O 11: Poster Session I: Plasmonics and nanooptics I

Time: Monday 10:30–12:30 Location: P

O 11.1 Mon 10:30 P

Fabrication and transfer of hexagonal gold nano-pyramid arrays on PDMS for SERS — •Peter Christian Simo[1], Florian Laible[1], Anke Horneber[1], Claus Burkhardt[2], and Monika Fleischer[1] — [1]Institute for Applied Physics, University of Tuebingen, Germany — [2]Natural and Medical Sciences Institute at the University of Tuebingen, Reutlingen, Germany

Surface enhanced Raman scattering (SERS) with pyramidal nanostructures increases the signal of Raman active analytes, since hotspots form at the edges and tip of a nano-pyramid under illumination. 2D hexagonal arrays of pyramidal nanostructures with a quadratic base are fabricated through cost-effective nano-sphere lithography and transferred onto PDMS. Under varying uniaxial strain the localized surface plasmon resonances (LSPRs) of the nanostructures on the PDMS can also be analysed. By making use of the (111) crystal plane of a silicon (100) wafer, an inverted pyramidal array is etched, which serves as the complementary negative for the gold nanostructures. Either a continuous gold thin-film with protruding pyramids or separate isolated nano-pyramids are produced. The use of a linker molecule between the PDMS and the gold is mandatory to increase the weak Au-PDMS adhesion. (3-Mercaptopropyl)triethoxysilane (MPTS) is able to bind to both PDMS and to the gold structures, thus strongly increasing stability for mechano-optical experiments. The SERS enhancement is verified by Raman mapping of 4-Mercaptobenzoic acid molecules.

O 11.2 Mon 10:30 P

Fabricating ultra-narrow gaps in bow-ties utilizing strain junctions — •Florian Laible[1], Kai Braun[2], Martin Eberle[2], Dieter P. Kern[1], Alfred J. Meixner[2], and Monika Fleischer[1] — [1]Institute for Applied Physics and Center LISA+, University of Tübingen, 72076, Tübingen, Germany — [2]Institute for Physical and Theoretical Chemistry and Center LISA+, University of Tübingen, 72076, Tübingen, Germany

Mechanically controllable break junctions (MCBJs) are widely used to create sub-1 nm gaps between two metal contacts. In this regime, the width of the gap can be controlled with Angstrom precision using the tunnel effect. The ability to create ultra-narrow gaps in bow-tie antennas is desirable for investigations on the interplay of localized plasmonics and electron tunneling, as well as for SERS applications since ultra-narrow gaps are promising highly enhanced near fields. The integration of nanoantennas into MCBJs is challenging since the localization of the plasmon and the mechanical properties of the break junction have to be preserved simultaneously. We present an approach to reach ultra-narrow gaps between two nanoantennas in the focus of a confocal microscope. A gapless bow-tie antenna is integrated into a mechanically controllable break junction. The nanostructure is optically decoupled from the electrical leads. The gap is created by bending the substrate, causing the nanoantenna to break at its thinnest point. The gap size is measured using electron tunneling and controlled by changing the bend of the substrate. Combined electrical and optical measurements will be presented alongside the fabrication process.

O 11.3 Mon 10:30 P

Ab-Initio study of plasmonic properties of metallic magnesium nanoclusters — •Oscar A. Douglas-Gallardo, Connor L. Box and, and Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, United Kingdom

The study of optical, electronic and catalytic properties of nanostructured plasmonic materials has been traditionally focused on gold and silver. In recent years, however, the plasmonic properties of a set of Earth-abundant materials (Al, Mg) have gradually gained increasing interest in the plasmonic area. These new plasmonic materials can potentially extend the application areas of standard plasmonic material (Au, Ag and Cu) adding more chemical variety whilst simultaneously reducing the production cost associated with coinage metals. In this context, the optical and electronic properties of a set of nanostructured metallic magnesium particles and surfaces have been explored by means of time-dependent density functional tight-binding (TD-DFTB) approach along with molecular dynamics with electronic friction (MDEF) simulation. The hot carrier distributions produced when Mg nanoclusters are exposed to light were computed and compared against silver nanoclusters. Finally, chemical interface damping due to molecular hydrogen/atomic hydrogen adsorption was also considered. The results obtained here represent the first step toward full characterization and assessment of this new variety of plasmonic material made of Earth-abundant elements.

O 11.4 Mon 10:30 P

Dramatic Enhancement of Tip-Enhanced Raman Scattering Mediated by Atomic Point Contact Formation — •Shuyi Liu[1], Borja Cirera[1], Yang Sun[2], Ikutaro Hamada[2], Melanie Muller[1], Adnan Hammud[3], Martin Wolf[1], and Takashi Kumagai[1,4] — [1]Department of Physical Chemistry, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]GREEN, National Institute for Materials Science, Ibaraki, Japan — [3]Department of Inorganic Chemistry, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [4]Center for Mesoscopic Sciences, Institute for Molecular Science, Okazaki, Japan

Tip-enhanced Raman scattering (TERS) in ångström-scale plasmonic cavities has drawn increasing attention. However, Raman scattering at vanishing cavity distances remains unexplored. In this presentation, I show the evolution of TERS in transition from the tunneling regime to atomic point contact (APC). A stable APC is reversibly formed in the junction between an Ag tip and ultrathin ZnO or NaCl films on the Ag(111) surface at 10 K. An abrupt increase of the TERS intensity occurs upon APC formation for ZnO, but not for NaCl. This remarkable observation is rationalized by a difference in hybridization between the Ag tip and these films, which determines the contribution of charge transfer enhancement in the fused plasmonic junction. The strong hybridization between the Ag tip and ZnO is corroborated by the appearance of a new vibrational mode upon APC formation, whereas it is not observed for the chemically inert NaCl.

