# Cluster – Surface Interactions

## Paris
## 1st – 4th Juin 2026

# Book of abstracts

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## Special Session on Nanoalloys Committee

The Special Session on Nanoalloys is organized on the 3rd and 4th of June, focusing on the interactions of nanoalloys with surfaces and other media. This session is organized with the support of a sub-committee:

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# Monday, 1st June
# Afternoon

# Biomembrane remodelling by ligand-protected metal clusters

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Ligand-stabilized metal clusters are a tunable nanoparticle platform whose size, shape, and surface chemistry can be engineered to control interactions with biological media. This tunability enables therapeutic and diagnostic uses, including bioimaging and drug delivery. A key opportunity is to use nanoparticles as interfacial agents that mechanically remodel lipid membranes.

Membrane fusion, in particular, is a topological transformation in which two membrane-bound compartments connect and then merge. In biology, fusion enables vesicular trafficking and communication, including neurotransmitter release, fertilization, and viral entry. Physically, fusion proceeds through highly curved metastable intermediates (stalk and hemifusion) whose formation and stability are set by curvature elasticity, membrane tension, and local packing defects. Ligand-stabilized clusters can act as synthetic fusogenic tools that reshape the free-energy landscape by stabilizing curvature and defect motifs at the interface.

Here we examine amphiphilic Au nanoparticles (NPs) bound to liposome surfaces as a minimal, adjustable fusogenic system [1]. Using coarse-grained Molecular Dynamics, we show that Au NPs adsorption and partial insertion can generate local curvature and packing defects that promote transitions toward stalk and hemifusion states. We relate the NP size [2] and vesicle curvature [3] to the stability of fusion intermediates. These results provide design principles linking the physico-chemical characteristics of clusters to membrane remodeling outcomes, supporting the rational development of synthetic fusogens for biomedical applications [4]. This suggests a route to engineer extracellular vesicle (EV)–like nanohybrids, where fusion between an endogenous EV and drug-loaded liposomes enables efficient cargo loading *in vitro* while preserving key EV surface features.

## References:

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# Engineering defects for electrochemical energy storage

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The increasing demand for efficient, high-power energy storage has accelerated research into technologies capable of delivering rapid charge–discharge capability, long cycle life, and high operational reliability. Among emerging and established storage systems, supercapacitors occupy an important position between conventional dielectric capacitors and rechargeable batteries. While batteries typically provide high energy density through bulk faradaic reactions, they are often limited in power output and cycle life due to slower reaction kinetics and structural degradation. Supercapacitors, by contrast, store energy through interfacial charge separation and/or fast surface redox processes, enabling exceptional power density and durability. In this talk I will describe our latest finding on energy storage based on Earth-abundant transition metal based electrodes, showing the possibility of engineer nanostructures defects to tune the final device performance. Electrochemical energy storage measurements further demonstrate that device performance is highly sensitive to defect density and type, as evaluated via transmission electron microscopy based methodologies.

These results indicate that the specific capacitance of transition metal-based nanostrucutres can be effectively tuned by controlling key synthesis parameters, highlighting the critical role of thermal treatment in optimizing electrochemical functionality.

## Acknowledgements:

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# Manipulating mechanical properties of thin films via nanoparticle incorporation

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The combination of a nanoparticle source with magnetron sputtering opens up plentiful potential for the fabrication of unique nanocomposite thin films. Nanoparticles (NPs) with tailored size, shape, distribution and volume density can be incorporated into a thin film matrix, without precipitation-related restrictions concerning phase diagrams and solubility. We use this approach to study deformation mechanisms in the resulting nanocomposite materials. In situ X-ray diffraction and resistance measurements during polymer-supported tensile testing are used to test the hypothesis that the intrinsic deformation mechanisms in brittle and ductile matrix films can be manipulated and improved via nanoparticles. The microstructures and nanoparticle concentrations are confirmed and characterized by TEM. For inherently brittle films (200 nm Mo), suffering from through thickness crack formation at low applied strains, incorporated nanoparticles (Al, 20 nm diameter) can significantly improve the electro-mechanical behavior. The observed changes in the developing crack pattern, through crack deflection at nanoparticles, correlates well with a lower electrical resistance at equivalent strains and changes in the stress-strain curve. For ductile films (25 - 200 nm Cu and Au) the observed influence of nanoparticles (W, Co, 4 nm diameter) observed softening or strengthening strongly depends on the grain size and film thickness. With further insights into the deformation behavior, nanoparticle incorporation via cluster sources is a powerful tool to tailor mechanical and functional properties of thin films for future devices.

# Atomic Engineering of Nanoparticles (Clusters)
# From Atomic Structure to Scale-Up and Applications

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"What would the properties of materials be if we could really arrange the atoms the way we want them? They would be very interesting to investigate theoretically. I can't see exactly what would happen, but I can hardly doubt that when we have some control of the arrangement of things on a small scale we will get an enormously greater range of possible properties that substances can have, and of different things that we can do".

So wrote Feynman in 1959, and the challenge to control materials on the atomic-scale is now being addressed vigorously, not least in the world of small nanoparticles (clusters of atoms). While Don Eigler made this quotation famous via his STM manipulation experiments in the 1990s, the cluster approach is more scalable than STM, and cluster production at the gram and and even kg scale is now within reach.

On the fundamental side, I will report recent studies of the atomic structure and dynamics of sub-10nm particles created by physical (as opposed to chemical) methods, specifically growth or deposition on surfaces in vacuum [1-3]. I will describe variable-temperature video imaging of individual (thus size-selected) clusters in the aberration-corrected (AC) electron microscope. The newest results concern the arrangements and dynamics of sub-5nm Au and Pt clusters. In the case of Au, the familiar competition between face-centred-cubic and decahedral structures is evident, validating the new method. In the case of Pt, we establish transition from the 5-fold Icosahedral and then Decahedral isomers to the bulk fcc structure as size increases from 150 to 450 atoms.

On the applications side, I will summarise the progress made by Swansea and the Grove spin-out company in translating materials prepared by physical methods in vacuum into solution. The resulting colloids have multiple applications, e.g., as multicoloured labels for lateral flow tests, catalysts, SERS substrates, light emitters and functional inks.

Together, the results provide a snapshot of progress towards realizing Feynman's vision in the world of nanoparticles and colloids.

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[1] H. Eliasson, Y. Niu, R.E. Palmer, H. Gronbeck, R. Erni, Nanoscale 15 19091 (2023).
[2] M. Dearg, C. Roncaglia, D. Nelli, E. El Koraychy, R. Ferrando, T.J.A. Slater, R.E. Palmer, Nanoscale Horizons 9, 143 (2024).
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# Promises Kept: the journey to the market of devices based on cluster-surface interactions

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The study of cluster-surface interactions has been a very active field of research [1]. Fundamental aspects have been deeply investigated, and new directions of research are constantly appearing. The opportunities related to practical applications of systems based on cluster-surface interactions have been always emphasized and considered as strong motivations to explore this field [2]. Here I will present some cases where promises have been kept, and devices based on CSI are on a particularly complex and challenging market such as that of medical devices [3]. The critical requisites for the transition from the lab to the market will be highlighted and discussed.

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[2] R.E. Palmer, R. Cai, J. Vernieres, Acc. Chem. Res. 51, 2296 (2018)
[3] B. Kearney, O. McDermott, Therap. Inn. Reg. Sci. 57, 783 (2023)

# Stained Glass as an Optical Interface: Surface–Nanoparticles Interactions for Designing Color

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Traditionally regarded as a decorative or heritage object, stained glass can also be understood as a true optical system in which the glass surface plays a central role in the formation of color. This contribution proposes to revisit historical and contemporary glass-painting techniques through the lens of surface–nanoparticle interactions.

We focus in particular on stain painting processes, where color does not arise from an opaque coating but from physicochemical modifications within the near-surface region of the glass. Ion exchange, diffusion of metallic species, and the subsequent nucleation and growth of nanoparticles in the glass matrix give rise to emblematic transparent colors such as silver yellow and copper red. At this scale, the surface is no longer merely a support: it becomes a reactive interface that governs ion penetration, reduction conditions, nanoparticle morphology, and ultimately the optical response.

This perspective creates a dialogue between the history of materials, glass chemistry, and nano-optics. We will show how modern concepts from plasmonics and optical modeling, including Mie theory, can be used to interpret and, in some cases, predict the resulting colors. At the intersection of art, physics, and chemistry, stained glass thus emerges as an original framework for thinking about surfaces not only as sites of aesthetic creation, but also as platforms for light engineering.

# Tuesday, 2nd June
# Morning

# Tuning the activity and stability of sub-nano clusters using deposition dynamics, support modifications, and cluster size

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The catalytic and electrocatalytic activity of sub-nano clusters can be quite high – higher than can be explained simply the surface availability of the catalytic metal atoms. The enhanced activity reflects electronic structure and active site geometries that are non-bulk-like, and which can be tuned by varying the cluster composition, size, and interactions with the support. The difficulty is that these small, undercoordinated metal centers are inherently unstable with respect to both sintering and poisoning, both of which deactivate them. This talk will explore three strategies for stabilizing sub-nano Pt-based cluster catalysts against deactivation, while maintaining high activity.

One approach is doping/alloying the Pt clusters with elements that can transfer electrons to or from clusters. This modifies the Pt chemical properties but also makes the cluster bonding ionic which tends to resist both Ostwald and Smoluchoski ripening, at least on ionic supports like alumina. This approach will be illustrated for Ge-doped Pt clusters on alumina supports, which are resistant to sintering and coking in high temperature hydrocarbon environments.

Another approach is to partially embed Pt clusters into an otherwise weak-binding support, disrupting both the support and cluster binding. This results in covalent Pt-support binding and creates new types of hybrid metal-support active sites. This approach will be illustrated by hydrogen evolution electrocatalysis by Pt clusters embedded in HOPG.

Finally, a weak-binding support (e.g. HOPG) can be modified by heteroatom implantation to create cluster binding sites that stabilize the clusters, and also modify their electronic and chemical properties. This approach will be illustrated for nitrogen- and metal-implanted HOPG supports for Pt electrocatalysts.

# When the Environment Matters: Symmetry Breaking and Shape Selection in Platinum Nanocrystals

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The shape of metal nanocrystals is commonly rationalized in terms of thermodynamic stability or facet-dependent growth kinetics. At the nanoscale, however, subtle symmetry-breaking mechanisms—strongly influenced by the surrounding environment—can determine the final morphology. Here, the growth of platinum nanocrystals is analyzed under two limiting conditions: gas-phase condensation and aqueous wet chemistry.

In an inert gas environment, where growth is governed exclusively by Pt–Pt interactions, size-selected naked nanocrystals evolve from truncated octahedra to octahedra and, at larger sizes, to tetrahedra. This transition originates from an intrinsic, defect-mediated kinetic pathway operating in an isotropic environment, without the involvement of ligands or adsorbates [1].

In solution, by contrast, the chemical environment plays a decisive role. During borohydride reduction, hydrogen released in situ selectively adsorbs on {100} facets. Density functional theory calculations on finite-size Pt clusters reveal a clear size dependence of hydrogen adsorption energies, highlighting the importance of facet dimensions at the nanoscale. The resulting environment-induced symmetry breaking leads to the formation of asymmetric pyramidal nanocrystals, a morphology that is not observed in vacuum, or when reducing agents that do not generate hydrogen are employed [2].

These results highlight two distinct routes to symmetry breaking—intrinsic kinetic mechanisms in the absence of external interactions and adsorbate-induced effects in solution—and demonstrate how controlled environment–nanoparticle interactions can be exploited to design asymmetric nanostructures, such as bimetallic Janus nanoalloys [3].

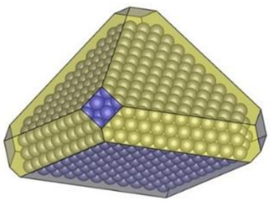

**Figure 1**: Platinum nanopyramid. This asymmetric shape requires the interaction with hydrogen in the solution to be formed.

## References:

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# Development of Metal Clusters as Co-Catalysts for Photocatalytic Water Splitting

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Photocatalytic water splitting allows producing green hydrogen without the need to be connected to the electric grid. Photocatalysts absorb light and generate electron hole pairs. Provided that the energy levels of the valence band and conduction band are positioned below and above the energy levels required for the oxygen and hydrogen evolution reaction, respectively, the absorbed light energy can be used to generate H2 and O2.[1] Photocatalysts consist typically of three components: the light absorbing material, the co-catalysts for facilitating the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER).

This presentation focuses on the use of atomic precise nanoclusters as HER and OER co-catalysts.[2] These nanoclusters can be synthesized with precision in the number of atoms forming the cluster and tailored for specific reactions by choosing a specific number of atoms forming a cluster. They can also be generated in gas phase cluster sources. The deposition of the clusters on surfaces requires conditions which avoid their agglomeration. Subsequent to the deposition the electronic structure needs to be determined such that the size of the clusters can be selected for a specific reaction. In this presentation the deposition and analysis of the electronic structure of Au, Ru and Pt clusters will be covered representing cases where agglomeration is avoided and occurs.

