MM 64: Nanomaterials - Miscellaneous

Time: Thursday 17:15–18:45 Location: H25

MM 64.1 Thu 17:15 H25

Plasmon resonances in Janus particles — •Sol Carretero-Palacios, Frank Jäckel, Theobald Lohmüller, and Jochen Feldmann — Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Department of Physics and Center for Nano-Science (CeNS), Amalienstr. 54, D-80799, München, Germany

Janus particles are particles whose surfaces have two or more different types of properties. Standard Janus particles used for optical manipulation consist of micro-silica core spheres half-coated with gold. The spherical asymmetry associated with Janus particles is the key point in many applications, including electrophoretic displays, nanoviscometers, and self-propelling micromachines. These systems possess a tunable plasmon resonance that can be controlled by changing the ratio of the core radius to the coating thickness.

We evaluate theoretically the extinction spectra of silica-gold Janus particles diluted in water, using a three-dimensional finite difference time domain (FDTD) method. We are able to tune the plasmon resonance from the near infrared to the optical regime by: i) half-coating the silica sphere with gold, but reducing the radius of the dielectric particle; ii) half-coating the silica particle with gold, but varying the ratio between radius and coating thickness; and iii) keeping both the radius and thickness fixed, but creating Dot-Janus particles, i.e., Janus particles which have a metallic coating covering $< 50\%$ of their surface area.

MM 64.2 Thu 17:30 H25

xcitons in solids captured with bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory — •Sangeeta Sharma, John Kay Dewhurst, Antonio Sanna, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

he ab-initio calculation of optical absorption spectra of nano-structures and solids is a formidable task. The current state-of-the-art is based on many-body perturbation theory: one solves the Bethe-Salpeter equation (BSE). Unfortunately, solving the BSE involves diagonalizing a large matrix making this method computationally very expensive.

Time-dependent density functional theory (TDDFT) is another method able to determine neutral excitations of a system. Although formally exact, the predictions of TDDFT are only as good as the approximation of the exchange-correlation (xc) kernel. There are only a few xc-kernels which correctly reproduce the excitonic effect, but these kernels suffer from either being computationally as expensive as solving BSE or depend upon external parameters.

In our latest work we propose a new approximation[1] for xc-kernel, and demonstrate that this kernel is nearly as accurate as BSE and has the correct 1/q^2 behavior. The computation cost for the bootstrap kernel is minimal and no system-dependent external parameter is required.

1. S. Sharma, J. K. Dewhurst, A. Sanna, E. K. U. Gross, Phys. Rev. Lett., 107, 186401 (2011).

MM 64.3 Thu 17:45 H25

Electrically Tunable Optical Gap Antenna — •Kai Chen and Bert Hecht — Nano-Optics & Biophotonics Group, Experimentelle Physik 5, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Optical gap antennas consist of two gold nanorods separated by gaps with a few nanometers in width. It is critical and desirable for a variety of applications to be able to actively tune the plasmon resonances of the gap antennas. Here, we demonstrated electrically tunable optical gap antennas fabricated from single crystalline gold flakes by focused ion beam (FIB). The antennas are suspended in air and hence charge accumulation induced by an applied DC voltage on the antenna results in a repulsive Coulomb force between the two nanorods leading to increased gap size. This technique provides an effective means for the fabrication of active plasmonic elements and allows to implement devices in which (nano-)optical and mechanical degrees of freedom are coupled.

MM 64.4 Thu 18:00 H25

Morphology of Fiber-Coatings by Thiol-Ene Photochemisty and their Mechanical Properties at the Interface — •Christian Kuttner[1], Michaela Eder[2], Helmut Schlaad[3], Ingo Burgert[4], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, 95447 Bayreuth, Germany — [2]Max-Planck Institute of Colloids and Interfaces, Department of Biomaterials, 14424 Potsdam, Germany — [3]Max-Planck Institute of Colloids and Interfaces, Colloid Chemistry, 14424 Potsdam, Germany — [4]ETH Zürich, Institute for Building Materials & Empa, Wood Lab, 8093 Zürich, Switzerland

Control of the interfacial properties is crucial for inorganic-organic composites. We studied the interfacial adhesion between inorganic surfaces grafted with macromolecular coatings and a given epoxy matrix. The aim was to develop a better understanding of adhesion principles in (fiber-reinforced) composites and thus optimizing composites.

