Clustermeeting 2021_**v2021_07_20**



Sunday July 18

14:00	Registration opens
14:00	Putting up posters Posters will be on display during the entire duration of the meeting
16:30	Welcome drink
18:00	Conference Opening Lecture Ludger Wöste Freie Universität Berlin, Germany 48 Years of Research on Metal Clusters
	Reception

Monday July 19

MoAM1	Chair: A	rmin Kleibert
8:30		Welcome by Martin Hof , Director of J. Heyrovský Institute of Physical Chemistry, Czech Republic
8:40-9:10	IL01	Marc Willinger ETH Zürich, Switzerland The dynamic behaviour of active catalysts revealed by multi-scale in-situ electron microscopy
9:10-9:30	IHT01	Yoshie Murooka Froschungszentrum Jülich, Germany Technical developments for light and high frequency excitations in transmission electron microscopy
9:30-9:50	HT01 Po24	Jaroslav Kočišek J. Heyrovský Institute of Physical Chemistry, Czech Republic Butadiene clusters as a model for nanoelectrets
9:50-10:00		Discussion of the session
10:00-10:30		Coffee Break

MoAM2	Chair: K	ersti Hermansson
10:30-10:50	IHT02	Ingo Barke University of Rostock, Germany Virtual plasmonic dimers and local excitation of electron-hole systems on silicon and molecule aggregates by means of particle plasmons
10:50-11:10	HT02 Po36	Vladimíra Petráková J. Heyrovský Institute of Physical Chemistry, Czech Republic Controlled assembly of plasmonic nanoparticles and fluorophores for sub- diffraction manipulation of light
11:10-11:40	IL02	Karl-Heinz Meiwes-Broer University of Rostock, Germany Cresting the coulomb barrier of polyanionic silver clusters
11:40-11:50		Discussion of the session
12:00-13:30		Lunch

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Monday July 19

MoPM1	Chair: In	Chair: Ingo Barke		
13:30-13:50	HT03 Po06	Mayara da Silva Santos Helmholtz-Zentrum Berlin für Material und Energie GmbH, Germany High-resolution X-ray absorption spectroscopy in a cryogenic ion trap as a tool to investigate 3d metal—oxygen bonds		
13.50-14:20	IL03	María Pilar de Lara-Castells AbinitSim Unit/CSIC, Spain First-principles modelling of subnanometer-sized catalysts and photocatalysts: TiO₂-supported coinage metal clusters as case studies		
14:20-14:50	IL04	Anatoly Frenkel Stony Brook University, United States Decoding reactive structures in catalytic clusters hidden in their X-ray absorption spectra		
14:50-15:00		Discussion of the session		
15:00-15:30		Coffee Break		

MoPM2	Chair: K	arl-Heinz Meiwes-Broer
15:30-15:50	HT04 Po46	Liana Socaciu-Siebert SPECS Surface Nano Analysis GmbH, Germany Routine operando studies with Near Ambient Pressure - XPS
15:50-16:10	IHT03	Stephan Bartling Leibniz Institute for Catalysis, Germany A near ambient pressure XPS setup and a nanofluidic reactor device for operando gas phase catalysis
16:10-16:30	HT05 Po19	Zdeněk Jakub CEITEC, Czech Republic Adsorbate-induced structural evolution changes the mechanism of CO oxidation on a Rh/Fe ₃ O ₄ (001) model catalyst
16:30-16:40		Discussion of the session
16:40-18:00		Flash talks – Posters with odd numbers
18:00-21:00		Poster Session I
		Posters with odd numbers

Poll for best posters of this session

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Tuesday July 20

TuAM1	Chair: M	larc Willinger
8:30-9:00	IL05	Armin Kleibert Paul Scherrer Institut, Switzerland Oxide shell growth kinetics and magnetism of cobalt nanoparticles during early stage oxidation
9:00-9:20	HT06 Po09	Veronique Dupuis Institut Lumiere Matiere, France Nanomagnets elaborated by Mass-Selected Low Energy Cluster Beam Deposition
9:20-9:40	IHT04	Chao Zhang Uppsala University, Sweden Modelling protonic double layer at metal oxide-electrolyte interfaces
9:40-9:45		Sponsor flash – Gustavo Santiso Quinones The nanocrystallography revolution: Eldico Scientific's novel 3D ED device
9:45-10:00		Discussion of the session
10:00-10:30		Coffee Break