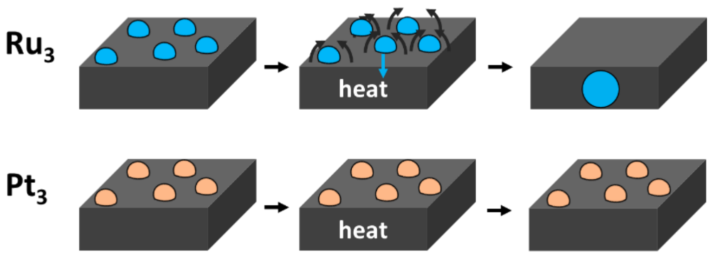


**Figure 1**: $Ru_3$ clusters embed and agglomerate when deposited onto $TiO_2$ while $Pt_3$ cluster neither embed nor agglomerate.

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# From cluster plasmon physics to electronics

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Atomic clusters (referred to as clusters), are multinuclear aggregates between atoms/molecules and macroscopic matter. They represent the initial ecology of condensed matter and are ideal models for associating macroscopic properties and microstructure of matter, which is of great significance for deep understanding and understanding of the law of matter transformation. This report will present the latest progress from the cluster plasmon physics to electronics.

Mass selection of clusters with high flow strength and wide mass range is realized, and the beam flow rate after mass selection reaches the level of more than 10 nA. On this basis, gold clusters with atomic numbers ranging from 100 to 70,000 are prepared, and a picture of the evolution process of plasmon physics from solid state to atomic-molecular evolution of gold clusters is constructed.

Developed the characteristic direction of single cluster transport, established single cluster capture and electrical measurement technology, and manufactured a series of single cluster devices, such as $Si_{170}$ and $Gd@C_{82}$. The first single-molecule electret has been discovered and its single-atom information storage capability has been demonstrated in the $Gd@C_{82}$ single-cluster device.

Realized the electrically controlled Zeeman effect in $Dy@C_{84}$ single-molecule transistors, thus revealing a transition in the magnetic moment. Density functional theory calculations further corroborate our realization of nonvolatile switching of single-atom magnetism, and the switching stability emanates from an energy barrier of 92 meV for atomic relaxation.

## References:

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# Stabilization of Au Nanoclusters into 2D Rafts by Carbon Support

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The question of metastability always underpins nanostructure fabrication. It is highly pertinent to the functional performance of nanomaterials. Here we explore the atomic structure of Au clusters (1-100 atoms) assembled from gold atoms sputtered onto amorphous carbon TEM supports. We find persistent evidence of 2D monolayer rafts competing with 3D cluster structures to at least size N=60 atoms and this is consistent with new DFT theory calculations.

The nuclearity and atomic structure were determined by aberration-corrected scanning transmission electron microscopy (STEM) in the high-angle annular dark field (HAADF) mode [1]. The cluster size measurements employed a two-step image analysis process, whereby the intensity of single atoms was determined to calibrate the intensity of the clusters themselves. The relationships between cluster size and cluster structure were obtained.

The main result from the analysis of the grown Au nanoparticles with size <100 atoms is the common formation of 2D rafts (typically one atom high). DFT calculations in addition to pair distribution function analysis indicate energetic and lattice match stabilization by the carbon support in the size regime of <100 atoms, demonstrating good competition with 3D structures also observed on the surface. These 2D cluster structures are expected to behave quite differently from a catalytic point of view than the competing 3D forms.

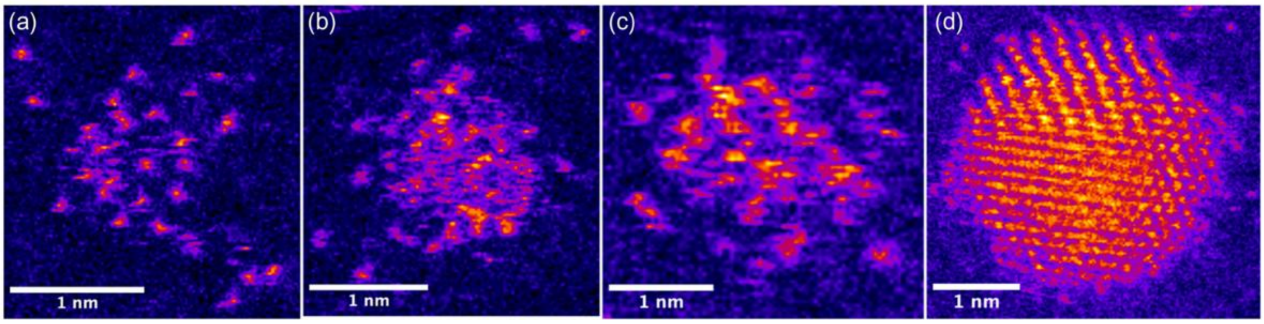


**Figure 1**: HAADF–STEM images of samples made by sputtering Au atoms onto an amorphous carbon support film. The sample contains isolated single atoms, a–c) 2D"rafts", and d) 3D clusters. The figures shown demonstrate 2D and 3D structures of sizes a) Au16, b) Au54, c) Au83, and d) Au1322 [2].

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# In situ growth of two-dimensional metallic islets suspend inside graphene pores

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Suspended two-dimensional (2D) metals (metallenes) have been widely predicted [1], yet direct observations remain scarce [2]. Here, we present an *in situ* method to synthesize few-nanometer islets (nanometallenes) of 2D zirconium (Zr) inside graphene pores using electron beam irradiation in a transmission electron microscope (TEM) [3]. Unlike epitaxial growth on metallic substrates, this approach yields free-standing 2D Zr islets with atomic precision.

Electron irradiation decomposes the Zr acetylacetonate precursor on graphene, generating Zr nanoparticles that transformed into 2D Zr islets embedded within the graphene lattice (Figure 1). Systematic observations reveal their formation, stability, and the role of defect engineering in confinement.

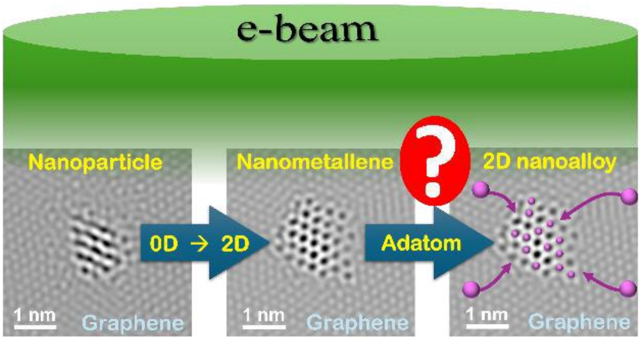


**Figure 1:** In situ growth of 2D Zr islets using TEM. A pathway toward 2D nanoalloys?

These findings reveal how electron beams drive the growth and degradation of 2D Zr islets, showing a new strategy for synthesizing atomically thin metals. Moreover, by combining different metal deposition methods with beam-driven dynamics, this approach can be extended to the fabrication of bimetallic nanometallenes, enabling controlled alloying at the atomic scale. Such capability opens pathways to explore other pure and alloyed 2D metals with superior electronic, magnetic and catalytic properties.

## References:

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[3] R. G. Mendes *et al. In Situ* Growth of Suspended Zirconene Islet inside Graphene Pores. *Adv. Funct. Mater.* 35 (2), 2025.

# Substitutional Mn dimers in graphene created by ultralow-energy cluster implantation

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Although adsorbed and defect-pinned clusters on 2D materials [1-3] have been widely explored, the substitutional incorporation of cluster-like species into 2D lattices remains comparatively under-studied. We investigated ultralow-energy (ULE) cluster implantation in monolayer graphene. Specifically, a beam of Mn2+ ions was accelerated to 82 eV and implanted into graphene on Cu(111). This approach yields adjacent substitutional Mn atoms, i.e., substitutional Mn2, within the graphene lattice. Low-temperature scanning tunneling microscopy (STM) observed a four-lobe feature and spectroscopic fingerprints, consistent with density-functional theory calculations. To understand the implantation mechanism, molecular dynamics simulations were conducted to track the impact sequence, including Mn2 fragmentation upon collision, carbon displacement, and vacancy formation. By combining the STM observations with impact-dynamics simulations, insight was obtained in the formation of substitutional Mn2 in graphene. Overall, this work highlights ULE cluster implantation as a promising strategy for creating substitutional multi-atom defects in 2D materials.

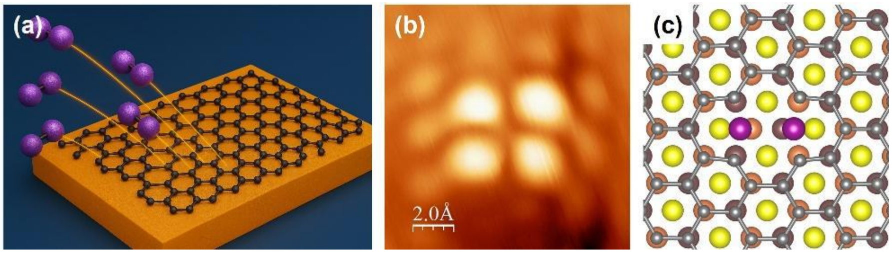


**Figure 1:** (a) Schematic of the ultralow-energy (ULE) cluster implantation into graphene/Cu(111). (b) Experimental STM topographies of a substitutional Mn2 and (c) corresponding atomic structure. (purple: Mn; gray: C; yellow: first layer of Cu; orange: second layer of Cu; brown: third layer of Cu).

## References:

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# A New Size-Selected Metal Cluster Source for Catalyst Research at Diamond Light Source

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Size-selected metal clusters composed of tens to thousands of atoms, supported on metal oxide thin films, provide a powerful model platform for probing size-dependent effects in heterogeneous catalysis and related surface processes[1,2]. Precise control over cluster size, composition, and deposition conditions is essential for establishing reliable structure–property relationships at the nanoscale.

At Beamline B07, Diamond Light Source, a fully integrated size-selected cluster deposition platform has been developed and commissioned, combining plasma sputtering, a gas-phase aggregation zone, in-line mass filtering, and an ultra-high vacuum (UHV) deposition chamber. Metal vapours are generated via inert-gas plasma sputtering of solid targets, followed by controlled nucleation and growth within the aggregation region. The system enables simultaneous sputtering from three targets, allowing accurate compositional tuning and alloy cluster synthesis. In-situ plasma spectroscopy provides real-time monitoring of sputtered atoms and plasma species, while automated sample handling and control systems regulate cluster coverage and kinetic energy to ensure stable and reproducible deposition.

A central technical challenge arises from the simultaneous formation of charged and neutral clusters within the plasma. Although an in-line quadrupole mass filter (QMF) enables precise mass selection and monitoring of charged cluster current and kinetic energy, neutral clusters remain unaffected and may compromise size selectivity. To overcome this limitation, finite element simulations (COMSOL Multiphysics) were performed to model charged particle trajectories and optimise electric field configurations within the deposition chamber. These results guided the design of a deflection system enabling the separation of charged from neutral clusters. As practical examples, size-selected Pd, Fe, and Cu clusters have been synthesised and deposited on oxide supports for model catalytic and surface studies. The size selectivity and narrow size distribution of the deposited clusters were confirmed by atomic force microscopy (AFM), verifying that cluster dimensions are consistent with the selected mass range.

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# Tuesday, 2nd June
# Afternoon

# Brain-like Computation with Percolating Networks of Nanoparticles

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Self-assembled networks of nanoparticles have emerged as important candidate systems for brain-like (or neuromorphic) information processing.[1] The essence of the approach is to take advantage of the intrinsic dynamical properties of these networks to implement brain-inspired approaches to computation.[2]

Our percolating networks of nanoparticles (PNNs) are self-assembled via simple deposition processes that are completely CMOS compatible, making them attractive for integration. The key to our approach is to terminate the deposition at the onset of conduction (the percolation threshold) when the electrical properties of the network are dominated by tunnel gaps between groups of particles.[3] At high voltages the memristive tunnel gaps turn out to have neuron-like properties, which means that PNNs can be viewed as networks of neurons.[4]

Both the structural and dynamical properties of PNNs have been shown to be brain-like[2] and, in particular, avalanches of neuron-like spiking events have been shown to be critical.[1] Criticality is a key feature of the biological brain that has been related to optimal information processing capability. We have explored brain-like computation with PNNs in two regimes, beginning with simulations[5,6,7] that allow us to understand the processes and refine parameters, and then moving to experimental demonstrations[8,9]. At low voltages, the devices are amenable to reservoir computation and we have successfully demonstrated time series prediction, non-linear transformation and spoken digit recognition.[5,8] In the high voltage regime, the spiking behaviour of the 'neurons' has been exploited to perform Boolean logic and MNIST classification[6], and, most recently, optimization tasks such as integer factorisation[7,9]. New experiments are now underway in which the aim is to achieve both neuron-like and synapse-like behaviour simultaneously, which should allow new kinds of learning behaviour.[10]

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# Accurate MLIPs for reactive/dynamic processes upon oxide-supported metal clusters

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Atomistic modelling of materials in general and metal-based nanomaterials in particular is currently undergoing a profound transformation, driven by advances in machine learning (ML). In this new paradigm, ML interatomic potentials enable at least a thousand-fold acceleration of structure sampling at near reference-level accuracy, while ML-based surrogate models allow rapid prediction of properties such as NMR or mechanical responses. ML is also reshaping reaction network exploration and the analysis of large-scale molecular simulation data through robust dimensionality reduction and clustering techniques. Together, these developments now make it possible to move beyond idealized models and begin addressing realistic catalytic materials that include defects, heterogeneous structures and their dynamic evolution.