Thiol-ene photochemistry was utilized to introduce a polymeric gradient on silica-like surfaces following a two-step approach by Schlaad et al. without additional initiator. Two grafting-techniques were applied: "Grafting-from" polymerization resulted in brush-like homopolymer films, whereas, "grafting-onto" deposition was suitable for diblock copolymer attachment. Both techniques were adapted to modify fiberglass. The resulting coating morphologies were nanostructurally characterized (AFM, SEM, SE, TGA). The interfacial shear strength of modified fibers in an epoxy matrix was measured by a single fiber pull-out experiment to benchmark the non-covalent fiber-matrix construction.

MM 64.5 Thu 18:15 H25

Nanomechanical characterization of soft matter fibers — •Daniel Kluge[1], Julia Singer[2], Hans-Werner Schmidt[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth, Germany — [2]Macromolecular Chemistry I, University of Bayreuth, Germany

Micro- and nanofibers are important structural elements in many functional materials. Their characterization requires highly advanced techniques beyond standard methods for macroscopic materials. In our contribution, we focus on nanoscale bending of free-standing fibers, which is suitable for a wide variety of fiber systems. We discuss major advantages of bending perpendicular and parallel to the substrate plane, especially the detailed investigation of the mechanical properties within and beyond linear elastic deformations. For the interpretation of the data, we use analytical as well as finite element models. In particular, we investigate supramolecular 1,3,5-Benzenetrisamides (BTAs), which allow combining the advantages of bottom-up and top-down techniques since they form well-defined fibers by self-assembly and melt electrospinning. We show that the morphology of self-assembled BTA fibers can be tailored via the substituents, establish mechanical structure-property relations and distinguish between size and material contributions. Furthermore, we compare self-assembled and electrospun fibers from the same BTAs and demonstrate that regardless of the preparation pathway, the fibers possess a remarkable mechanical stiffness. This is a striking result, since only supramolecular interactions and no covalent bonds are present in these systems.

MM 64.6 Thu 18:30 H25

Nanoscale materials and electronic transport: from ballistic to hopping approaches — •Velimir Meded[1,2], Angela Poschlad[2], Franz Symalla[1], Denis Danilov[1], and Igor Beljakov[1] — [1]Institute of Nanotechnology, KIT, Karlsruhe — [2]Stainbuch Centre for Computing, KIT, Karlsruhe

In recent years we have developed simulation methods that describe the conformation and electronic properties of materials built based on well-defined nanoscale constituents. The methods were used to describe ballistic in nanoscale devices. Here we discuss applications on single-molecule electronics, specifically molecular wires (metallic and organic) and the development of an atomic transistor [1,2,3,4].

Secondly, we present multiscale methods to describe function of organic light emitting diodes [5] by deploying morphology simulations with Monte Carlo methods, quantum mechanical analysis of the generated morphology, and hopping charge transport.

Finally, I will discuss the integration of these methods into a European framework for multiscale materials modelling, MMM@HPC, which aims at making general simulation methods accessible to a wide audience of interested scientists, by seamlessly integrating HPC re-

sources from within its graphical user interface [6].

1. R, Maul, W. Wenzel, Phys, Rev. B, 80, 045424 (2009). 2. F. Xie, et al., Adv, Mat„ 22, 2033 (2010). 3. V. Meded, et al., SMALL,5, 2218 (2009). 4. V. Meded, et al., Phys. Rev. B, 83, 245415 (2011). 5. J. J. Kwiatkowski, et al., Phys, Chem. Chem. Phys., 10(14), 1852 (2008). 6. The MMM@HPC webpage: www.multiscale-modelling.eu