

## O 68: Poster Wednesday: Nanostructures

Time: Wednesday 17:45–20:00

Location: Poster B2

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**Simulation of Brass Nanoparticles using a Neural Network Potential** — ●JAN WEINREICH, MARTÍN LEANDRO PALEICO, and JÖRG BEHLER — Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

High-dimensional neural network potentials (HDNNPs) are a powerful method to study complex systems, because they offer the accuracy of density functional theory (DFT) calculations at the computational costs of simple empirical potentials thus enabling large-scale Monte Carlo and molecular dynamics simulations. In this work we construct a HDNNP for brass nanoparticles, which are important industrial catalysts for methanol synthesis. The potential is applied to determine the most stable structures of large brass clusters of varying composition and size. The analysis of the surface structures emerging in Monte Carlo simulations reveals that depending on the system size the copper to zinc ratio in the surface layers can strongly differ from the interior of the particles.

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**Iridium dioxide catalysts for water electrolysis - From Wulff shape to atomic structure and beyond** — ●JAKOB TIMMERMANN, DANIEL OPALKA, CHRISTOPH SCHEURER, and KARSTEN REUTER — Technische Universität München, Germany

Iridium oxide is currently the preferred material to develop highly active and chemically stable nanoparticle catalysts for the electrochemical oxygen evolution reaction (OER) in proton exchange membrane electrolyzers. Computational models provide important support for the rational design of novel nanoparticle catalysts with optimal size, shape and stability. While the Wulff construction is often adopted to model single-compound nanocrystals, little is known about the influence of edge and corner atoms on the dimensional stability of ultra small IrO<sub>2</sub> nanoparticles as used in state-of-the art OER catalysts. In order to validate the inherent approximations of the Wulff construction, we compare relaxed, mono-facet IrO<sub>2</sub> Wulff nanoparticles of varying shape, size and stoichiometry to respective slab models for extended facets in a comprehensive structure analysis. We demonstrate that the geometry relaxation of IrO<sub>2</sub> nanoparticles strongly depends on the termination and, hence, thermodynamic parameters of the environment, prohibiting the application of the Wulff construction for certain IrO<sub>2</sub> surfaces. We further present an analysis of the contributions of facets, edges and corners to the surface free energy for selected nanoparticle models.

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**Cluster-surface interaction of plasmonic silver particles on silicon** — ●KATHARINA ENGSTER<sup>1</sup>, KEVIN OLDENBURG<sup>1</sup>, JEAN LERMÉ<sup>2</sup>, SYLVIA SPELLER<sup>1</sup>, and INGO BARKE<sup>1</sup> — <sup>1</sup>University of Rostock, Institute of Physics, 18059 Rostock, Germany — <sup>2</sup>Université de Lyon, Institut Lumière Matière, 69622 Villeurbanne Cedex, France

Plasmonic nanoparticles interact with semiconductor surfaces in various ways. On the one hand the plasmon resonance is highly sensitive to the polarizable substrate on an atomic scale [1]. On the other hand plasmonically enhanced excitation of electron-hole pairs is expected to give rise to spatial variations of surface photovoltages (SPV), unless metallic surface states result in equilibration of the surface potential [2]. For size-selected Ag nanoparticles deposited on silicon we show that photoemission electron microscopy (PEEM) enables precise quantification of the SPV based on the spectrally resolved electron yield. The role of the plasmon resonance energy of individual particles, the detailed properties of the substrate (doping, surface states), and effects induced by the experimental setup are being discussed.

[1] K. Oldenburg et al., under review.

[2] K. Sell et al., Phys. Status Solidi B **247**, 1087-1094 (2010).

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**Growth and Morphology of Metal Clusters on HOPG** — ●CHRISTOPHE NACCI<sup>1</sup>, ALEXANDER SCHIFFMANN<sup>2</sup>, FLORIAN LACKNER<sup>2</sup>, PHILIPP THALER<sup>2</sup>, WOLFGANG E. ERNST<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Department of Physical Chemistry, University of Graz, 8010 Graz, Austria — <sup>2</sup>Institute of Experimental Physics, TU Graz, 8010 Graz, Austria

Clusters are a unique class of materials with extraordinary electronic, optical, and catalytic properties [1]. Gold nanoparticles are one of the most studied classes of nanoparticles due to their biocompatibility, high chemical and physical stability, the ease of surface functionalization with organic molecules and the optical properties related to surface plasmons. We have produced gold clusters by helium droplet synthesis and deposited them under clean ultrahigh vacuum (UHV) conditions onto an inert HOPG surface, where they were characterized by scanning tunneling microscopy (STM). Extended ramified structures were identified when depositing clusters on the surface kept at room temperature. In particular, the metallic structures exhibit a fractal-like pattern. The temperature dependence of their shapes has been explored by repeated post-deposition thermally annealing: A cross-over from fractal-like to smoother structures could be observed. To shed some light on the growth processes, Au clusters have been further deposited on an HOPG surface exhibiting defects created by ion sputtering in mild conditions.