In this talk we will discuss recent developments in the area of machine learned interatomic potentials (MLIPs), including the shift from from-scratch training to finetuning of so-called foundation models,[1] the application of gpu-optimized architectures for simulation speed-up, and the implementation of these methods towards dynamics-influenced structure determination on supported small metallic cluster systems. We will illustrate these techniques with example cases involving the dynamics of Pt cluster migration/sintering on silicate supports,[2,3] coinage metals on alumina, and the generalization of catalytic reaction schemes for propane epoxidation.[4]

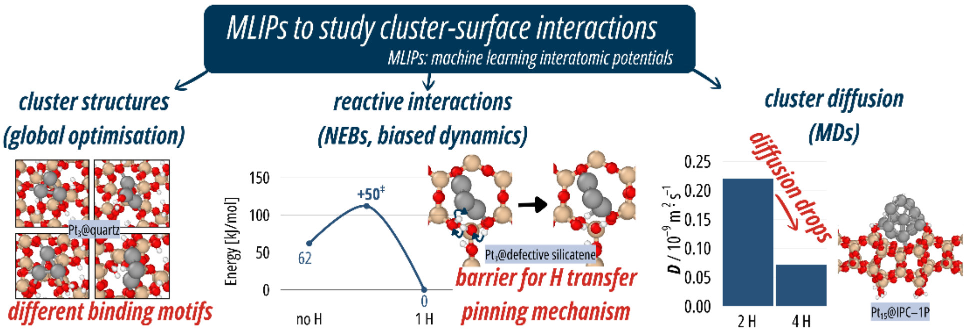


**Figure 1**: Schematic depiction of MLIP usage for studying supported metal cluster dynamics

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# Controlled Deposition of Nanocluster Superatoms on Organic Surfaces

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Among various gas-phase nanoclusters and their characteristic functionalities explored during the past several decades, nanoclusters formed with a highly symmetrical geometry and an electronically closed shell are known as "superatoms (SAs)," which mimic the chemical properties of atoms with clusters. So far, we have succeeded in mass synthesis of SAs, e.g. metal encapsulating Si SAs as ($M@Si_{16}^{+/-}$) as well as $Al_{13}^-$ (and $B@Al_{12}^-$) SA through a bottom-up magnetron sputtering technique [1], where they are promising candidates for the fabrication of SA assembled nanomaterials. To stably immobilize these SAs, preserving their favorable charge states in the gas phase, controlled deposition of these SAs is required using appropriate substrates, which facilitate desired cluster-surface interactions.

Here, we show that the choice of organic substrate can allow molecular control of charge transfer interactions at the cluster–surface interface and stabilize SAs on the surface. Since the localized interactions between the pre-decorated organic molecules and the deposited NCs are enhanced compared to those of a clean bulk metal or semiconductor substrate, the organic substrate is key to the immobilization of the deposited NCs, in which the NC aggregation caused by two-dimensional gas behaviors is suppressed.

For $Al_{13}^-$ (and $B@Al_{12}^-$) SA, exhibiting "superhalogen" property, it can be stably immobilized on a pre-deposited organic surface with p-type hexabenzocoronene (HBC) divertive, where its distinct chemical stability at the deposited phase is characterized by X-ray photoelectron spectroscopy (XPS) and oxidative reaction measurements[2].

On the other hand, the chemical properties of $M@Si_{16}$ can be designed by selecting the central metal atom based on their 68 $e^-$ shell closure. We found that the chemical robustness of alkali-like $M@Si_{16}$ (M = V, Ni, and Ta:69 $e^-$ at neutral) enhances by deposition on an n-type $C_{60}$ substrate, and halogen-like $M@Si_{16}$ (M = Lu) SAs show better stability on HBC derivative like a $Al_{13}^-$[3]. Currently the research is further extending to the discovery of periodic table of SAs based on $M@Si_{16}$ or $M@Ge_{16}$[4].

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# Size effects in Pd nano-catalysts for methane oxidation

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Size effects in heterogeneous catalysts nanoparticles are well established and are generally explained as due to a combination size-dependent changes in the coordination of metal atoms and their electronic structure. X-ray photoelectron spectroscopy (XPS) is an obvious technique to study such changes in the chemical composition and electronic structure of catalyst nanoparticles. However, as XPS is an averaging technique, experiments require a narrow distribution of cluster sizes in order to pinpoint size effects. Traditional methods of catalyst synthesis by impregnation/calcination of support powders lead to very large particle size distributions (typically ± 50 %) which are not suitable for such studies. We therefore use an alternative approach designed to enable XPS analysis in vacuum and under reaction conditions, whereby nanoparticles are synthesized by gas condensation and passed through a mass filter, which allows size selection in the range from one to more than 10,000 atoms typically with accuracy of a few percent. These particles are deposited onto a thin $Al_2O_3$ film, which mimics the properties of conventional alumina supports while being conductive enough to avoid any charging-related artefacts in the XPS spectra.

Changes in the chemical composition of Pd nanoparticles were studied by near-ambient pressure (NAP)-XPS under dry and wet reaction conditions for methane oxidation ($CH_4$ + $O_2$ [+ $H_2O$]) in the temperature range between 150°C and 450°C [1]. Under these conditions oxidation was observed for all particles, whereby the level of oxidation depends on the particle size. The presence of water leads to very significant changes in the oxidation behaviour of Pd, which are more pronounced for small particles. Sintering during the temperature ramp cannot be excluded, especially for the smaller particles, and may be part of the reason for the different behaviour under wet conditions. This study also shows a clear correlation between catalytic activity and the level of oxidation which – in turn – is particle-size dependent. It demonstrates the possibilities of fine-tuning catalytic activity if better size-control can be achieved in catalyst synthesis.

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# Modelling nanoparticle transformations in reactive environments

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The improvement of spectroscopic techniques has enabled the in-situ characterization of catalysts under operating conditions, often revealing a highly dynamic behavior of the active phase. Metals and metal-oxides usually employed as catalysts frequently undergo significant chemical and structural transformations during operation. In contrast, the design of structural models used to rationalize the catalytic properties of such materials has traditionally relied on a rather static picture of the catalyst substrate. In addition to this so-called environmental or dynamic complexity, the structural complexity of nanostructured catalytic materials further hinders the characterization of their response to reaction conditions [1].

Establishing reliable structural models of working catalysts is particularly relevant in computational modeling studies relying on quantum mechanical calculations. To overcome these challenges, novel computational approaches have been developed to determine the structure and composition of targeted materials and conditions, combining quantum mechanics, structure prediction (i.e. global optimization) algorithms, ab initio thermodynamics, and, more recently, machine-learning methods [2,3].

During my talk, I will introduce the efforts of our group in developing and applying novel global optimization techniques, focusing on recently developed grand canonical approaches tackling nanostructured materials under reaction conditions. I will showcase their capacity and limitations, presenting different case studies within thermal and electrocatalysis.

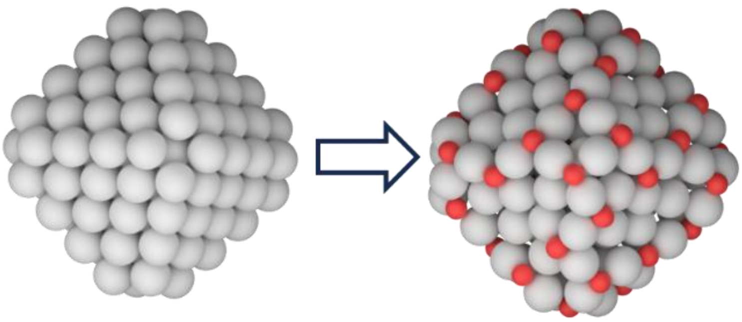

**Figure 1**: Example oxidation of metal nanoparticles

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# Revealing the Interplay of Inertial, Frictional, and Viscous Forces in Cluster Interaction Dynamics Using Physics-Informed Machine Learning

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We use molecular dynamics (MD) to investigate dynamic regimes in spreading of molecular clusters on solid surfaces. To analyze the underlying physical behavior, we use an approach based on the physics-informed neural network (PINN) droplet analysis introduced recently [1]. Spreading is commonly described by the power-law relation $r = \beta t^{\alpha}$ between contact radius $r$ and time $t$[2]. We quantify the influence of droplet size, surface wettability, and system temperature on the exponent $\alpha$ and the prefactor $\beta$, and assess the limitations of inertial [3], viscous [3], and frictional [4] scaling laws in describing the process. First, we establish a robust procedure for characterizing the droplet state during spreading and derive a new equation for $r$ based on the radius of gyration $R_{\mathrm{g}}$[5]. The new PINNs trained on MD data predict that $\alpha \to 0.1$ during the late stages on hydrophilic surfaces, independent of temperature, and consistent with Tanner's viscous regime. However, $\alpha \to 0$ for highly hydrophobic systems. We demonstrate that increasing the temperature does not lead to a superdiffusive regime. Second, we introduce a data-driven machine learning approach to determine the appropriate characteristic length scale in existing spreading scaling laws. When line tension effects are important, the relevant length scale is the equilibrium contact radius rather than the initial droplet radius. Moreover, the viscous scale provides the most consistent description of the entire spreading process, leading to the collapse of $\beta$ values. The results indicate that viscous forces dominate the spreading dynamics, inertial effects are relevant early, and frictional effects govern the transition between the two regimes. These findings highlight the combined roles of the active forces and provide clarity on previously conflicting interpretations.

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# Size-histogram determination of mass-selected clusters: beyond the spherical approximation

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The reliable size determination of clusters is often a pre-requisite to interpret various measurements on cluster assemblies [1]. The use of transmission electron microscopy images is one of the best experimental methods available to infer the size distribution, for particles of a few nanometers diameter: it offers a very good resolution and a statistical analysis of many particles (hundreds) is possible in a reasonable time. It can be automated with image softwares, involving some filtering and threshold-selection steps. However, standard observations (as opposed to tomography studies) only provide information on the projected area of particles in the sample plane (usually a thin carbon layer) so that assumptions need to be made concerning the out-of-plane dimension of clusters in order to deduce the effective size of particles. This effective size, which we call equivalent diameter $D_{eq}$ is that of a sphere having the same volume as the one of the true particles (often not a perfect sphere!). Even the in-plane projected area A may differ from a disk, so that a better approximation than the spherical approximation is desirable. In this widely used approximation, the measured A of each particle, is used to compute its hypothetical volume V, and thus its equivalent diameter corresponding to $D_{eq}=D_{sph}=(4A/\pi)^{1/2}$.

Here we will discuss other approximations [2] going beyond the spherical model : they can be very easily implemented because, in addition to the area A, they only use standard shape descriptors, namely the roundness r and the circularity C (equal to $4\pi A/P^2$ where P is the perimeter). I will show how the diameter $D_{eq,ellips}=r^{1/6}D_{sph}$ and $D_{eq,grain}=C^{1/6}D_{sph}$ naturally emerge, respectively with an “ellipsoidal” approximation or a “grain” approximation where particles are assumed to consist of touching grains without any coalescence. I will then discuss the extension of this “grain” model to the case of a partial coalescence. Taking advantage of the existence of well-defined multimers (dimers, trimers etc.) in the case of random deposition of mass-selected clusters [3], the benefits of this improved approach will be put into evidence [2]: the volume of multimers should indeed necessarily correspond to an integer number of incident particles (monomers) volume. In the end, the proposed approximations for improved size-histogram determination go beyond the spherical hypothesis (and in fact encompass it), which is found to often overestimate the cluster size, and allow us to keep using the concept of equivalent diameter, even with obviously non-spherical particles [2].

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# Nucleation of Carbon Nanoparticles in Gas Phase Plasma

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Gas-phase plasmas enable the synthesis of nanoparticles with tailored properties, but their unintentional formation can disrupt plasma stability and process efficiency—posing both a challenge and an opportunity for plasma technology.

Gas-phase plasmas are highly reactive media capable of generating solid particles in the gas phase. Understanding their formation, growth, and interaction (or coupling) with the discharge is critical for many reactive plasma processes. Enhanced comprehension of these mechanisms allows for the optimization of processes, improved stability, and better control over the quantity, structure, and quality of the resulting particles.

Particle nucleation in reactive plasmas occurs via the dissociation of feed gas compounds, followed by the growth of molecular or ionic precursors. This nucleation can proceed through multiple pathways, as illustrated in Figure 1.

