Topical Talk

Tunable bandgaps and excitons in doped semiconducting carbon nanotubes made possible by acoustic plasmons — 

Catalin Spataru and Francois Leonard — Sandia National Laboratories, Livermore, California, USA

Doping of semiconductors is essential in modern electronic and photonic devices. While doping is well understood in bulk semiconductors, the advent of carbon nanotubes and nanowires for nanoelectronic and nanophotonic applications raises some key questions about the role and impact of doping at low dimensionality. Here we show that for semiconducting carbon nanotubes, bandgaps and excitonic binding energies can be dramatically reduced upon experimentally relevant doping, and can be tuned gradually over a broad range of energies in contrast to higher dimensional systems. The later feature, made possible by a novel mechanism involving acoustic plasmons, establishes new paradigms for the understanding and design of nanoelectronic and nanophotonic devices.

Electronic Excitations in Single-Wall Carbon Nanotubes: Building-Block Approach — 

Ralf Hambach, Christine Giorgetti, Xochitl Lopez-Lozano, and Lucia Reining — LSI, École Polytechnique, CNRS, CEA/DSM, Palaiseau, France — European Theoretical Spectroscopy Facility — University of Texas at San Antonio, United States

Parameter-free calculations of electron energy-loss spectra for low-dimensional systems like single-wall carbon nanotubes can become numerically very demanding or even unfeasible for large diameters.

We overcome this problem by means of a building-block approach: Combining effective-medium theory and ab-initio calculations we can describe the collective excitations in nanostructures (like carbon nanotubes) starting from the microscopic polarisability of their building blocks (bulk graphite). To this end, Maxwell’s equations are solved using the full frequency- and momentum-dependent microscopic dielectric function \( \varepsilon(q, \omega) \) of the bulk material. The latter is calculated from first principles within the random phase approximation [1].

Besides an important gain in calculation time this method allows us to analyse the loss spectra of nanostructures in terms of their normal-modes excitation. We apply the building-block approach to study angular resolved loss spectra for graphene and single-wall carbon nanotubes and find a very good agreement with full ab-initio calculations of these systems and corresponding experiments.


Functionalized Tips Leading to Atomic-Resolution Force Microscopy — 

Nikolaj Moll, Leo Gross, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer — IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Performing atomic force microscopy (AFM) with a molecule or an atom at the tip the resolution can be dramatically enhanced as the resolution crucially depends on the chemical nature of the tip termination. A pentacene molecule is imaged with atomic resolution with a tip functionalized with a CO molecule. The interactions between the CO tip and the pentacene are studied with first principles calculations. The different energy contributions are analyzed, and the Pauli energy is computed. The source of the high resolution is Pauli repulsion, whereas van-der-Waals and electrostatic interactions only add a diffuse attractive background. To validate the usefulness of AFM with functionalized tips the natural product cephalanole A is studied. The measurements together with first principle calculations demonstrate that the direct imaging of an organic compound with AFM facilitates the accurate determination of its chemical structure. The method might be developed further towards molecular imaging with chemical sensitivity, and could solve certain classes of natural product structures.