[1] W. A. de Heer, Rev. Mod. Phys. **65**, 611 (1993)

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**Manipulation of silver clusters in Ionic Liquids via added ligands.** — ●DAVID MÖNKEBÜSCHER, ALEXANDER KONONOV, PHILIPPE POULET, and HEINZ HÖVEL — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany

Ionic Liquids (IL), e.g. BMIM-PF<sub>6</sub>, delay the aggregation of nanoparticles due to their high viscosity and a formation of an ion layer around the clusters, which separates them electrosterically. Preformed silver clusters with an average size of 2 nm were deposited into different ILs [1]. The temperature dependent aggregation of the nanoparticles can be measured in-situ and ex-situ via UV/vis spectroscopy [2]. Ligands such as Dodecanethiole can be used to manipulate the aggregation of cluster due to the formation of a shell [3]. In order to investigate this influence, such mixed samples are compared with pure samples of different ILs. Another method to examine nanoparticles is AFM. It is used to detect silver clusters deposited on a MoS<sub>2</sub> surface to determine the cluster size distribution.

[1] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. C **120**, 6239 (2016). [2] S. Roese, A. Kononov, J. Timoshenko, A.I. Frenkel, H. Hövel, Langmuir **34**, 4811 (2018). [3] O. P. Khatri et al, Langmuir **24**, 7758 (2008).

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**Mass selected iron clusters on thin oxide films** — ●KEVIN FORYT, ALEXANDER KONONOV, DOMINIK WOLTER, and HEINZ HÖVEL — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany

Clusters are the bridge between atomic and solid-state physics, they show strong size dependent properties. In our cluster beam facility a magnetron sputter gas aggregation source produces a wide range of clusters. Mass selection is performed with a semicontinuous time-of-flight mass selector [1]. For deposition in a load-lock chamber attached directly to the mass selector a new setup of ion optics was simulated with SIMION [2] and has been put into operation. Iron clusters, e.g. Fe<sub>1790±30</sub>, are deposited on an indium tin oxide (ITO) substrate which should be usable for magneto-optical studies. Afterwards ex situ UV/vis spectroscopy and AFM measurements are carried out.

[1] B. von Issendorff, R. E. Palmer, Review of Scientific Instruments **70**, 4497 (1999). [2] Scientific Instrument Services, Inc (2003-2012), <http://simion.com>.

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**An effective nanopatterning strategy for controllable fabrication of high-density sub-3-nm gaps** — ●QUN FU<sup>1,2</sup>, HUAPING ZHAO<sup>1</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — <sup>2</sup>Institute of Nanochemistry and Nanobiology, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China

The realization of large-scale high-density gaps with size as small as possible between neighboring nanostructures is crucial for designing ultrasensitive surface-enhanced Raman scattering substrates. As known, the ultra-thin alumina mask (UTAM) surface nanopatterning tech-

nique allows to fabricate large-scale ( $>1$  cm<sup>2</sup>) ultrahigh-density (1010-1012 cm<sup>-2</sup>) 5-nm nanogaps in periodic nanostructure arrays. However, it is still difficult to realize reliable sub-5-nm gaps distribution on large area only by traditional one-step pore-widening process for UTAM technique, because of the collapse of the UTAM pore wall in the excessive pore-enlarge process at high operating temperature (30 C). Here, a two-step high-low temperature pore-widening process in the UTAM fabrication was reported as an efficient solution to precisely control the gap size into the range of sub-3-nm. This two-step pore-widening method enable to effectively avoid the fragmenting of the membrane and to obtain the large enough pore diameter to 97-99 nm steadily at appropriate lower temperature. As a result, large-scale nanoparticle arrays with high-density sub-3-nm gaps have been realized with the as-prepared UTAM as nanostructuring template.