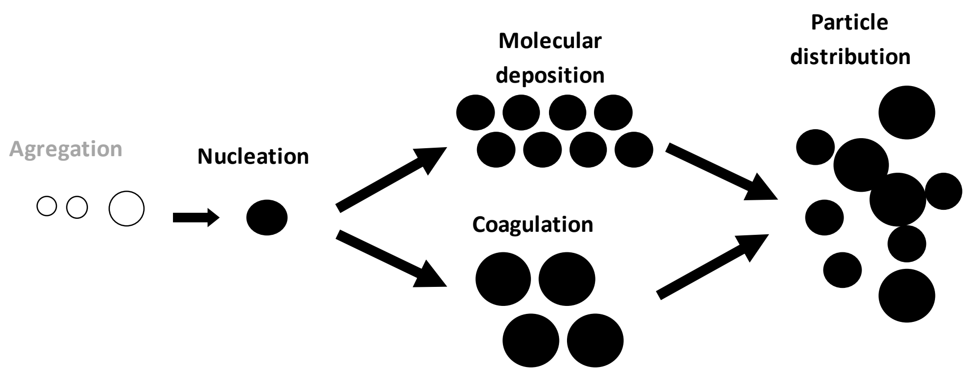


**Figure 1** : schematic of particle formation in gas phase plasma.

Once formed, the particles become charged, grow through molecular deposition and coagulation, and are transported within the discharge. The resulting particle size distribution (shown in Figure 1) strongly depends on local plasma conditions. The cloud of charged particles, in turn, influences the discharge equilibrium, plasma kinetics, molecular growth, and even the nucleation of new particle generations. This creates a strong coupling between particles and the discharge—commonly referred to as the *dusty plasma effect*.

In this presentation, we will highlight several plasma scenarios that lead to the formation of solid particles, whether intended or detrimental to process stability. We will discuss particle formation pathways under various plasma conditions and illustrate, through examples, the coupling effects between discharge dynamics, molecular growth, and the aerosol dynamics of growing dust.

# Wednesday 3rd June
# Morning

# From SERS (Surface Enhanced Raman Scattering) to PIERS (Photo Induced Enhanced Raman Scattering)

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Surface Enhanced Raman Scattering (SERS) has been known for about fifty years. The enhancement occurs when the molecules under study are in close proximity to a nanostructured metallic substrate, allowing SERS to increase Raman intensity by a factor of $10^6$ to $10^8$. The reasons for this enhancement are generally attributed to two effects : on the first hand an electromagnetic effect due to a stronger field near the nanostructures and on the other hand a chemical effect. The latter arises from charge transfer between the metallic nanostructures and the analyte.

In 2016, it was demonstrated that this amplification could be further increased if the metallic nanostructures were deposited on a semiconductor surface and exposed to UV radiation prior to detection. A few dozen articles have investigated this Photo Induced Enhanced Raman Scattering (PIERS) effect, but none have succeeded in making it last more than one hour. In this presentation, we will show that by co-depositing gold nanoparticles with a $TiO_2$ matrix, it is possible to extend this duration to at least 8 days. To better understand the specificity of our sample structuring, we conducted cathodoluminescence experiments. The results suggest that UV exposure reduces the width of the depletion zone of the Schottky barrier between gold and $TiO_2$, thereby enhancing the chemical effect.

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# Interaction of Individual Supported Nanoparticles with their Environment: Photoemission and Electron Loss Spectroscopy

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The electronic structure of deposited metal clusters and nanoparticles are highly sensitive to the optical properties and local geometry of the substrate, down to the atomic scale. Here we present spatially resolved electron spectroscopy of single silver particles deposited from the gas phase and excited close to their plasmon energy using photoemission electron microscopy (PEEM) and electron energy loss spectroscopy (EELS). The focus is on the role of the particles' local environment and of the substrate which includes supports such as Si(111)-(7x7) and amorphous carbon. We report on the formation of image dipoles, resulting in a breakdown of the quasistatic limit [1], as well as on the photoelectron momentum distribution which can be controlled via the laser polarisation. The role of the localized plasmon in the photoemission process is being discussed in view of resonant and non-resonant excitation [2].

Insight into the detailed geometry of involved plasmon modes is enabled by EELS conducted in a scanning transmission electron microscope (STEM). Silver particles are deposited from a beam on a narrow rim of a carbon support and investigated in a cross-sectional view. We observe pronounced symmetry breaking, and a partially lifted degeneracy of the dominant dipole modes. An intriguing finding is that the strongest substrate effect is found at locations farthest away from the particle, which we refer to as a *nonlocal substrate effect* [3].

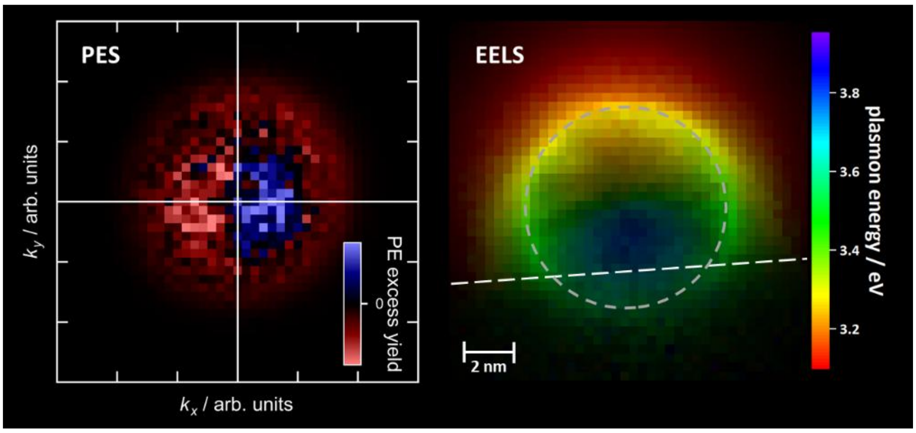


**Figure**: Single-particle electron spectroscopy: momentum distribution (left) measured by *k*-space PEEM, and plasmon energy distribution (right) obtained from STEM-EELS.

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# Synthesis of nanoparticles using a plasma-in-liquid process

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Plasmas in liquids for materials science is a rapidly growing field, characterized by the strong coupling between an electric discharge located above and/or within a liquid and the complex chemistry of the different species present in the system, including the solvent, dissolved compounds, and even nearby solids. Material synthesis and modification are most often governed by the liquid-phase chemistry and/or by the presence of high concentrations of solvated electrons, and many of these processes are being investigated with specific targeted applications such as nanoparticle synthesis [1] or surface functionalization [2].

Recently, the plasma-in-liquid process (PLI) has been used to synthesize different metal oxide nanoparticles [3, 4]. In a bottom-up approach, the plasma generated species are able to react with the metal ions present in the solution, leading to the oxide formation. This technique is considered as environmentally friendly since no additional chemicals are needed; most of the metal precursors are soluble in water which avoids using toxic solvents; and it has low heating requirements when carried out at ambient temperature.

We use the PLI process in order to produce silver- and iron- based oxide particles from aqueous solutions containing the dissolved corresponding salt. Pulsed plasma discharges are generated using platinum wires as the electrodes, which are immersed in the solution, and positioned in a pin-to-pin configuration. The effect of the electrode length, metal precursor concentration and applied voltage on the material production is studied.

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# Thermal stability of high entropy nanoalloys: myth or reality?

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High Entropy Alloys nanoparticles (HEA NPs) has attracted a huge interest since the last decade due to their exceptional properties in electrocatalysis, magnetic applications, and mechanical characteristics, such as corrosion resistance, which make them ideal for industrial uses, including integration into microelectromechanical systems (MEMS) [1]. In addition, the entropy-driven stability of high entropy alloy nanoparticles gives hope of developing more stable nanomaterials for high-temperature applications. Nevertheless, the enhanced thermal stability of nearly equiatomic nanoalloys containing at least 5 metals is nothing more than theoretical speculations about the impact of thermodynamic contributions on their structural properties and remains to be proven.
In this context, studying the thermal behavior of HEA NPs is a necessary first step to evalutate their structural stability as a function of increasing temperature. Moreover, our current state of knowledge on atomic diffusion in HEA is still far from complete and experimental evidence of the existence of the sluggish diffusion in HEA NPs is lacking.
In this presentation, we will present the results of a combined *in situ* aberration-corrected TEM study and atomistic simulations to reveal the thermal behavior of AuCoCuNiPt nanoparticles (NPs) at the atomic scale from 298 K to 973 K. Both experimental and theoretical results show the formation and melting of an AuCu layer at the surface of NPs at high temperature. This phase separation that appears progressively with temperature is driven by atomic diffusion that is surprisingly more active in these quinary nanoalloys than in binary subsystems. Furthermore, this study allows distinguishing kinetic and thermodynamic effects on their structural properties, which is an essential prerequisite to better control the synthesis of complex nanomaterials [2,3].
In the second part of the presentation, we will present how this high temperature behavior is modified under pure $H_2$ and $O_2$ atmosphere. We will explore the modifications of the NPs structure (mass transfer, oxygen-induced demixing of components, nanovoid nucleation, formation of oxides) of the NPs during an in-situ experiment under $H_2$ and $O_2$ environment at atmospheric pressure during a progressive heating at 973 K [4].

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# Characterization of physically synthesized Cu@$Cu_2O$ and of Cu NPs deposited on B/HOPG substrate

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In this paper physical synthesis and characterization of Cu nanoparticles (NPs) with oxide shells will be presented. $Cu_2O$ is promising as a photocathode material in photoelectrochemical cells for hydrogen production, owing to its visible-range band gap and suitable band-edge positions for water splitting. The incorporation of metallic Cu nanoparticles (NPs) can further enhance light absorption and extend the absorption range of $Cu_2O$ towards the red and near-infrared, due to the excitation of localized surface plasmon resonances (LSPRs) within the metal NPs. On the other hand, the possibility of coupling plasmonic NPs with 2D systems (like for instance Borophene) opens fascinating possibilities in fundamental physics and optoelectronic applications. Cu@$Cu_2O$ NPs were prepared by molecular beam epitaxy and thermal treatment in oxygen atmosphere, tuning the NP size, composition and oxide shells size. Microscopy and spectroscopy techniques were used to characterize morphology, structure and optical properties. Cu NPs were also prepared with gas phase synthesis assisted by a magnetron source and deposited on Boron films grown previously on HOPG. Atomic force microscopy reveals a complex islanded structure of the B/HOPG films which increases the diffusion of Cu NPs, revealing a possible lubricant action of the substrate.

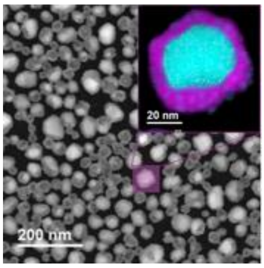


**Figure 1**: STEM image of Cu NPs annealed in an $O_2$/$N_2$ flux after annealing in UHV at 773 K for 60 min; Inset: EELS maps of a single NP, in which the $Cu^0$ concentration is reported in cyan and the $Cu^{1+}$ concentration is in magenta.

## Acknowledgments:

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# Increasing the atom-type number in multimetallic nanoalloys to induce a chemical disorder

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High-Entropy Alloys (HEAs), constitute an original class of materials, composed of five or more elements mixed with atomic concentrations ranging from 5 to 35 atomic percent. The concept of HEAs is that when increasing the number of elements in the alloy and combining them in this range of composition, the configurational entropy contribution becomes significant compared to the compound's formation enthalpy, the formation of chemically disordered solid solutions is favored, and the formation of undesired intermetallic phases is suppressed. At the nanoscale in metallic alloys, the high surface-to-volume ratio makes surface energy a major contribution to the total free energy, while finite-size effects significantly influence electronic and thermodynamic properties. In multimetallic nanoalloys[1], these nanoscale effects interplay with compositional complexity, leading to competing phenomena such as lattice strain, atomic segregation, and local compositional fluctuations driven by differences in atomic size, surface energy, and chemical affinity, and not by configurational entropy alone. A key challenge lies in disentangling the respective roles of thermodynamic and kinetic factors in systems where composition, size, and surface effects are strongly coupled. To achieve this goal, a combination of advanced characterization techniques is employed: grazing-incidence wide-angle and small X-ray scattering (GIWAXS-GISAXS) to probe structure and investigate morphology, and high-resolution electron microscopy (HRTEM/STEM) to image atomic arrangements and chemical ordering at a more local scale. These measurements are performed mainly in situ and in real time during the formation and thermal evolution of nanoalloys composed of 2 to 5 metallic elements (Pt, Cu, Ni, Rh, Pd) via atomic vapor deposition under ultra-high vacuum, carried out on amorphous substrates (a C /$SiO_2$ /Si).[2,3]

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# Wednesday, 3rd June
# Afternoon

# Gas-phase Synthesis of Multielement Nanoparticles. Towards the formation of Hybrid Systems for Improving Electrocatalysis

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In this talk we will present the gas phase synthesis of multi-element nanoparticles (NPs). In particular, the synthesis of 4 and 5 transition metals NPs using a Multiple Ion Cluster Source [1] connected to an ultra-high vacuum system. The morphological, structural and chemical characterization of the NPs presented differences between the 4-element and 5-element cases. In the 4-element NPs we observed a segregation of the elements creating core-shell NPs, while having 5 elements end up with a solid solution, revealing the formation of high entropy alloys (HEA) NPs. Molecular Dynamic simulations performed on both systems gave more insights on the nucleation process of such complex nanoparticles and magnetic measurements evidenced that nanoparticles smaller than 8 nm diameter presented room temperature ferromagnetism in the case of 4-element NPs.
The HEA NPs were further used to fabricate hybrid $Ti_3C_2T_x$ MXenes – HEA NPs systems. The high electrical conductivity and large specific surface area of MXenes make them excellent candidates for hybrid materials. Functional groups on their surfaces facilitate efficient integration with metal nanoparticles, serving as versatile platforms for engineering advanced nanomaterials [2]. In addition, HEA NPs combine their intrinsic properties of HEA with low dimensional effects, making them particularly interesting for applications like catalysis. This hybrid system was further deposited onto Ni foams, revealing a good electrocatalytic performance towards Oxygen Evolution Reaction.

