



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

Kludie 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
Welcome by the Organizers

16:50 **Martin Hof**
Word by the Director of HIPC

17:00-17:25 IL **Beatriz Roldán Cuenya**
Conference opening lecture
From single atoms to clusters and nanoparticle catalysts
in energy conversion

17:25-17:50 IL **Atsushi Nakajima**
Molecularly controlled support effect on catalytic activity
of Metal Subnanoclusters

17:50-18:15 IL **Alessandro Fortunelli**
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 The optimal size of catalytic nanoparticles
9:05-9:30	IL	Cafer Yavuz NiMoCat: Coke and sintering resistant nanocatalyst for reforming hydrocarbons with CO ₂ to make zero carbon fuels
9:30-9:45	HT P15	Olga Lushchikova CO ₂ activation by Cu clusters in superfluid helium nano-droplets
9:45-10:00	IHT	Grant Johnson Atomically precise clusters in advanced energy applications
10:00-10:10		Discussion of the session
10:10-10:40		<i>Coffee Break</i>
MoAM2		Chair: Scott Anderson
10:40-10:50		Introduction by the Chair
10:50-11:05	HT P21	Jan Balajka The atomic structure of reconstructed Al ₂ O ₃ (0001) surface
11:05-11:20	IHT	Zdenek Dohnálek Dynamics of single Rh atoms in Fe ₃ O ₄ (001) surfaces under reaction conditions
11:20-11:35	IHT	Christian Durante 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 P14	Seok-Jin Kim Engineering catalyst support for improved ammonia decomposition
11:50 -12:00		Discussion of the session
12:00-13:30		<i>Lunch</i>



Monday, June 19 – afternoon session

MoPM1	Chair: Emil Roduner	
13:30-13:40		Introduction by the Chair
13:40-14:05	IL	Armin Kleibert Towards optical control of magnetism at the nanoscale
14:05-14:30	IL	Xiangzhong Chen Piezoelectric and magnetoelectric catalysis: emerging fields yet to be explored
14:30-14:45	HT P23	Kateryna Biliak Reactive-sputter-based synthesis of group IV transition metal nitride nanoparticles
14:45-15:00	HT P06	El yakout El koraychy 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		<i>Coffee Break</i>
MoPM2	Chair: Grant Johnson	
15:40-15:50		Introduction by the Chair
15:50-16:05	HT P38	Ji Yujing Low-temperature oxidation of CO by Fe-C-Al sites generated on Fe-oxide/Al ₂ O ₃ surface prepared by TR-CVD method
16:05-16:20	HT P10	Elisa Jimenez-Izal Pt:Ge ratio as a lever of activity and selectivity control of PtGe clusters
16:20-16:35	HT P34	Rares Banu Chiral gold nanoclusters as promising catalysts for asymmetric reactions
16:35-16:50	HT P17	Micha Polak 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 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 Growth, structure, reactivity and magnetic properties of single layer 2D transition metal silicates
8:35-9:00	IL	Ulrike Diebold Surface structure, defects, and adsorption on a model (photo-)catalyst material: $\text{In}_2\text{O}_3(111)$
9:00-9:25	IL	Jeroen van Bokhoven Nano-sized particles under pressure
9:25-9:50	IL	Paolo Milani 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		<i>Coffee Break</i>
TuAM2		Chair: Mauro Stener
10:30-10:40		Introduction by the Chair
10:40-11:05	IL	Francesca Baletto Nanofaceting and catalysis
11:05-11:30	IL	David Wales Energy landscapes: From molecules and nanodevices to machine learning
11:30-11:45	HT	Chris Heard Accelerated modelling of supported Pt clusters via reactive machine learning potentials
11:45-12:10	IL	Timo Jacob On the role of surface oxides on Pt-based catalysts
12:10-12:20		Discussion of the session
12:20-13:30		<i>Lunch</i>



Tuesday, June 20 – afternoon session

TuPM1		Chair: Armin Kleibert
13:30-13:40		Introduction by the Chair
13:40-14:05	IL	Pascal Andreazza Ageing of out-of-equilibrium Ag-Pt nanoalloys in temperature and under gas exposure
14:05-14:30	IL	Anatoly Frenkel Monomers, dimers and trimers: characterization and control of catalytic ensembles
14:30-14:55	IL	Janis Timoshenko Tracking the evolution of copper clusters, nanoparticles and nanocubes by time- resolved X-ray absorption spectroscopy and machine learning
14:55-15:10	HT P47	Liana Socaciu-Siebert NAP-XPS instrumentation and applications: Quo Vadis?
15:10-15:25	IHT	Thorsten Bernhardt Isolated calcium manganese oxide clusters: Bioinspired model systems for sustainable catalytic water splitting
15:25-15:35		Discussion of the session
15:35-16:00		<i>Coffee Break</i>
TuPM2		Chair: Claude Henry
16:00-16:10		Introduction by the Chair
16:10-16:35	IL	Scott Anderson Size-selected catalysis and electrocatalysis: effects of cluster electronic structure and fluxionality on activity and stability under reaction conditions
16:35-16:50	HT P03	Gunther Andersson Atomic layer deposited overlayers on metal clusters
16:50-17:15	IL	Jan Macak Atomic layer deposition of noble metal nanoparticles for catalytic applications
17:15-17:40	IL	Yu Lei Synthesis of well-defined heterogeneous catalysts using atomic layer deposition
17:40-17:50		Discussion of the session
18:00		<i>Departure of the bus for the Conference Dinner (Social Evening)</i>



