-situ characterization of the semi-model catalytic systems as a key to understanding structure-function relationships in dry methane reforming

P21 **Jan Balajka**
The atomic structure of reconstructed $Al_2O_3$(0001) surface

P22 **Emanuela Pitzalis**
Covalent triazine framework-supported nickel nanoparticles for catalytic transfer hydrogenations of nitroaromatics with ammonia borane

P23 **Kateryna Biliak**
Bimetal Ag/Cu/ polyethylene glycol nanofluids prepared by gas aggregation cluster sources

P24 **Abdul Selim**
Highly selective oxidation of biomass to glucaric acid over the $ZrO_2$ supported Au/Pt nanocatalyst

P25 **Federico Loi**
Oxidation of size-selected $Ag_n$ clusters on graphene: a combined experimental and theoretical XPS study

P26 **Mirko Vanzan**
A computational insight on Au-based nanoalloys

P27 **Caitlin McCandler**
Modeling dynamic behaviors in ligand-stabilized gold nanoclusters

P28 **Zhonghua Xue**
Sustainable electrochemical reduction of nitrate into ammonia by a boron-processed Nickel foam

P29 **Deborah Perco**
The highest oxidation state observed in graphene-supported sub-nanometer iron oxide clusters

P30 **Iria Rodriguez Arias**
Propylene oxidation on supported $Ag_5$ clusters

P31 **Kristýna Pokorná**
Accuracy evaluation of reactive neural network potentials for Pt nanoparticles on hydroxylated silica

P32 **Mykhailo Vaidulych**
Low-temperature selective oxidative dehydrogenation of cyclohexene by titania-supported Pd, Pt and Pt-Pd catalysts

P33 **Cesare Roncaglia**
Gold nanoparticles fluctuations: every atom counts

P34 **Rares Banu**
Chiral gold nanoclusters as promising catalysts for asymmetric reactions

P35 **Johanna Sandoval Menjivar**
Cobalt functionalization of carbon-based materials for hydrogen storage

P36 **Tereza Benešová**
Silicate-supported Pt clusters: Structure prediction via machine learning global optimisation

P37 **Nicholas Smith**
Applying the divide-and-conquer paradigm to cluster global optimisation

P38 **Ji Yujing**
Low-temperature oxidation of CO by Fe-C-Al sites generated on Fe-oxide/$Al_2O_3$ surface prepared by TR-CVD method

P39 **Jakub Szmitek**
Pt cluster diffusion in zeolites with machine learning potentials

P40 **Antonija Mravak**
$CO_2$ conversion on monometallic and bimetallic Pd-doped copper tetramer clusters at zirconia support

P41 **Alexander Macion**
A benchtop approach for determination of ionization potentials of clusters in molecular beam experiments in the VUV range

P42 **Mattia Parnigotto**
Improved activity and stability of Pt NPs supported on $CeO_2$/C as electrocatalysts for oxygen reduction reaction: novel insights in the synthesis and physico-chemical characterization

P43 **Feng Zhang**
GPU-based parallelization and optimization of GCR for solving Helmholtz Equation in GRAPES

P44 **Thantip Roongcharoen**
Revealing oxidation and de-alloying of PtMn and its catalytic performance for methanol aqueous-phase reforming: A computational investigation

P45 **Martin Mergl**
Magnetotransport properties of graphene decorated with $Co_{xx}O$ clusters

P46 **Karolína Simkovičová**
Propane combustion over alumina-supported copper nanoparticles

P47 **Liana Socaciu-Siebert**
NAP-XPS instrumentation and applications: Quo Vadis?

P48 **Hannes Frey**
Visualizing platinum-induced hydrogen spillover on iron oxide in real-time and space using quantitative techniques

P49 **Libor Novák**
MicroReactor for in situ SEM imaging of chemical processes

P50 **Stanislav Valtera**
Evolution of the activity and oxidation state of subnanometer Pt clusters with cluster size and support in CO oxidation

P51 **Sarita Kolay**
Role of the capping ligands in regulating the optical properties of the metal nanoclusters

P52 **Noelia Barrabés**
Bimetallic active sites designed with atomic precision using metal nanoclusters: structural evolution and reactivity by operando spectroscopy