CPP 113: Nanostructured Surfaces and Thin Films III: Dots, Particles, Clusters (joint session O/CPP)

Time: Friday 10:30–13:00 Location: WIL B321

CPP 113.1 Fri 10:30 WIL B321

Reconfigurable Polaritonics using Phase Change Materials — •Christina M. Spägele[1], Xinghui Yin[1], Michele Tamagnone[1], Kundan Chaudhary[1], Stefano L. Oscurato[1,2], Jiahan Li[3], Christoph Persch[4], Ruoping Li[1], Noah A. Rubin[1], Luis A. Jauregui[5], Kenji Watanabe[6], Takashi Taniguchi[6], Philip Kim[1], Matthias Wuttig[4], James H. Edgar[3], Antonio Ambrosio[1,7], and Federico Capasso[1] — [1]Harvard University, USA — [2]Unina, Italy — [3]KSU, USA — [4]RWTH, Germany — [5]UCLA, USA — [6]NIMS, Japan — [7]CNST-IIT, Italy

Polaritons garnered significant interest due to their ability of confining light to the nanoscale. They arise when light couples strongly to material excitations such as excitons, plasmons or phonons. To date, methods to control these highly confined states of light are not well-suited for free-form manipulation of polaritons. Moreover, they create systems that are unalterable after the initial fabrication process.

Placing the hyperbolic vdW-material hexagonal boron nitride on the phase change material (PCM) Ge3Sb2Te6, we successfully achieved spatial control of the propagation of surface phonon polaritons (SPhP) by structuring the PCM. The exponentially decaying tail of the guided SPhP modes interacts with the PCM, which can be optically switched to a higher refractive index crystalline phase, slowing the SPhP. We demonstrate rewritable waveguides and refractive optical elements such as lenses and prisms for mid-IR polaritons. Moreover, we will discuss reconfigurable metalenses that allow for precise wavefront engineering and diffraction-limited focusing.

CPP 113.2 Fri 10:45 WIL B321

Synthesis of 3D ZnO nanostructures on different substrates for gas sensor applications — Hanaa Seso, Stefan Ostendorp, •Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische-Wilhelms-Universität, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Three-dimensional (3D) ZnO nanostructures have been synthesized via atomic layer deposition (ALD) on different types of templates to act as a gas sensing active material. The used template structures range from anodic aluminum oxide (AAO) template synthesized by a two-step anodization method, a polymer template prepared by infiltration of a polymer solution into an AAO structure to a porous gold template fabricated by de-alloying of an Au-Ag solid solution. The morphology of the templates and the nanostructured ZnO-based carbon monoxide (CO) sensors were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The gas-sensing performance of sensors based on the different templates was measured successfully in terms of electrical response to detect CO as a hazardous gas. The tremendously increased surface to volume ratio of ZnO on an AAO (alike) template or porous gold template is thereby supposed to provide an enhanced sensing capability compared to 2D thin film or bulk sensor structures.

CPP 113.3 Fri 11:00 WIL B321

Thinking inside the box: Quantum corrals as artificial atoms and molecules — •Saoirse Freeney, Jaap Harteveld, Sam Borman, and Ingmar Swart — Utrecht University, Utrecht, Netherlands

The electronic behaviour that underlies the field of chemistry is essentially a result of the confining potential of an atom's nucleus on its electrons. Due to their confinement, the allowed energies that electrons can take in an atom are quantised, and their wavefunctions are well-defined . If we were to create our own potential that confines electrons within, we could emulate real atoms and change their properties at will. In fact, a quantum corral is exactly this. To create one, adsorbates on a metal surface are accurately manipulated with an STM tip to predetermined positions. Much like a particle-in-a-box, the surface state electrons are then confined, exhibiting discrete energy levels analogous to an atom. We can liken the measured wavefunctions to those of s, p, d etc orbitals in an atom. Beyond this, we can pair two quantum corrals together and observe that bonding and antibonding orbitals arise. Here, we use CO molecules to scatter the Cu(111) surface state and investigate the relation of size and shape on the energy and wavefunction, and secondly we tailor the strength of coupling in "molecular" quantum corrals. Several artificial lattices have been made before with the CO/Cu(111) platform. The information presented is useful for designing such lattices.