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**Fabrication of metallic microstructures on optical fibers** — ●ALEXANDER FASSBENDER and STEFAN LINDEN — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Fiber cavities have emerged to be a promising tool for the fabrication of a quantum memory cell. Based on the compactness and robustness of atom/ion traps that can be realized with fiber cavities, they are a candidate for the realization of quantum repeater nodes. We report on the fabrication of metallic microelements on optical fibers. A polymer mask is created on a cleaved end of the fiber using three-dimensional laser writing based on the principle of two photon absorption. A layer of gold is then thermally evaporated. After the removal of the polymer mask, four gold electrodes remain, separated by thin stripes that arise from the shadow of the polymer mask. The core of the fiber is protected as well, so the in- and outcoupling of light is not affected by the microstructures. When using these fibers in a cavity, the light-matter action can be manipulated. We envision that our microstructured fibers can be employed to realize compact ion traps inside of a fiber resonator.

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**Chemical properties of metal-silicates rendered by metal exchange reaction** — ●FRANZ KÖNIGER<sup>2</sup>, ROBERTO C. LONGO<sup>1</sup>, PETER THISSEN<sup>2</sup>, and ALEXEI NEFEDOV<sup>2</sup> — <sup>1</sup>University of Texas at Dallas, Materials Science and Engineering 800 W. Campbell Road, RL 10 Richardson, TX, USA 75080 — <sup>2</sup>Karlsruher Institut für Technologie (KIT), Institut für Funktionelle Grenzflächen (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Calcium-Silicates and Calcium-Silicate-Hydrates (CS and CSH) form the most important building material, cement. Both phases react fast with CO<sub>2</sub> from the atmosphere and, due to the porosity of cement and concrete, such reaction goes deep into the material, producing phase transformations and crack formation and propagation. The aim of this work is twofold. In the first part, we compare the reaction of CO<sub>2</sub> with CSH phases and with Magnesium-Silicate-Hydrates (MSH).

Surprisingly, MSH did not show any contamination of carbonates in the infrared spectra. While the reaction of CO<sub>2</sub> with CSH has been well studied and explained, there is currently no explanation about the resilience of MSH to the interaction with CO<sub>2</sub>. For the first time, the atomistic details of the reaction of CO<sub>2</sub> with MgSiO<sub>3</sub> are shown, and the chemical resistance of MgSiO<sub>3</sub> against CO<sub>2</sub> and other relevant chemicals for corrosion of cement and concrete is explained. Secondly, we demonstrate that Mg and other metals can undergo an exchange in situ process in CS and CSH phases. Depending on the type of metal exchanged, a completely new platform for rendering the properties of cement and concrete surfaces against corrosion is developed.

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**Mechanism of SeO<sub>x</sub>- Immobilization by  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> Microsphere with Surface Oxygen Vacancies** — ●LONG LIU<sup>1</sup>, HUAPING ZHAO<sup>1</sup>, CHENGLIN ZHANG<sup>1</sup>, YANG XU<sup>1</sup>, DONGJIANG YANG<sup>2</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — <sup>2</sup>School of Environmental Science and Engineering, 266071 Qingdao, China

Removal of the toxic selenium compounds, e.g., selenite (SeO<sub>3</sub><sup>2-</sup>) and selenate (SeO<sub>4</sub><sup>2-</sup>), from contaminated water is imperative for environmental protection and drinking water safety. But conventional ion exchange and physical adsorption approaches are insufficient to achieve the required drinking water standard of selenium compounds with a concentration below 10  $\mu$ g/L. Here we report that the preparation of microsphere-like  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> with surface oxygen vacancies for efficiently capturing toxic SeO<sub>x</sub>- (SeO<sub>3</sub><sup>2-</sup> and SeO<sub>4</sub><sup>2-</sup>) anions from aqueous solutions with superior capacity and fast uptake rate. The SeO<sub>x</sub>- immobilization mechanism is attributed to the existence of surface oxygen vacancies, and implies the utilization of surface defects as highly efficient and adsorptive sites to capture specific toxic species.

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**Dielectric Waveguide Fabrication by Direct Laser Writing** — ●FRANK BRÜCKERHOFF-PLÜCKELMANN, ALEXANDER FASSBENDER, and STEFAN LINDEN — Physikalisches Institut, Rheinische Friedrich-Wilhelms Universität Bonn, Nußallee 12, D-53115 Bonn, Germany

Direct laser writing allows the fabrication of three dimensional polymer structures from a negative tone photoresist by two photon absorption with an accuracy of a few hundred nanometer. By choosing the refractive index of the polymer slightly larger than the one of the glass substrate, we can use an external laser to excite guide modes in the printed structure [cf. Landowski, Freymann et al. '17]. For an efficient coupling we exploit the high refractive index difference between the polymer and air e.g. by designing a prism shaped coupler that uses total internal reflection at the polymer air interface. We study different coupler geometries and the overall performance of the polymer waveguides. In order to design larger optical networks we also test a simple beam splitting device.