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# Cluster beam deposition of bimetallic nanoalloys: From gas-phase growth to catalytic function

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Beam deposition of mass-selected bimetallic clusters produced in a laser ablation source provides a powerful platform to investigate cluster–surface interactions and to establish structure–activity relationships in well-defined catalytic systems. The combination of controlled gas-phase growth, soft landing, and detailed post-deposition characterization enables systematic studies of structural, chemical, and electronic properties of supported nanoalloys before, during, and after reaction.

Deposition of gas-phase produced $Au_xCu_{1-x}$ clusters (x = 1, 0.75, 0.5, 0.25 and 0) onto $TiO_2$ nanotubes was found to significantly enhances photoelectrochemical water splitting. Detailed structural and chemical analysis reveals segregation-driven formation of bifunctional catalytic sites composed of metallic Au/AuCu domains in contact with a copper oxide surface layer. These findings highlight how cluster composition and restructuring upon deposition determine interfacial properties and catalytic performance [1].

To bridge cluster-based model studies and realistic catalytic environments, a dedicated microreactor was developed to probe minute quantities of beam-deposited nanoparticles under elevated pressures (up to 40 bar) and temperatures (up to 250 °C). $PdZnO_x$ and $CuZnO_x$ clusters soft-landed on oxide and carbon supports were investigated for $CO_2$ hydrogenation via the reverse water–gas shift reaction [2] and methanol synthesis [3]. By tuning alloying and oxidation during cluster growth through the aggregation atmosphere, catalytic activity and selectivity can be systematically controlled.

These results demonstrate how cluster beam deposition links gas-phase nanoalloy formation with surface-supported functionality, providing insight into alloying, segregation, metal–support interactions, and their impact on catalytic performance.

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# Influence of the cooling rate on the microstructure and mechanical behaviour of non-equiatomic Zr-Hf-Ti-Cu-Ni-Co-Al High Entropy Alloys

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Two non-equiatomic high-entropy bulk metallic glasses (HEBMGs) with comparable compositions and significant glass forming ability (GFA) have been recently reported in the literature [1, 2]. Nonetheless, directly comparing their GFA presents a challenge because of the different processing techniques used in their manufacturing. Furthermore, there is insufficient information concerning the initial crystalline phase/s that develop during cooling and their influence on mechanical behavior. To shed light on this, two novel non-equiatomic compositions of the identical alloy system have been created at two distinct cooling rates (~1000 K/s and ~250 K/s, for 2 and 4 mm diameter samples, respectively): $Zr_{27.5}Hf_{11.1}Ti_{6.2}Cu_{32.4}Ni_{10.7}Co_{5.5}Al_{6.6}$ and $Zr_{29.7}Hf_{16.8}Ti_{5.2}Cu_{6.3}Ni_{12.1}Co_{8.4}Al_{21.5}$ at. %. For the $Zr_{27.5}Hf_{11.1}Ti_{6.2}Cu_{32.4}Ni_{10.7}Co_{5.5}Al_{6.6}$ alloy, the mechanical properties variation between the highest and lowest cooled regions, from the narrow amorphous ring edge (nanoindentation hardness H = 8.2 ± 0.42 GPa) to the centre of the largest sample (H = 8.8 ± 0.35 GPa), is very small.

This phenomenon can be ascribed to minor microstructural variations, primarily the development of a solid solution BCC crystalline phase, albeit with some presence of the HCP phase. The amorphous phase exists in a highly relaxed condition, about to crystallize. However, for the $Zr_{29.7}Hf_{16.8}Ti_{5.2}Cu_{6.3}Ni_{12.1}Co_{8.4}Al_{21.5}$ alloy, more significant microstructural variations, and consequently mechanical properties, are observed between the regions that have cooled the most and those that have cooled the least. From a fully amorphous region far from equilibrium (H = 8.5 ± 0.44 GPa) to a solid solution of BCC (~80 % vol.) and HCP (~20 % vol.) crystalline phase (H = 10.8 ± 0.6 GPa) and free from brittle intermetallic phases. This indicates that the latter alloy represents a composition closer to the eutectic point, making its microstructure more susceptible to variations in the cooling rate. This is an important factor to consider when designing microstructures for engineering applications.

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# Enhancing Synergistic Interactions between PtGe Nanoalloys and 2D Materials for PEMFC Applications

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In this work[1], we have systematically investigated the stability, CO poisoning resistance, and catalytic performance toward the hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR) of small monometallic Pt and bimetallic PtGe nanoclusters supported on various 2D materials. Using global minimum searches and mechanistic studies at the density functional theory (DFT) level, including an implicit solvent model, we performed a comprehensive screening of cluster size, composition, and support to identify optimal catalyst formulations.

Alloying and support effects operate synergistically. The support enhances cluster stability and alters its electronic structure through metal–support interactions, while the cluster, in turn, modifies the electronic properties and catalytic behavior of the support depending on its size and composition. Notably, 2D supports reduce the CO poisoning tendency of pure Pt clusters, an effect that is further strengthened by Ge alloying. In some cases, such as $Pt_5Ge_5$ supported on germanene, CO adsorption even becomes thermodynamically unfavorable, effectively suppressing catalyst poisoning.

Concerning catalytic activity, all systems exhibit excessively high overpotentials for the ORR under acidic conditions, mainly due to overly oxophilic active sites that overbind oxygenated intermediates. In contrast, the combined effect of Ge alloying and 2D supports leads to significant improvements in HOR performance. Overall, the simultaneous tuning of cluster composition and support emerges as an effective strategy for rationally optimizing catalytic properties.

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# Surface−Driven Growth and Structural Evolution in Au−Cu Nanoalloys: Atomistic Insights

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The properties of metallic nanoparticles strongly depend on their structure and chemical distribution. In bimetallic nanoalloys, morphology and elemental ordering are intimately coupled, and even small changes in growth conditions can significantly affect surface composition, strain and stability. Atomistic simulations provide a powerful tool to identify the fundamental driving forces controlling nanoparticle growth and structural evolution under kinetically controlled conditions.

Here we explore surface−driven growth and restructuring phenomena in pure Au and AuCu nanosystems through molecular dynamics simulations. In the first example, we analyze the growth of pure Au nanoparticles, highlighting how surface diffusion and kinetic effects influence morphological selection during cluster formation [1]. The simulations reveal the atomic−scale mechanisms that steer the system toward specific structural motifs as growth proceeds.

In the second example, we focus on bimetallic growth pathways in AuCu systems. We investigate Cu shell deposition on Au and AuCu seeds, demonstrating how lattice mismatch strain and surface energetics compete with interdiffusion processes, leading to morphology−dependent segregation and partial alloying [2]. We also examine the reverse process – Au deposition on Cu and AuCu seeds – revealing distinct growth pathways and structural outcomes arising from the asymmetry in elemental surface energetics and atomic mobility [3].

Together, these studies provide a unified atomistic picture in which surface energy, strain relaxation and chemical ordering tendencies act as competing driving forces that dictate nanoalloy structure and stability at the nanoscale.

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# Chemical structure and environment effects in nanoalloys: from alloy miscibility to UV plasmonics

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Combining metals at the nanoscale provides a powerful way to tune the physicochemical properties of nanoparticles. In nanoalloys, these properties are governed not only by size and composition, but also by chemical structure and interaction with the surrounding environment. Variations in elemental distribution, chemical order, and surface reactivity can therefore strongly modify optical and electronic properties, particularly in the sub-10 nm size range where surface effects dominate [1]. In this talk, I will present two complementary studies addressing how chemical structure and environmental interactions control the properties of surfactant-free nanoalloys. In the first part, we investigate Au–Ag nanoalloys in the 4–10 nm size range, with the specific goal of disentangling intrinsic alloy thermodynamics from extrinsic effects such as oxidation, surface reactivity, and environmental interactions. We show that the intrinsic chemical ground state consists of a miscible alloyed core with a gradual Ag-enriched shell, while other chemical ordering reported in previous studies is strongly influenced by extrinsic effects and metastability, rather than by intrinsic alloy property at its fundamental state [2]. In the second part, we address $In_2Au$ system for deep-UV plasmonics at the few-nanometer scale. We show that uncontrolled surface oxidation suppresses the plasmonic response, while embedding the nanoparticles in oxide matrices enables stabilization of a chemically ordered phase with a robust localized surface plasmon resonance near 280 nm. Ensemble UV–Vis spectroscopy and single-particle low-loss STEM-EELS are employed to probe the plasmonic behavior of these systems. Related work on alumina-embedded silver clusters shows that stable surface plasmon resonances can be achieved in oxide matrices for small metal nanoparticles [3], further highlighting the importance of cluster–surface interactions in preserving plasmonic behavior in sub-10 nm systems. Together, these results show how controlling nanoalloy interactions with surrounding surfaces and matrices can unlock physical regimes that are otherwise inaccessible.

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# Thursday, 4th June
# Morning

# Transition-metal nanoalloys in hydrogenation and dehydrogenation reactions

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Catalyzed hydrogenation and dehydrogenation reactions play an essential role in the chemical industry, for the synthesis of chemicals, agrochemicals, or the development of green energy solutions. These reactions are fundamental for obtaining ethylene, the organic compound with the largest annual production. To produce ethylene through the non-oxidative dehydrogenation of ethane, Pt-based catalyst suffers from a low selectivity and deactivates due to coking. Here we will demonstrate how nanoalloying Pt with Ge can be an effective strategy to optimize the catalytic performance and the lifetime of surface-mounted Pt nanoclusters [1]. The effect of Ge content in supported PtGe cluster alloys on the activity toward ethane dehydrogenation, selectivity against deeper dehydrogenation and coking, and sintering resistance will be deciphered. Subsequently, ethylene purification can be achieved through the semi-hydrogenation of acetylene using Pd. Inspired by previous experimental findings [2], in this talk we will also present our theoretical results on the PdTi bimetallic catalyst by combining two different approaches [3]: PdTi subnanoclusters of different sizes and compositions deposited on $\gamma$-$Al_2O_3$ (100), and a series of larger nanoparticles with different core/shell motifs and PdTi mixing patterns. Monometallic Pd and Ti are too reactive for the semi-hydrogenation of acetylene. However, at low proportions of Ti, Ti helps to anchor the clusters to the surface, producing sintering resistant catalysts, and modifying the electronic structure of Pd to create a more selective catalyst.

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# Structural motifs and stability of CuNiPdPtRh High-Entropy Nano-Alloys

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High Entropy Nano-Alloys (HENA) represent a new class of nanostructured materials composed of multiple elements in near-equiatomic proportions, where the high configurational entropy stabilizes unique solid phases and complex microstructures [1]. This multi-element configuration provides interesting mechanical, thermal, and catalytic properties compared to conventional alloys [2]. The structural, chemical, and thermodynamic properties of equiatomic CuNiPdPtRh HENA were investigated. Global optimization methods were employed to determine the most stable nanoparticle geometries across different sizes and structural motifs. The behavior of the HENAs was systematically analyzed as a function of nanoparticle size and geometry, revealing clear correlations between structure, chemical ordering, and stability. Thermodynamic properties were further investigated through Molecular Dynamics and Monte Carlo simulations, enabling the identification of possible phase transitions.

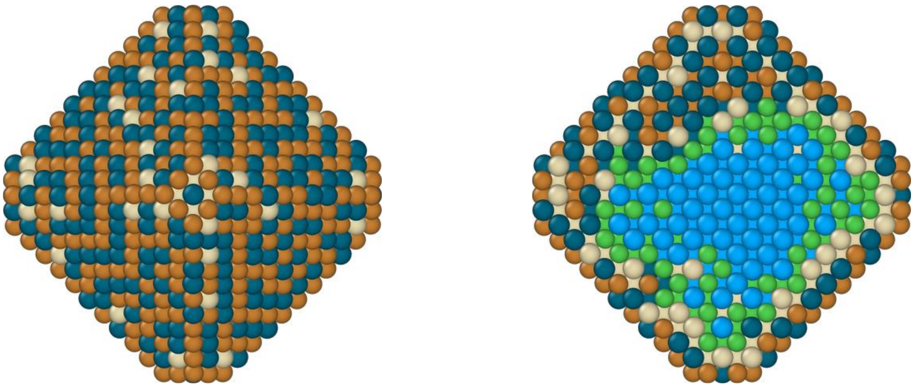

**Figure 1:** Optimal chemical ordering of equicomposed CuNiPdPtRh truncated octahedron with 2225 atoms.

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# Analysis of the IR-MPD spectroscopy of mixed metal clusters: in search of a unifying model

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This presentation will document our recent work which seeks to provide an over-arching framework to understand the IR-MPD spectra of mixed metal clusters. Specifically, I will discuss a range of silicon-based clusters containing one or more group elements (Mn, Re), and show how the interplay of metal-metal and metal-silicon bonding leads to the complex spectroscopic signatures. The relatively high symmetry of many of these clusters allows group theory to be used with some success to assign the various bands. I will also discuss more recent work on mixed Al/Nb clusters, where the degeneracy or near degeneracy of levels in the Nb 4d band leads to complex structural distortions (1st and 2nd-order Jahn-Teller distortions), the signatures of which can be identified in the vibrational spectra.