CPP 113.4 Fri 11:15 WIL B321

Ordered structures with functional units from artificial alumina membranes — •Wenxin Wang — Photonic Materials Group, College of Physics and Optoelectronic Engineering, Harbin Engineering University,15001 Harbin, China

Constructing ordered structures with functional units (OSFU) gives opportunities to improve, modify intrinsic performances of ordered structures, even render novel properties. Here I report an approach to realize OSFU through artificial alumina membranes (AAMs), single and multi-order structure(s) are functionalized with plasmonic and (or) smart polymer unit to check their mesoscopic optical behaviors. For instance, AAMs are directly used as OSFU to achieve structural color imaging with high reflectivity. Second, functionalize units with plasmonic materials to obtain enhanced local field and resonance modes hybridization, in order to manipulate the linear and nonlinear optical performances. Third, functionalize units with polymer to realize reversible structures for dynamic optical modulation. Finally, multi-order OSFU is designed by inducing diverse lattice arrangements for photonic band engineering. The second-order elements are embedded on special points that corresponding high symmetry points in k-space that will arise Dirac cone and flat band.

CPP 113.5 Fri 11:30 WIL B321

Comsol modeling of the role of nanostructured current collectors in supercapacitor — •Maximilian Kaupenjohann, Long Liu, Huaping Zhao, and Yong Lei — Technische Universität Ilmenau, 98393, Ilmenau, Germany

Current collector is an important component in supercapacitors and its main role is to transport charge carriers from/to electroactive materials during the charge-discharge process. The charge transport efficiency is believed to be dominated by the resistance at the electroactive-material/current-collector interfaces. Owing to the large specific surface area, nanostructured current collectors have been designed, fabricated, and investigated intensively for supercapacitors. Especially for pseudocapacitive materials that have theoretically high specific capacitance but intrinsically low electric conductivity, nanostructured current collectors enable one to achieve a much higher specific capacitance even nearly reach the theoretical value. The improved performance is generally attributed to the improved electrical and ionic transport kinetics endowed by nanostructured current collectors. In this work, the role of nanostructured current collectors in supercapacitor electrode is further identified by using COMSOL Multiphysics simulations in combination with the experiment results.

CPP 113.6 Fri 11:45 WIL B321

Global Optimization of Copper Clusters on ZnO Surfaces Utilizing a Neural Network Potential — •Martín Leandro Paleico and Jörg Behler — Universität Göttingen, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany

The catalyst used in the industrial synthesis of methanol is composed of large copper and zinc oxide nanoparticles. Studying the structure of this system requires a simulation method capable of handling thousands of atoms with ab initio accuracy, but with computational efficiency comparable to classical empirical potentials. To meet these requirements, a Neural Network Potential (NNP) has been trained to reproduce the potential energy surface of the system based on DFT reference calculations.

We have utilized this potential to carry out the tens of thousands of energy and force evaluations required to perform global optimization searches employing genetic algorithms. With this, we are able to optimize pure copper and binary copper-zinc clusters with up to 30 atoms on two different zinc oxide surfaces. This allows us to investigate structural and energetical trends in cluster growth and cluster-substrate interactions, as well as to identify possible active sites and their distribution in the clusters.