TuAM2	Chair: (Claude Henry
10:30-11:00	IL06	Vlasta Bonačić-Koutecký Humboldt Universität Berlin/University of Split, Croatia Concepts guiding joint theoretical and experimental approaches from catalysis to bioimaging
11:00-11:20	HT07 Po16	Andreas Hauser Graz University of Technology, Austria Mixed-method and artificial intelligence-enhanced strategies toward the modelling of metallic nanostructures
11:20-11:40	HT16 Po52	Kevin Rossi Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland A Next-Gen site-counting method to link size, shape, and activity of metallic nanocatalysts for the electrochemical reduction of small molecules
11:40-11:50		Discussion of the session
12:00-13:30		Lunch

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Tuesday July 20

Chair: N	Chair: Noelia Barrabés		
IL08	Claude Henry CINaM CNRS/Aix-Marseille University, France Reactivity of regular arrays of Pd clusters supported on a nanostructured alumina thin film: from nanoparticles, clusters to single atoms		
IL09	Alessandro Fortunelli CNR-ICCOM, Istituto di Chimica dei Composti Organometallici, Italy Theoretical approaches to nanocluster catalysis		
HT08 Po20	Ewald Janssens KU Leuven, Belgium Methanol dehydrogenation by cationic vanadium clusters		
	Discussion of the session		
	Coffee Break		
	IL08 IL09 HT08		

TuPM2	Chair: A	llessandro Fortunelli
15:30-15:50	IHT05	Christopher Heard Charles University in Prague, Czech Republic Stabilization, migration and sintering of zeolite- encapsulated metal clusters
15:50-16:20	IL10	Scott Anderson University of Utah, United States Cluster model catalysts: improved stability, size-selected electrocatalysis, and single cluster/atom electrocatalysis
16:20-16:50	IL11	Anastassia Alexandrova UCLA, United States Dynamic fluxionality and metastable nature of active sites of supported cluster catalysts
16:50-17:20	IL12	Nuria López Institute of chemical Research of Catalonia, Spain Speciation in low-nuclearity catalysts: the frontier to robust structure- activity relationships
17:20-17:30		Discussion of the session
18:00-22:00		Conference Dinner
18:00		Departure by bus from Conference venue/Clarion hotel to the Castle Liblice
		Return to Prague around 22:00

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Wednesday July 21

WeAM1	Chair: E	Chair: Ewald Janssens		
8:30-8:50	IHT06	Detre Teschner Max-Planck-Institute for Chemical Energy Conversion, Germany Key role of chemistry versus bias in electrocatalytic oxygen evolution		
8:50-9:20	IL13	Noelia Barrabés Institute of Materials Chemistry / TU-Wien, Austria Atomically designed catalysts by bimetallic metal nanoclusters: insights into the structure dynamics by operando spectroscopy		
9:20-9:50	IL14	Angelika Brückner Leibniz-Institut für Katalyse, Germany Impact of synthesis and test conditions on nanostructure and electron transfer in Pt/metal sulfide/C ₃ N ₄ semiconducturs during photocatalytic H ₂ production		
9:50-10:00		Discussion of the session		
10:00-10:30		Coffee Break		

WeAM2	Chair: l	Jlrike Diebold
10:30-11:00	IL15	Kersti Hermansson Uppsala University, Sweden Size dependent oxygen chemistry of CeO ₂ nanoparticles
11:00-11:20	IL16	Richard Palmer Swansea University, United Kingdom Challenges for nanoparticle deposition: predicting the catalytic performance of nanoalloys and scale-up to manufacturing
11:20-11:50	IL17	Pascal Andreazza ICMN Université d'Orléans CNRS, France Real-time analysis of the incorporation of Co or Ni heteroatoms into Ag clusters and vice versa
11:50-12:00		Discussion of the session
12:00-13:30		Lunch
13:30-14:00		Lunchtalk Štefan Vajda Introduction of the J. Heyrovský nanocatalysis program: Catalysis by nano- and subnanometer size catalysts
14:00		Tour of the Nanocatalysis labs / Free Afternoon

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Thursday July 22

ThAM1	Chair: Pascal Andreazza		
8:30-9:00	IL18	Panagiotis Grammatikopoulos OIST Graduate University/ETH Zurich, Japan Nanoparticle scaffold for multilayered Si-based Li-ion battery anodes	
9:00-9:30	IL19	Petr Krtil J. Heyrovský Institute of Physical Chemistry, Czech Republic Optimization of activity of electrocatalytic oxides on local level - top down and bottom up strategies in materials' design	
9:30-10:00	IL27	M.A. López-Quintela University of Santiago de Compostela, Spain Synthesis at pilot scale	
10:00-10:10		Discussion of the session	
10:10-10:40		Coffee Break	