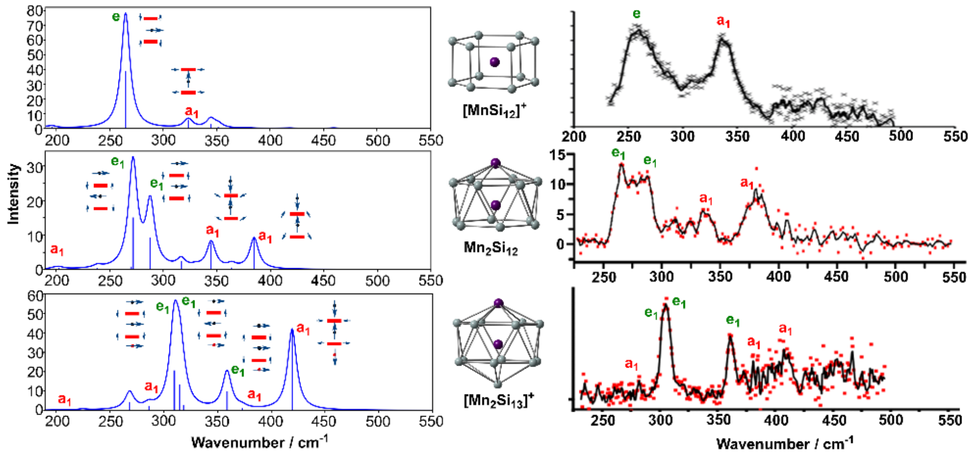


**Figure 1**: *IR-MPD spectra of Mn and $Mn_2$-containing silicon clusters.*

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[1] Evolution of Vibrational Spectra in the Manganese–Silicon Clusters $Mn_2Si_n$, *n* = 10, 12, and 13, and Cationic $[Mn_2Si_{13}]^+$. V. Khanna, R. Singh, P. Claes, M.-T. Nguyen, A. Fielicke, E. Janssens, P. Lievens, J.E. McGrady, *J. Phys. Chem. A*, **2022**, *12*, 11.

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# Alloy NanoStructures for the Oxygen Reduction Reaction

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The widespread adoption of proton-exchange membrane fuel cell (PEMFC) devices for electrochemical energy conversion is currently limited by the lack of appropriate catalysts. Highly active and durable (under acidic condition) platinum-based catalysts would in fact be indispensable to accelerate the sluggish oxygen reduction reaction (ORR), but their development face serious issues [1,2]. In the present talk, I will present recent results of experimental/theoretical studies to single out the factors affecting activity and stability of Pt-based systems under ORR conditions [3], and to propose novel systems exhibiting state-of-the-art catalytic activity and robustness [4]. Descriptor quantities, describing strain and stoichiometry phenomena, defined on experimental and theoretical observables, and correlating with oxygen binding energy and the experimentally determined ORR activity, will be used to discuss and rationalize the results of extensive ML-accelerated Global Optimization stochastic first-principles searches. The proposed systems surpass DoE 2025 target in terms of catalytic activity and durability, and set the stage for future further developments [4].

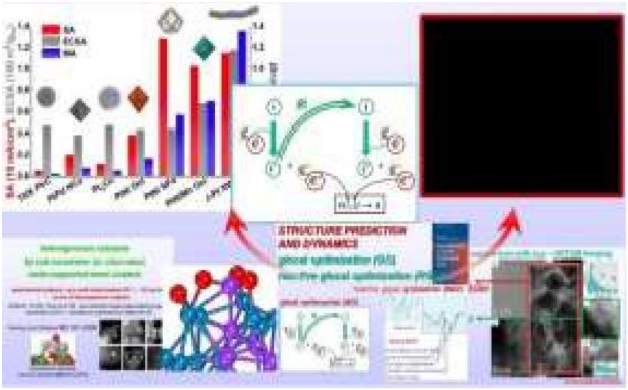

Figure 1. Theoretical Approaches to Pt-based ORR Catalysts.

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# Surface plasmons in unconventional nanoalloys

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The conventional plasmonic materials most widely used in applications as nanoalloys are the coinage metals gold and silver. However, their plasmon energies lie in the visible and the near-UV ranges. Their replacement with materials that are on the one hand cheaper and that on the other hand promise surface-plasmon resonances in the far UV is the matter of intense studies. In particular, alloying of gold and silver with aluminum and indium have been shown to be promising [1].

In the present work, we show that alloying of silver with indium produces indeed the expected blue-shifts of the SPR energies. Our results using real-time time-dependent density-functional theory are validated by comparison with other approaches. We discuss the physics that causes the shifts, in particular the role of the In d electrons compared with those in Ag. Finally, we demonstrate the differences in the behavior of alloys containing Au instead of Ag.

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# Support-induced strain engineering of the chemical order of anchored nanoalloys

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Alloy NPs can be described in terms of their physical ordering (size, shape, crystallinity, etc.) and their chemical ordering; namely, the pattern in which the different elements are arranged. There are three main parameters that determine whether a stable structure of an alloy NP falls into a mixing or a non-mixing class [1]: (i) the enthalpy of mixing; (ii) surface energy differences between various elements; and (iii) strain energy considerations. If all parameters work together, identifying chemical order is straightforward. However, they often compete with each other, making the prediction of the final arrangement of atoms challenging; it is difficult to anticipate which parameter is dominant for every individual nanoalloy, especially since their influence changes with NP size.

Of all three parameters, strain energy is the only one that can be manipulated. Therefore, the key scientific question of this work is: can we strain-engineer the chemical order of alloy NPs for specific applications?

To this day, the equilibrium structures of multi-elemental NPs have been investigated thoroughly, but always with the implicit assumption that the particles are in vacuum [1]. For clusters in vacuum the strain energy parameter is usually less important than the other two; however, for NPs strongly bound on supports it can become dominant. Indeed, gas-phase deposited clusters can bind strongly on supports, thus introducing strain to their own lattice

[2]; a portion of them (all, if small enough) can become epitaxially aligned with the support even if their lattice-constant mismatch is significant. So far, this has been demonstrated only for monometallic NPs.

This work combines these two considerations, i.e., investigate supported alloy NPs, revealing design opportunities which, to this day, have been hiding in plain sight. We propose a strain-engineering method to control atomic arrangement by anchoring bimetallic clusters to flexible supports and use atomistic computer simulations to provide initial proof-of-concept validation of our proposal.

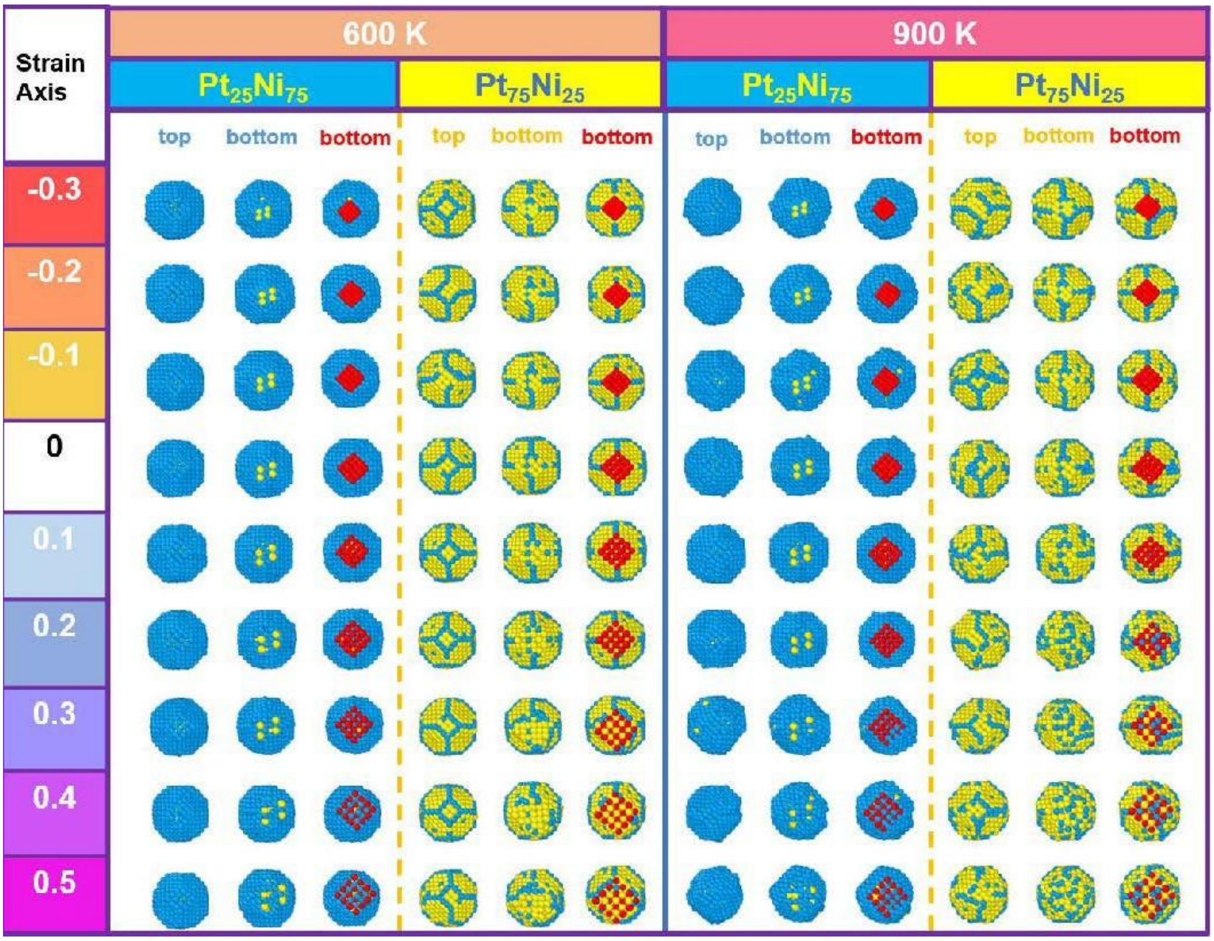


**Figure 1**: collection of snapshots for equilibrated 586-atom NiPt nanoalloys under a complete straining routine (including the equilibrium structures prior to straining). For each group of NiPt nanoalloys with a specified temperature and composition, three columns of snapshots are presented along the strain axis: the leftmost column shows a top viewpoint, the middle corresponds to a bottom viewpoint; the third column shows the same bottom viewpoint but with marking fixed atoms (at the bottom layer) in red, to highlight the leaching atoms.

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# Posters

# Pt aggregation on Graphene/Ir(111): Role of defects and moiré sites for planar nanocluster formation

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The growth of metal clusters on two-dimensional materials is governed by a subtle interplay between surface diffusion, local environment, and aggregation kinetics. In a previous combined experimental–theoretical study, we demonstrated that Pt atoms deposited on epitaxial graphene supported on Ir(111) exhibit an ultra-low diffusion barrier, leading to highly mobile monomers and the formation of flat nanoclusters at very low temperatures [1]. In the present work, we extend this investigation through detailed theoretical modeling to disentangle the atomistic mechanisms governing Pt aggregation on the graphene/Ir(111) moiré surface. Knowing that Pt aggregation is a stochastic process occurring at distinct regions of the moiré unit cell, with local symmetry playing a decisive role in cluster morphology, we explored the possible role of defects in graphene surface and the kinetics of Pt monomers aggregation. Our calculations reveal that Pt monomers arriving at defect sites are strongly anchored, serving as nucleation centers for subsequent growth. Additional monomer attachment leads predominantly to planar clusters, whose calculated core-level shifts fall within the range reported in our previous experimental study.

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# Facet-Dependent Adhesion of Au Clusters on Fe Substrate

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The interaction between gold and iron at the nanoscale is of significant interest for the development of multifunctional bimetallic nanoparticles. The FCC Au unit cell, after a 45° rotation, aligns almost perfectly with the face diagonal of the BCC Fe unit cell. This nearperfect lattice match, together with the fact that iron is more cohesive than gold, promotes the formation of core-shell structures. Such architectures are particularly relevant for nanomedicine, as they combine the magnetic properties of the iron core with the biocompatibility of the gold shell. The thermodynamic stability and equilibrium morphology of these systems are governed by adhesion energies and lattice matching. In this context, we present a computational study of gold adhesion on both (100) and (110) iron surfaces and growth dynamics on iron clusters. We first compute adhesion energies of two-dimensional Au islands on BCC Fe(100) and Fe(110) surfaces (Figure 1) using Density Functional Theory (DFT). These *ab initio* results serve as reference for evaluating different parametrizations of the Gupta potential. We identify a parametrization that best matches the DFT interface energies, reproducing the markedly stronger Au adhesion on Fe(100) compared with Fe(110). Using this potential, we perform molecular dynamics (MD) simulations of Au deposition on cubic and rhomboidal Fe clusters to investigate growth mechanisms on (100) and (110) facets, respectively. These simulations reveal how facet-dependent adhesion energetics dictate the wetting behavior and the resulting equilibrium morphology of Au–Fe nanoalloys.