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 Chirality in metal clusters: Computational approaches for plasmons, Circular Dichroism and ligand dynamics
9:05-9:30	IL Vlasta Bonačič-Koutecký Metallic quantum clusters and surrounding for catalysis and bioimaging
9:30-9:45	HT P09 Petra Simoncic 3D-electron diffraction: Revealing the growth mechanism of nanoparticles
9:45-10:10	IL Arturo López-Quintela Metal clusters of 5 atoms: Are they especially unique in catalysis?
10:10-10:20	Discussion of the session
10:20-10:45	<i>Coffee Break</i>
WeAM2	Chair: Alessandro Fortunelli
10:45-10:55	Introduction by the Chair
10:55-11:20	IL María Pilar de Lara-Castells Unsupported and graphene-supported atomic copper clusters and silver atoms: soft-deposition, stabilization, aggregation, and oxidation
11:20-11:45	IL Gareth Parkinson Probing the fundamentals of hydroformylation on Single-atom catalysts
11:45-12:10	IL Richard Palmer Nanoclusters in the real world: Insights into deposited clusters from aberration-corrected electron microscopy
12:10-12:25	HT P52 Noelia Barrabés 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	<i>Lunch</i>
WePM	
14:30	<i>Departure of the bus to NanoCat Labs Excursion / Free Afternoon</i>



Thursday, June 22 – morning session

ThAM1		Chair: Jan Macak
8:30-8:40		Introduction by the Chair
8:40-9:05	IL	Claudio Evangelisti 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 Photocatalysts for environmental remediation: Studies from rutile TiO ₂ to TiO ₂ /cement composite
9:30-9:45	HT P04	Moritz Eder 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		<i>Coffee Break</i>
ThAM2		Chair: Noelia Barrabés
10:30-10:40		Introduction by the Chair
10:40-11:05	IL	Marc Willinger On the many faces of strong metal-support interactions
11:05-11:25	HT P48	Hannes Frey Visualizing platinum-induced hydrogen spillover on iron oxide in real-time and space using quantitative techniques
11:25-11:50	IL	Yoshie Murooka 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 NAP-XPS study of Mo/HZSM-5 under methane dehydroaromatization conditions
12:05-12:15		Discussion of the session
12:15-13:30		<i>Lunch</i>



Thursday, June 22 – afternoon session

ThPM1	Chair: Thorsten Bernhardt
13:30-13:40	Introduction by the Chair
13:40-14:05	IL Julia Stähler Ultrafast Quasiparticle Dynamics and the role of screening at complex interfaces
14:05-14:20	HT P19 Mihai Vaida 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 Ultrafast dynamics of strongly correlated metal oxide clusters
14:35-14:50	HT P13 Eva Klimešová Ultrafast dynamics in clusters and nanodroplets at ELI Beamlines
14:50-15:00	Discussion of the session
15:00-15:30	<i>Coffee Break</i>
ThPM2	Chair: Alessandro Baraldi
15:30-15:40	Introduction by the Chair
15:40-16:05	IL Martin Kalbáč From graphene functionalization to functional devices
16:05-16:20	HT P35 Johanna Sandoval Menjivar Cobalt functionalization of carbon-based materials for hydrogen storage.
16:20-16:35	HT P29 Deborah Perco The highest oxidation state observed in graphene-supported sub-nanometer iron oxide clusters
16:35-16:50	HT P25 Federico Loi 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 Reactive-sputter-based synthesis of group IV transition metal nitride nanoparticles
9:05-9:30	IL	Roman Bulánek Metal clusters encapsulated within zeolite support: Synthesis and catalytic applications
9:30-9:45	HT P16	Luis Molina DFT simulations of structure and chemical reactivity of small Pt clusters doped with Zr
9:45-10:00	HT P37	Nicholas Smith Applying the divide-and-conquer paradigm to cluster global optimisation
10:00-10:10		Discussion of the session
10:15-10:45		<i>Coffee Break</i>
FriAM2		Chair: Yoshie Murooka
10:45-10:55		Introduction by the Chair
10:55-11:10	HT P12	Shashikant Kadam CoFe ₂ O 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 Locally excited plasmon resonances of size-selected silver nanoparticles
11:25-11:40	HT P05	Björn Bastian Plasmon resonance quenching of a single Au nanoparticle in the gas phase
11:40-11:55	HT P02	Benajmin Demirdjian Plasmonic sensing to follow the reactivity on Pt nanoparticles and clusters
11:55-12:10	HT P01	Abdul Rahman Abid Soft ionization of water cluster by resonant photoexcitation in doped helium nanodroplets at AMOLine ASTRID2
12:10-12:25	HT P31	Kristýna Pokorná Accuracy evaluation of reactive neural network potentials for Pt nanoparticles on hydroxylated silica
12:25-12:35		Discussion of the session
12:35		<i>Polls results announcements: Best Poster Awards</i>
13:00		<i>Farewell</i>



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 TiO₂(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**
Water cluster microconfinement effects in protonic zeolites via machine learning
- 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**
CoFe₂O₄/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**
CO₂ 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 Al₂O₃(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 ZrO₂ 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 Ag₅ 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/Al₂O₃ surface prepared by TR-CVD method
- P39 **Jakub Szmitek**
Pt cluster diffusion in zeolites with machine learning potentials
- P40 **Antonija Mravak**
CO₂ 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 CeO₂/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_xO 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