ThAM2	Chair: Martin Srnec		
10:40-11:00	IHT07	Hazar Guesmi CNRS-ICGM-Montpellier, France Modeling the effect of reactive gas on alloy catalysts from single-atom sites to nanoparticles of thousands of atoms	
11:00-11:30	IL20	Vladimír Matolín Charles University, Czech Republic <i>Hydrogen – fuel for sustainable energy</i>	
11:30-12:00	IL21	Mauro Stener Trieste University, Italy Excited states and metal clusters: computational studies from optical properties to photocatalysis	
12:00-12:10		Discussion of the session	
12:10-13:30		Lunch	

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Thursday July 22

Chair: Maria Pilar de Lara-Castells		
IL22	Laurent Piccolo IRCELYON, University of Lyon, France Reaction-induced changes in structure and activity of supported platinum catalysts investigated in situ: from single atoms to clusters	
IL23	Gareth Parkinson TU Wien, Austria Unravelling CO adsorption on model single-atom catalysts	
IHT08	Maria J Lopez Universidad de Valladolid, Spain Reactivity of Pd-Cu nanoalloys towards hydrogen adsorption and dissociation	
	Discussion of the session	
	Coffee Break	
	IL22	

ThPM2	Chair: Maria J Lopez		
15:30-15:50	HT10 Po12	Michal Fárník J. Heyrovský Institute of Physical Chemistry, Czech Republic Pickup and reactions of molecules on carbonaceous from the perspective of atmospheric and interstellar processes	
15:50-16:10	HT11 Po14	Estefania German Universidad de Valladolid, Spain DFT study of TM ₆ (TM: V, Co, Pd) adsorption on boron-graphdiyne layer	
16:10-16:30	HT12 Po42	Gustavo Santiso-Quinones Eldico Scientific AG, Switzerland 3D-ED continuous rotation method in nanocrystallography: a dedicated device for structural elucidation of nanocrystalline particles	
16:30-16:40		Discussion of the session	
16:40-18:00		Flash talks – Posters with even numbers	
18:00-21:00		Poster Session II	
		Posters with even numbers	
		Poll for best posters of this session	

Start of the poll for best HTs

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Friday July 23

FrAM1	Chair: Laurent Piccolo		
8:30-8:50	HT13 Po32	Kinga Mlekodaj J. Heyrovský Institute of Physical Chemistry, Czech Republic Splitting of O ₂ at room temperature over distant binuclear transition metal centers in zeolites for direct oxidation of methane to methanol	
8:50-9:20	IL24	Ulrike Diebold TU Wien, Institute of Applied Physics, Austria Direct assessment of the acidity of individual surface hydroxyls on oxides	
9:20-9:50	IL25	Robert Schlögl Fritz Haber Institute of Max Planck Society, Germany On the relation between dynamics, nanostructure and catalytic activity of materials	
9:50-10:00		Discussion of the session	
10:00-10:30		Coffee Break	

FrAM2	Chair: Christopher Heard		
10:30-11:00	IL26	Martin Srnec J. Heyrovský Institute of Physical Chemistry, Czech Republic On the role of asynchronicity in C-H bond activation	
11:00-11:20	HT14 Po38	Muhammad Irfan Qadir J. Heyrovský Institute of Physical Chemistry, Czech Republic Selective CO ₂ hydrogenation to olefin-rich hydrocarbons driven by FeO _x nanorods decorated with Cu nanoparticles	
11:20-11:40	HT15 Po26	David Kubička University of Chemistry and Technology Prague, Czech Republic Copper clusters for environmentally friendly hydrogenolysis of esters to alcohols – effects of support properties and copper introduction method	
11:40-11:50		Discussion of the session	
12:30		Announcement of Best Posters & Best Hot Topic Talks	
12:30-13:00		Closing event, farewell	



POSTERS - MONDAY

Po01 Olesya Ablyasova

Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

XAS study of electronic structure of cold gas-phase manganese oxide clusters

Po03 Jose Eduardo Barcelon

Universita di Parma, Italy

Surface assisted synthesis, characterization and electronic properties of pristine and oxygen-exposed graphene nanoribbons on Ag(110)