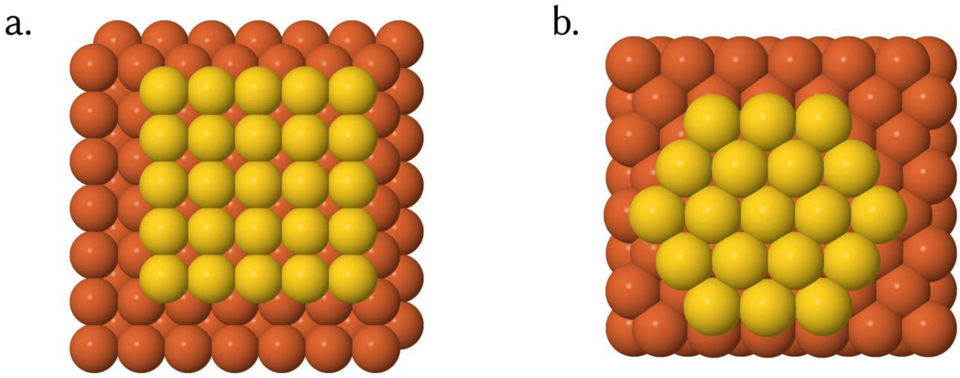


**Figure 1**: Relaxed atomic configurations of 2D Au islands on (a) Fe(100) and (b) Fe(110)

# Multiphoton Orders and Polarisation Dependence of Individual Silver Nanoparticles

Waqas Pervez[1,2], Moha Naeimi[1,2], Frithjof Harmsen[1,2], Kevin Oldenburg[2], Sylvia Speller[1,2], and Ingo Barke[1,2]

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Resonant laser excitation of nanoparticles at frequencies matching the localised plasmon energy can gives rise to a vastly enhanced photoemission yield. Here we study size-selected silver particles produced in a magnetron sputtering cluster source and deposited *in-situ* onto silicon substrates. By carefully tuning the parameters of the cluster source, we produce single particles ("monomers") as well as agglomerates ("dimer", "trimers", etc), as revealed by transmission electron microscopy (TEM). Using wavelength-dependent photoemission electron microscopy (PEEM), most particles show plasmon resonances near 400 nm, enabling single-particle plasmon mapping [1]. When excited near 800 nm, we observe multiphoton orders ranging from 3 to 7, depending on particle shape, laser intensity, and final-state energy of the emitted photoelectrons. On silicon with a native oxide layer, we achieved selective $k$-space maps of a single nanoparticle whose emission characteristics could be controlled by the polarisation. Larger agglomerates show a complex polarization dependence of the total electron yield, with distinct spectra for certain polarisation directions. We discuss the plasmon participation in the photoemission process in view of contributing plasmon modes [2], multiphoton excitation of plasmon resonances [3], and observed photon orders.

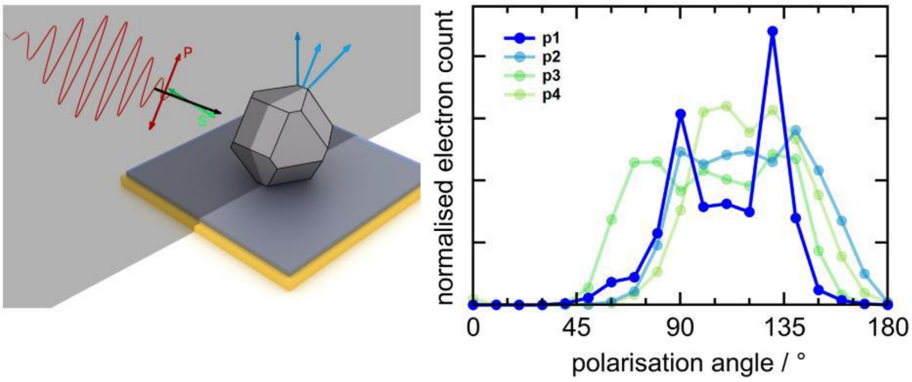


**Figure**: left: geometry of the PEEM experiment (courtesy of M. Bednov and D. Bauer, University of Rostock). Right: polarisation-dependent photoelectron yield of a few different Ag nanoparticles.

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# Modelling the Asymmetric Growth of Janus Metallic Nanoparticles via DFT and Kinetic Monte Carlo Simulations

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Janus bimetallic nanoparticles, characterized by asymmetric chemical ordering, are promising nanomaterials for applications in heterogeneous catalysis, active nanomotors, and multifunctional devices. Their potential arises from the coexistence of chemically distinct surface regions, enabling spatially separated reactions or directional activity. However, achieving controlled and robust chemical asymmetry during synthesis remains challenging. The aim of this work is to identify bimetallic combinations and atomic-scale surface processes that favor asymmetric growth *via* Density Functional Theory (DFT) and Kinetic Monte Carlo (KMC) simulations.

The strategy for developing this project is based on recent experimental results [1,2]. Here, deeply truncated octahedral Pt nanoparticles (nanopyramids) are synthesized, exposing a large (100) facet opposite to several (111) facets. From here, we deposit atoms of different species (Ag, Au, Pd, Rh), on the hypothesis that the asymmetry of the seed promotes preferential accumulation of the deposited species on the (100) facet, which is typically preferred due to the larger coordination number.

Several competing processes may counteract this mechanism and must be quantitatively evaluated. Under isotropic deposition conditions, effective accumulation on a single facet requires sufficiently fast surface diffusion. Deposited atoms must remain at the surface without exchanging with seed atoms, which would lead to alloying rather than segregation. Furthermore, once a bimetallic region forms, continued growth must be energetically preferred on that region over adsorption on the remaining uncovered facets.

To address this, the surface physical effects are studied with DFT calculations, including determination of adsorption energies, diffusion barriers, and exchange energetics on different facets and edges, for multiple metal pairs. A model, based on the DFT results, is developed and simulated, adapting KMC algorithm to the non-trivial surface of the seed [3].

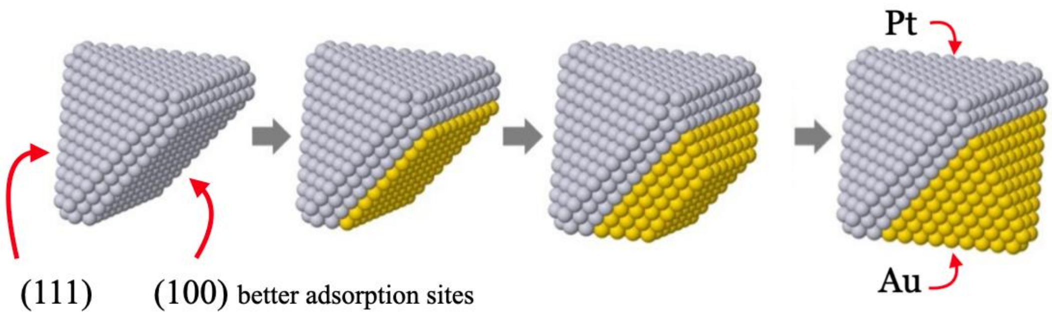


**Figure 1**: The desired growth of a Janus nanoparticle, an example with Pt, Au

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# Exciton Distribution and Dynamics in Rubrene Nano- and Microstructures in the Presence of Silver Nanoparticles

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Controlled exciton transport in organic semiconductors is key to improve the performance of light-harvesting and optoelectronic devices. Rubrene is a particularly promising material as it offers one of the largest hole mobilities and can be prepared with high quality due to recent advances based on high partial-pressure techniques [1-3]. Here we present quasi-one-dimensional rubrene wires on silicon to support highly anisotropic exciton migration along the wire axis, driven by photo-induced mobile carriers. A combination of Kelvin probe force microscopy (KPFM), fluorescence lifetime mapping (FLIM), and photoemission electron microscopy (PEEM) is used to characterize and track the excitonic properties. Silver nanoparticles deposited from the gas phase result in a time-dependent photoemission intensity, producing stochastic photoelectron bursts. The underlying mechanisms are being addressed by time-of-flight PEEM, enabling electron spectroscopy as a function of space and time.

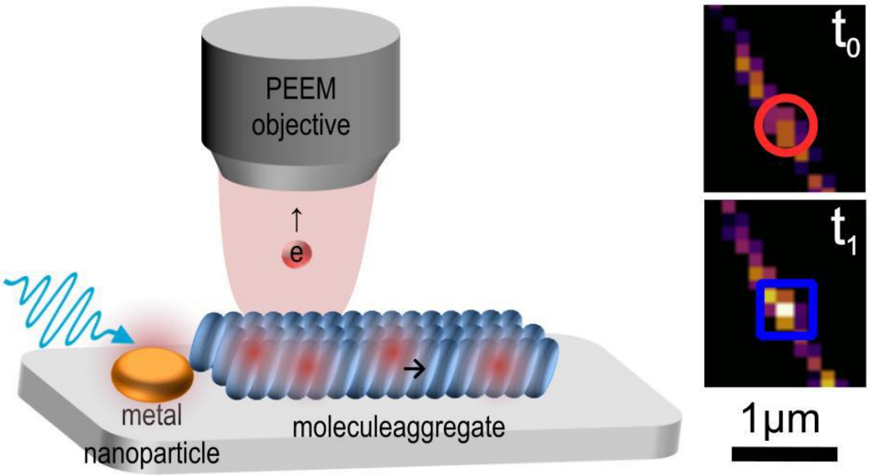


**Figure:** Scheme of the PEEM experiment aiming to trace excitons within molecule aggregates under local coupling to metal nanoparticles. Top right: Photoelectron yield along a quasi 1D rubrene strand in the vicinity of a silver nanoparticle (marking) at two different points in time.

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# Tuning Hydroxyl Defects to Control Sintering Resistance of Silica-Supported Platinum Clusters

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A persistent hindrance to using supported noble metal atoms and sub-nanometer clusters in real-life catalytic applications is their susceptibility to sintering. Because these processes are challenging to understand experimentally, many studies aim to provide an atomistic picture via modelling.[1] Recently, cluster dynamics simulations have advanced beyond the limits of classical force fields and short-scale ab initio methods, due to the emergence of machine learning interatomic potentials (MLIP).

Recently, we studied interactions of Pt atoms and clusters with a silica(tene) surface with an in-house trained MLIP.[2] We observe non-Ostwald ripening sintering coalescence pathways, driven by particular, size-specific cluster-surface interactions. Moreover, in the presence of hydroxyl defects, Pt species interact reactively with surface hydroxyls, leading to electrostatic pinning which suppresses sintering even at high temperatures relevant to catalytic experiments. The observed stabilisation mechanism of hydroxyls was then tested on different industry-relevant siliceous surfaces. Using a fine-tuned MACE foundation model,[3] we observe that while clusters bind strongly to a fully hydroxylated layer of quartz, the dynamic stability is no longer maintained, as new diffusive mechanisms emerge. On the other hand, on IPC–1P zeolitic monolayer with medium hydroxyl density, the sintering resistance can be achieved by selecting the clusters of specific sizes. Our simulations provide an atomistic, mechanistic underpinning of cluster-surface interactions that illustrate the importance of considering the dynamic behaviour of supported metal clusters at the smallest scales.

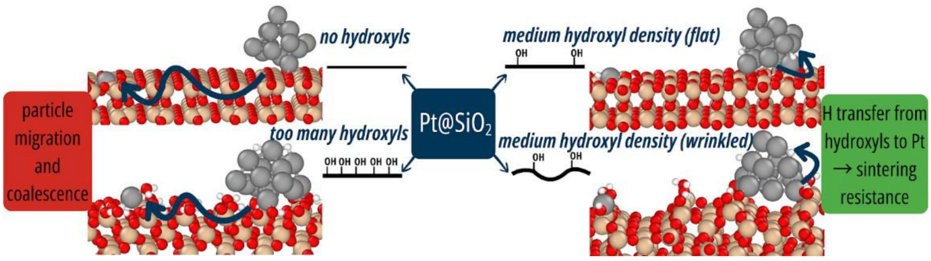


**Figure 1:** Reactive interactions between surface hydroxyl groups and Pt atoms and clusters enhance the sintering resistance by the H transfer mechanism.

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# A computational framework for quantitative predictions of protein-nanomaterial interactions

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Understanding the formation of protein corona on nanomaterials is critical for predicting their biological identity and behavior in physiological environments [1]. In this study, we employ coarse-grained molecular dynamics simulations using the Martini3 force field [2] to investigate the adsorption of human serum albumin (HSA) – taken here as a representative case study of serum proteins – onto graphene [3], a widely studied nanomaterial with biomedical applications. Clustering algorithms were applied to simulation trajectories to identify distinct HSA adsorption modes. To characterize the geometry of the adsorption events, we introduce a novel polyhedral approximation in which each protein face is defined by the intersections of planes defined by HSA beads in contact with the graphene surface, enabling estimation of geometric adsorption probabilities from the corresponding polyhedral contact face areas. For selected modes, we carried out free energy calculations to estimate their binding free energy, and then identified a transferable, computationally efficient proxy to easily predict adsorption energies for any other serum protein. The combination of data from the geometric and free energy analyses allows for the development of a probabilistic framework that integrates both thermodynamic and structural criteria to describe adsorption mode preferences. Such a model provides a physically grounded basis for predicting protein–nanomaterial interactions and can be extended to explore more complex corona formation scenarios involving multiple proteins and heterogeneous surfaces. Our results advance the understanding of protein adsorption mechanisms at the nanoscale and offer new tools for modeling protein corona formation on nanoparticles with implications in nanomedicine.