CPP 113.7 Fri 12:00 WIL B321

Deposition and annealing of Fe_xNi_{1-x} nanoparticles on a W(110) surface — •Mahboobeh Ravankhah, Dennis Jagenburg, and Mathias Getzlaff — Institute of Applied Physics, University Düsseldorf

3d bimetallic nanoparticles have received lots of attention because of their technological application. In comparison to pure Fe and Ni, alloys of Fe_xNi_{1-x} have much more complex structural phases under different conditions. Different FeNi alloys are used: $Fe_{0.50}Ni_{0.50}$, $Fe_{0.25}Ni_{0.75}$ and $Fe_{0.75}Ni_{0.25}$. All nanoparticles are prepared by a magnetron sputtering source under UHV condition on a W(110) surface, therefore contaminations are avoided. The deposited nanoparticles are subsequently annealed between 500-800K. Particle's size, shape and structure will be investigated by Transmission Electron Microscopy (TEM) and Scanning Tunneling Microscopy (STM). We report on the influence of different parameters like size of nanoparticles, stoichiometry and annealing temperature on the melting behavior.

CPP 113.8 Fri 12:15 WIL B321

Cu2+ Detection by Carbon Quantum Dots Derived from Water Hyacinth (Eichhornia crassipes) — •Eduardo Magdaluyo Jr[1], Gerald Mari Quiachon[2], and Persia Ada de Yro[2] — [1]Department of Mining, Metallurgical and Materials Engineering, University of the Philippines, 1101 Diliman, Quezon City, Philippines — [2]Materials Science Division, Industrial Technology Development Institute, Department of Science and Technology, Bicutan, Taguig, Metro Manila, Philippines

Preparation of carbon quantum dots (CQDs) was derived from water hyacinth (Eichhornia crassipes) leaves as a carbon source using facile approach of hydrothermal treatment in acidic medium. The as-synthesized CQDs exhibited coagulation in aqueous solution and a strong blue fluorescence under UV light at 365 nm. Infrared spectra analysis confirmed the presence of functional groups such as hydroxyl (OH), carboxyl (COO) and carbonyl (CO) on the surface of the CQDs. The functional groups were analyzed using zeta potential and was found to induce surface charges which allow the attraction of copper ions and bind with the CQDs. These surface charges were utilized in the application of the CQDs as a biosensor for the detection of Cu2+ ions based on ion-induced fluorescence quenching of CQDs. The photoluminescence spectra confirmed this process and it was found to have excellent affinity toward Cu2+ as the PL of CQD with copper solution was quenched relative to pure CQD solution. The highest quantum yield of the CQD sample being measured against deionized water was found to be at 6.48.

CPP 113.9 Fri 12:30 WIL B321

Electronic and optical properties of quantum-confined nanoparticles — •Marius Buerkle and Vladimir Svrcek — National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

We discuss the electronic and optical properties of semiconducting nanoparticles in the quantum-confinement regime. Here we focuse on how do quasi-band-like features emerge from finite electronic states with increasing particle size. This is discussed for Si, SiC, and Sn nanoparticles. Particularly interesting is the transition from an indirect to direct bandgap semiconductor for ultra-small Sn nanoparticles.

CPP 113.10 Fri 12:45 WIL B321

Developing a GAP machine-learned potential for iridium dioxide nanoparticles — •Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Iridium dioxide is currently the preferred material for highly active, yet chemically stable nanoparticle catalysts enabling the electrochemical oxygen evolution reaction (OER) in proton exchange membrane electrolyzers. Full ab initio molecular dynamics (MD) simulations of the reactive processes at the electrified nanoparticle surface would be highly desirable for mechanistic catalyst improvement, but are computationally not tractable for a foreseeable time. To overcome the limitations regarding system size and propagation time, MDs based on machine-learned interatomic potentials are an appealing alternative.

Here, we present a corresponding Gaussian Approximation Potential (GAP) for IrO_2 combining two-body and smooth overlap of atomic positions (SOAP) descriptors to capture the atomic environment. The potential is trained with density-functional theory (DFT) data comprising IrO_2 bulk, various surface slabs, Wulff shape nanoparticles, as well as semi-amorphous structures iteratively obtained from short MD trajectories based on the developing GAP. The final GAP is found to faithfully provide a wide range of static geometric and energetic key parameters. MD simulations based on this GAP now provide first insight into stability and special OER active sites offered by nanoparticles of varying size and shape.