Po05 **Sebastian Cisneros**

Leibniz Institute for Catalysis, Germany

Modulating the chemical state of Ru supported on TiO₂ to control CO₂ hydrogenation selectivity

Po07 Xingchao Dai

Leibniz Institute for Catalysis, Germany

Extending the potential of CuO_x catalysts for valorization of biomass-based platform molecules by downsizing clusters to active single sites

Po09 Veronique Dupuis

Institut Lumiere Matière, France

Nanomagnets elaborated by Mass-Selected Low Energy Cluster Beam Deposition

Po11 Katharina Engster

Institute of Physics, University of Rostock, Germany

Clusters as nanoscale light sources: electron excitations on silicon and tetracene crystallites

Po13 Max Flach

Helmholtz Zentrum Berlin, Germany

Charge transfer in L-edge x-ray absorption spectra of diatomic gas-phase iron halide cations: beyond the oxidation state

Po15 Lena Haager

TU Wien, Austria

Comparison of single Rh adatoms on α -Fe₂O₃(1102) and TiO₂(110) stabilized by adsorbed water

Po17 Guillermo Herrera - to be presented by Veronique Dupuis

Institut Lumière Matière, France

Size and surface/interface effects on the magnetic behavior of B2- like supported FeRh nanoclusters

Po19 Zdeněk Jakub

Central European Institute of Technology (CEITEC), Czech Republic

Adsorbate-induced structural evolution changes the mechanism of CO oxidation on a $Rh/Fe_3O_4(001)$ model catalyst

Po21 Kevin Anthony Kaw

Quantum Solid-State Physics, KU Leuven, Belgium

The wavelength-dependent non-linear absorption and refraction of Au_{25} and Au_{38} monolayer-protected clusters

Po23 Monika Klusáčková

J. Heyrovský Institute of Physical Chemistry, Czech Republic Photoelectrochemical activity and selectivity of SrTiO₃ nanocubes

Po25 Jaroslav Kočišek

J. Heyrovský Institute of Physical Chemistry, Czech Republic Electron Attachment to Fe(CO)₅ Aggregates on Ar Clusters



Po27 Anastasia Kurbanova

Charles University, Czech Republic

Preparation of Fe@zeolite composite hydrogenation catalysts with metallic nanoparticles by reductive demetallation of Fe-zeolites

Po29 Ang Li

Charles University, Czech Republic

Tracing the stability of subnanometric metal clusters on layered zeolite by in- situ TEM investigation

Po31 Peter Matvija

Charles University, Czech Republic

Ceria-supported metal clusters studied by STM and NAP-XPS

Po33 Shashikant Kadam

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Design and application of capillary-based reactor for microactivity reference catalytic testing

Po35 Vladimíra Petráková

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Modified absorption of dye molecules is related to specifically treated silver nanoparticles and is not a general phenomenon in metallic nanoparticles

Po37 Pavel Pleskunov

Charles University, Czech Republic

Reactive magnetron sputtering and gas condensation of tantalum oxynitride nanoparticles with architecture and band gap controlled by design

Po39 Ali Rafsanjani-Abbasi

Technische Universität Wien / Vienna University of Technology, Austria Thermal stability and CO-induced mobility of single Pt adatoms supported on the α -Fe₂O₃(11 $\overline{\ 0}$ 2) surface

Po41 Leo Sala

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Stability of gold nanoparticle-DNA origami conjugates under gamma irradiation

Po43 Barbora Sedmidubská

J. Heyrovský Institute of Physical Chemistry, Czech Republic Low-energy electron attachment to L- Valine.(H₂O)_n clusters

Po45 **Panukorn Sombut**

Institute of Applied Physics, TU Wien, Austria

Polarons in single atom catalysts: case study of Me₁=[Au₁, Pt₁, Rh₁] on TiO₂(110)

Po47 Marija Stojkovska

University of Genova, Italy

Monitoring oxidation and reduction of iron oxide islands on Pt(111)

Po49 Mykhailo Vaidulych

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Cluster deposition instrument: from a single atom to nanoscale clusters

Po51 Arik Beck - to be presented by Marc Willinger

ETH Zürich, Switzerland

Following the structure of copper-zinc-alumina across the pressure gap in carbon dioxide hydrogenation

Po53 Dianwei Hou

Charles University, Czech Republic

Theoretical insights into zeolite encapsulated subnanometer platinum



POSTERS - THURSDAY

Po02 Öyküm Naz Avcı

CNR-ICCOM, Italy

Oxygen evolution reaction (OER) mechanism and activity on spinel oxide-type catalysts