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# Energy Differences between Competing Structural Isomers of Deposited Pt and Au Nanoclusters from Variable-Temperature Aberration-Corrected STEM Imaging

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The potential energy surface (PES) of a nanoscale system describes the energy in terms of the atomic arrangements, where minima correspond to locally stable atomic structures. It regulates the dynamical behaviour of the system. For Au and Pt clusters, both important nanocatalysts, one typically finds several competing structural isomers. An understanding of the PES, and thus how temperature affects the emergence of different active sites, is key to the production of more selective nanoparticle catalysts.

A method pioneered by the group provides a rare experimental and quantitative insight into the PES [1]. The method employs atomic-resolution aberration-corrected STEM imaging of nanoclusters as a function of temperature [2]; comparison to a simulation atlas identifies the cluster structural motif (Fig.1). Competing isomers are treated as states of a Boltzmann distribution (1), from which the energy difference between the states can be found.

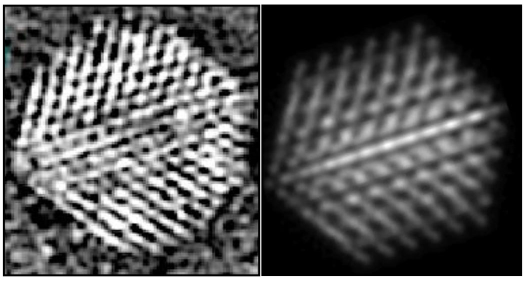

**Fig. 1 :** HAADF-STEM image of a 413±5% atom Au nanocluster taken at 200°C (Left) and the corresponding simulated Au561 image used to identify its structure as decahedral (dh) rotated to an angle of α=50°, β=0°. (right)

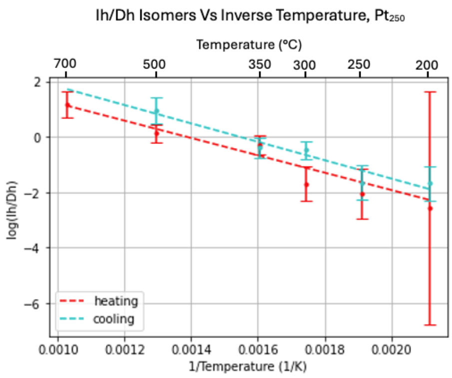


**Fig. 2** : Boltzmann plot of the icosahedral and decahedral isomers of Pt250 imaged between 150 and 700°C. Using the Boltzmann formula, Average ΔE = 280±79 meV and average ΔS = 0.41±0.13.

The original work of 2018 [1] imaged arrays of size-selected clusters that were heated up from room temperature by a precision thermal chip. Since then, we have demonstrated that video imaging of a single clusters captures the same competition (indeed fluctuations) between isomers – and means that mass-selection of the array is not needed. Here we combine the video method with precise heating, and also cooling, to extract energies. Over 30 sizes of Au and Pt nanoclusters between 100 and 600 atoms were video imaged from 150°C and 700°C and back to 150°C. General agreement between heating and cooling data is obtained, confirming the equilibrium state of the system assumed by the method. ΔE and ΔS values are calculated in each case – we hope this will prove a valuable body of reference data, eg, for theoretical simulations. In future such measurements may be feasible with gas exposure.

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# Machine Learning Force Fields for C3 Upgrading: Oxidation on $Cu_xAg_y$ Clusters Supported on Alumina

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Metal–oxide clusters are pivotal in selective hydrocarbon oxidation, where both metal composition and surface hydroxyl coverage may dictate stability,[1] activity and product selectivity. Here, we develop a machine-learning interatomic potential [2] for Cu, Ag, and mixed CuAg oxide clusters supported on hydroxylated alumina, enabling rapid, near-DFT exploration of propane ($C_3H_8$)-to-propylene ($C_3H_6$) and propylene-to-propylene oxide ($C_3H_6O$) conversion pathways [3]. A reference dataset of DFT energies, activation barriers, and forces for all relevant intermediates was used to train a message-passing neural network within the MACE framework. The resulting model accurately reproduces DFT-level energetics while permitting extended molecular dynamics simulations, capturing cluster structural rearrangements, molecular diffusion, and dynamic interactions with reactants. Using this approach, we systematically investigate the influence of surface-hydroxyl coverage on reactivity and selectivity, providing a predictive and scalable platform for designing oxide-supported metal catalysts for C3 hydrocarbon upgrading.

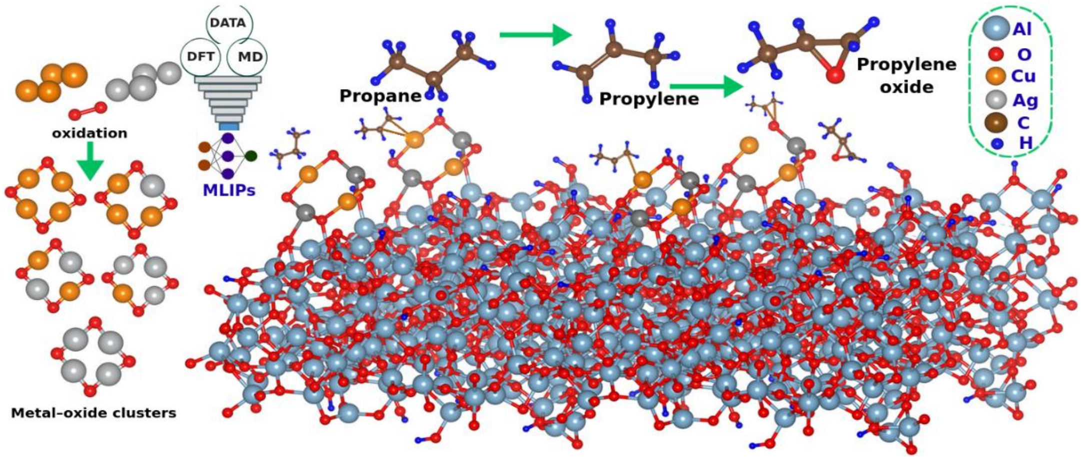


**Figure 1**: Modeling Propane-to-Propylene and Propylene-to-Propylene Oxide catalytic conversion on $Cu_xAg_y$ clusters using MLIPs.

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# Structure and Reactivity of Cobalt–Vanadium Alloy Nanoclusters on Organic Molecular Substrates

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Nanoclusters (NCs), consisting of a few to several dozen atoms, exhibit size-dependent physical and chemical properties when their atomicity is precisely controlled. Therefore, the creation of functional nanomaterials using NCs as building units has attracted considerable attention. In alloy NCs, core–shell structures are key structural motifs that can give rise to unique chemical reactivity, as exemplified by $X@Al_{12}$ [1] and $M@Si_{16}$ [2] ("@" denotes encapsulation within a cage). Among them, cobalt–vanadium alloy NCs ($Co_nV_m$) are predicted to form minimal core–shell, represented by $V@Co_{12}$, composed of early and late transition metal elements [3,4]. For practical applications such as heterogeneous catalysis, it is essential to establish surface-supported methods that suppress aggregation while controlling the charge state of NCs.

In this study, size-selected cationic and anionic $Co_{12}V$ and $Co_{13}$ NCs were soft-landed (0.6 ML) onto organic molecular substrates. The substrates consisted of *n*-type fullerene ($C_{60}$) and *p*-type hexa-*tert*-butyl-hexa-*peri*-hexabenzocoronene (HB-HBC), both of which were deposited on graphite [5,6]. Ultraviolet photoelectron spectroscopy (UPS, He I$\alpha$: 21.22 eV) and X-ray photoelectron spectroscopy (XPS, Mg K$\alpha$: 1253.6 eV) measurements were conducted under ultra-high vacuum ($10^{-8}$ Pa) to investigate the charge states and chemical states of the supported NCs. The chemical reactivity toward oxygen molecules ($O_2$) was also evaluated by stepwise $O_2$ exposure in Langmuir units at room temperature, followed by XPS analysis.

UPS measurements reveal substrate-dependent charge transfer between $Co_{12}V/Co_{13}$ NCs and the organic molecular layers. On $C_{60}$, $Co_{12}V$ becomes positively charged while the substrate is negatively charged, whereas on HB-HBC the opposite charge transfer is observed. A similar behavior is confirmed for $Co_{13}$, demonstrating that the charge state of supported NCs can be tuned via substrate selection. On $C_{60}$, XPS measurements show that $Co_{12}V$ exhibits higher oxidation resistance than $Co_{13}$, with an approximately one-fifth lower reactivity, indicating the preservation of a stable icosahedral core–shell structure ($V@Co_{12}$). In contrast, on HB-HBC, $Co_{12}V$ exhibits initial oxidation of the V atom followed by Co oxidation, suggesting a surface-exposed exterior V atom in the negatively charged state. These results highlight the importance of controlling the charge-state of NCs through cluster-substrate interactions, which optimize their geometric structure and chemical reactivity.

## References:

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# Deterministic control of cobalt nanoparticle growth via non-equilibrium cooling in MS-IGC

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Controlling the structure and size of metallic nanoparticles synthesized by gas-phase methods remains a major challenge due to the inherently non-equilibrium nature of the growth process. In magnetron sputtering inert gas condensation (MS-IGC), nanoparticle formation is governed by the interplay of sputtered atom injection, gas-phase cooling, and residence time, yet the dominant atomistic growth mechanisms remain poorly resolved.

Here, we develop a reactor-resolved molecular dynamics framework to investigate cobalt nanoparticle growth under realistic MS-IGC conditions. The model explicitly incorporates directional sputter injection, spatially varying thermal environments, and collision-driven energy dissipation. By selectively thermostating the inert gas while allowing cobalt species to evolve freely, we demonstrate that hot cobalt atoms undergo rapid cooling through collisions with argon without inducing artificial clustering in the gas phase, confirming that argon acts as a physically consistent thermal bath.

Our results reveal that nanoparticle growth proceeds through non-equilibrium pathways, where nucleation, aggregation, and coalescence occur sequentially as cobalt atoms traverse plasma, buffer, and aggregation zones, with aggregation-driven cluster–cluster coalescence governing late-stage growth. The cooling rate, controlled by gas density and temperature gradients, governs the transition between nucleation- and aggregation-dominated growth regimes and strongly influences cluster formation kinetics and final size distributions. In particular, we show that this coalescence-driven growth dominates over monomer attachment under typical MS-IGC conditions.

These findings establish a direct mechanistic link between experimental control parameters, including sputtering power, gas pressure, and reactor geometry, and nanoparticle morphology. More broadly, this work provides a physically consistent, atomistically resolved framework for understanding and tuning non-equilibrium nanoparticle synthesis in gas-phase reactors.

## References:

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# CSI Paris 2026

## Cluster-Surface Interactions
## 1st-4th June 2026
## Paris, France

| | Monday 01 June 2026 | Tuesday 02 June 2026 | Wednesday 03 June 2026 | Thursday 04 June 2026 |
|---|---|---|---|---|
| 08:00 | | Breakfast @ The hotel Restaurant | Breakfast @ The hotel Restaurant | Breakfast @ The hotel Restaurant |
| 09:00 | | Scott L. ANDERSON<br>Diana NELLI | Nathalie LIDGI-GUIGUI<br>Ingo BARKE | Elisa JIMENEZ-IZAL<br>Luca BENZI<br>John E. MacGrady |
| 10:00 | | Gunther ANDERSSON | Arlette VEGA GONZALEZ | Alessandro FORTUNELLI |
| | | Coffee break | Coffee break | Coffee break |
| 11:00 | | Fengqi SONG<br>Sean LETHBRIDGE<br>R. G. MENDES | Christian RICOLLEAU<br>Sergio d'ADDATO | Hans Christian WEISSKER<br>Panagiotis GRAMMATIKOPOULOS |
| 12:00 | Rgistration & welcome | Chen HE<br>Ali KHATIBI | Pascal ANDREAZZA | Closing |
| 13:00 | | Lunch @ The hotel Restaurant | Lunch @ The hotel Restaurant | |
| | Opening | | | |
| 14:00 | Giulia ROSSI<br>Maria Chiara SPADARO | Simon BROWN<br>Christopher James HEARD | Lidia MARTINEZ<br>Ewald JANSSENS | |
| 15:00 | Barbara PUTZ | Masahiro SHIBUTA | S. GONZALEZ-SANCHEZ<br>Jose M. MERCERO | |
| | Refreshments | Refreshments | Refreshments | |
| 16:00 | Richard E. Palmer<br>Paolo MILANI | Georg HELD<br>Albert BRUIX<br>Esmaelian FARSAD | El Yakout EL KORAYCHY<br>Murilo MOREIRA | |
| 17:00 | | Florent TOURNUS<br>Armelle MICHAU | | |
| 18:00 | Cultural evening lecture: metallic nanoparticles in stainless glass | Poster session Sponsord by Groove nanomaterial | | |
| 19:00 | Reception | GROVE nanomaterials | Reception drink Sponsored by the IRN Nanoalloy | |
| 20:00 | Dinner @ The hotel Restaurant | Dinner @ The hotel Restaurant | Dinner @ The hotel Restaurant | |
| 21:00 | | | | |