O 11.5 Mon 10:30 P

Dipolar coupling of nanoparticle-molecule assemblies: An efficient approach for studying strong coupling — •Jakub Fojt[1], Tuomas P Rossi[2], Tomasz J Antosiewicz[3], Mikael Kuisma[4], and Paul Erhart[1] — [1]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Department of Applied Physics, Aalto University, Aalto, Finland — [3]Faculty of Physics, University of Warsaw, Warsaw, Poland — [4]Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland

Strong light-matter interactions facilitate not only emerging applications in quantum and non-linear optics but also modifications of materials properties. In particular the latter possibility has spurred the development of advanced theoretical techniques that can accurately capture both quantum optical and quantum chemical degrees of freedom. These methods are, however, computationally very demanding, which limits their application range. Here, we demonstrate that the optical spectra of nanoparticle-molecule assemblies, including strong coupling effects, can be predicted with good accuracy using a subsystem approach, in which the response functions of the different units are coupled only at the dipolar level. We demonstrate this approach by comparison with previous time-dependent density functional theory calculations for fully coupled systems of Al nanoparticles and benzene molecules. While the present study only considers few-particle systems, the approach can be readily extended to much larger systems and to include explicit optical-cavity modes.

O 11.6 Mon 10:30 P

Boosting Light Emission from Single Hydrogen Phthalocyanine Molecules by Charging — •Vibhuti Rai[1], Lukas Gerhard[1], Qing Sun[1], Christof Holzer[2], Taavi Repaen[3], Marjan Krstic[2], Liang Yang[3], Martin Wegener[3], Carsten Rockstuhl[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

The aspect of light emission from single molecules on insulating layers studied by scanning tunneling microscopy induced luminescence (STML) has made considerable progress. Many fundamental aspects of light emission, however, remain unclear for the future prospect of

device applications. Here, we used STML to investigate light emission from individual Hydrogen-Phthalocyanine (H_2Pc) molecules thermally evaporated onto bi- and trilayers of NaCl on Au(111). Combining STML measurements, full-wave electrodynamics, and quantum chemical calculations, we show that the emitted light from a charged H_2Pc couples more efficiently to the far-field than its neutral form [1]. This boost can be explained by the development of a vertical dipole moment normal to the substrate, facilitating out-coupling of the local excitation to the far-field. Since this effect is not related to the specific molecule, it provides a general pathway for enhancing the quantum efficiency of light emission from a molecular junction.

[1] Rai et al. Nano Letters 2020, 20 (10), 7600-7605.

O 11.7 Mon 10:30 P

Design of periodic structures by surface plasmon polaritons excitation — •Pavel N. Terekhin[1], Jens Oltmanns[2], Andreas Blumenstein[2], Dmitry S. Ivanov[1,3,4], Frederick Kleinwort[2], Martin E. Garcia[3], Baerbel Rethfeld[1], Juergen Ihlemann[2], and Peter Simon[2] — [1]Department of Physics and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institut für Nanophotonik Göttingen e.V., 37077 Göttingen, Germany — [3]Theoretical Physics Department, University of Kassel, 34132 Kassel, Germany — [4]Quantum Electronics Division, Lebedev Physical Institute, 119991 Moscow, Russia

Laser irradiation of solids can lead to the spontaneous formation of periodic structures on the surface. They are known as laser-induced periodic surface structures (LIPSS) and have unique properties with a broad spectrum of applications. For their controlled fabrication, it is essential to understand the basic governing mechanisms of energy deposition.

We demonstrate the influence of surface plasmon polaritons (SPP) on the process of LIPSS formation after irradiation of a step edge structure in a single-pulse experiment. The absorption of laser energy is described by an analytical source term, which considers the excitation of SPP. The further surface structures development is traced by a hybrid atomistic-continuum model. The theoretical predictions are fully confirmed by experimental observations. The developed method can be used to study the mechanisms of laser energy absorption and to design surface structures under controlled conditions.

O 11.8 Mon 10:30 P

Dependency of aggregate absorption on near field polarization — •Sidhartha Nayak[1], Fulu Zheng[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany

Strong interaction between transition dipoles of molecules leads to the formation of delocalized excitonic eigenstates of molecular aggregates. To understand their optical and transfer properties, knowledge of these eigenstates is required. Using near-field radiation stemming from a metallic tip which is scanned over the aggregate one can record position-dependent absorption spectra [1]. From these spectra, it is possible to reconstruct excitonic wavefunction [2]. In this contribution, we focus on the situation when the tip is irradiated by linear polarized light. We show that there is a strong dependence of the near field spectra on the polarization and propagation direction of the incident light, which can be used to facilitate the wavefunction reconstruction. Finally, we explain this orientation dependency using three basic functions which depend on tip position and eigenfunctions but not on the orientation of the incoming radiation.

[1] X. Gao and A. Eisfeld, *J. Phys. Chem. Lett.* 9, 6003 (2018)
[2] F. Zheng, X. Gao and A. Eisfeld, *Phys. Rev. Lett.* 123, 163202 (2019)