Po04 Lucinda Blanco Redondo

Charles University, Czech Republic

Ir-decorated Pt nanoparticles as bifunctional catalyst for unitized regenerative proton exchange membrane fuel cells

Po06 Mayara da Silva Santos

Helmholtz-Zentrum Berlin für Material und Energie GmbH, Germany

High-resolution X-ray absorption spectroscopy in a cryogenic ion trap as a tool to investigate 3d metal—oxygen bonds

Po08 Alina M. Darabut

Charles University, Czech Republic

Preparation and characterization of thermally expanded graphite. Applications for PEM FCs technology

Po10 Andreas Erlebach

Charles University Prague, Czech Republic

Cluster confinement in zeolites: insights from accurate neural network potentials

Po12 Michal Fárník

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Pickup and reactions of molecules on carbonaceous clusters from the perspective of atmospheric and interstellar processes

Po14 Estefania German

Universidad de Valladolid, Spain

DFT study of TM₆ (TM: V, Co, Pd) adsorption on Boron-graphdiyne layer

Po16 Andreas Hauser

Graz University of Technology, Austria

Mixed-method and artificial intelligence-enhanced strategies toward the modelling of metallic nanostructures

Po18 Vana Chinnappa Chinnabathini

KU Leuven, Belgium

Composition-tuned AuAg bimetallic clusters-modified TiO₂ films as efficient self-cleaning surfaces under visible light

Po20 Ewald Janssens

KU Leuven, Belgium

Methanol dehydrogenation by cationic vanadium clusters

Po22 Elisa Jimenez-Izal

University of the Basque Country (EHU/UPV) /Donostia International Physics Center (DIPC), Spain

Doping Pt with Ge to reduce the deactivation of the catalyst

Po24 Jaroslav Kočišek

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Butadiene clusters as a model for nanoelectrets

Po26 David Kubička

University of Chemistry and Technology Prague, Czech Republic

Copper clusters for environmentally friendly hydrogenolysis of esters to alcohols – effects of support properties and copper introduction method

Po28 Florian Lackner

Graz University of Technology, Austria

Rhodamine B covered Au nanoparticles separated by an intermediate spacing layer in helium nanodroplets



Po30 Aleš Marek

HVM PLASMA, spol. s r.o., Czech republic

Long-term stability of nanoparticle source operation for semi- industrial application and role of reactive admixtures

Po32 Kinga Mlekodaj

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Splitting of O_2 at room temperature over distant binuclear transition metal centers in zeolites for direct oxidation of methane to methanol

Po34 Daniil Nikitin

Charles University, Faculty of Mathematics and Physics, Czech Republic

Silver nanofluids prepared by direct transfer of magnetron-sputtered nanoparticles to liquid polymer

Po36 Vladimíra Petráková

Heyrovsky Institute of Physical Chemistry, Czech Republic

Controlled assembly of plasmonic nanoparticles and fluorophores for sub-diffraction manipulation of light

Po38 Muhammad Irfan Qadir

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Selective CO_2 hydrogenation to olefin-rich hydrocarbons driven by FeO_x nanorods decorated with Cu nanoparticles

Po40 Thantip Roongcharoen

Institute for the Chemistry of OrganoMetallic Compounds, Italy

Catalysts design by predictive modelling of aqueous phase reforming of liquid renewable feedstocks

Po42 Gustavo Santiso-Quinones

Eldico Scientific AG, Switzerland

3D-ED continuous rotation method in nanocrystallography: a dedicated device for structural elucidation of nanocrystalline particles

Po44 Karolína Simkovičová

J. Heyrovský Institute of Physical chemistry, Czech Republic

CO₂ conversion on Cu/Fe nanostructured catalysts

Po46 Liana Socaciu-Siebert

SPECS Surface Nano Analysis GmbH, Germany

Routine operando studies with Near AmbientPressure - XPS

Po48 Rika Tandiana

Université Paris Saclay, France

Investigation on the adsorption geometry of substituted aromatic compounds on the surface of gold nanoparticles: quantum chemical topology and vibrational study

Po50 Stanislav Valtera

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Subnanometer cluster-based catalysts for highly selective oxidative dehydrogenation of cyclohexene

Po52 **Kevin Rossi**

Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

A Next-Gen site-counting method to link size, shape, and activity of metallic nanocatalysts for the electrochemical reduction of small molecules