

HL 11: C/diamond

Time: Monday 11:00–13:00

Location: EW 202

HL 11.1 Mon 11:00 EW 202

Discontinuity of the loss function at large momentum transfers in graphite. — ●RALF HAMBACH^{1,2}, CHRISTINE GIORGETTI¹, FRANK ORTMANN², KARSTEN HANNEWALD², FRANCESCO SOTTILE¹, APOSTOLOS G. MARINOPOULOS³, FRIEDHELM BECHSTEDT², and LUCIA REINING¹ — ¹Laboratoire des Solides Irradiés, CEA-CNRS UMR 7642-Ecole Polytechnique, 91128 Palaiseau Cedex, France and European Theoretical Spectroscopy Facility (ETSF), Palaiseau, France — ²IFTO, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — ³Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA

The loss function of graphite was studied for momentum transfers q beyond the first Brillouin zone. Surprisingly, near Bragg reflexes, the spectra are highly dependent upon very small changes in q , which reminds the non-analyticity of the loss function in the optical limit ($q \rightarrow 0$). The effect is investigated by means of first principle calculations within the random phase approximation (RPA). We find crystal local field effects to be crucial and propose a simple 2×2 model dielectric function.

HL 11.2 Mon 11:15 EW 202

Optical properties and electronic structure of size- and shape-selected nanodiamonds — ●LASSE LANDT¹, KATHRIN KLÜNDER¹, TREVOR WILLEY², TONY VAN BUUREN², JEREMY DAHL³, ROBERT CARLSON³, THOMAS MÖLLER¹, and CHRISTOPH BOSTEDT¹ — ¹Technische Universität Berlin, Germany — ²Lawrence Livermore National Laboratory, USA — ³MolecularDiamond Technologies, USA

Diamondoids can be considered the smallest possible cage-like subunits that can be excised from diamond lattice closing the gap between large hydrocarbon molecules and nanodiamonds. Diamondoids are fully sp^3 -hybridized and show no surface reconstruction due to full hydrogen-passivation.

The optical and electronic properties of perfectly size- and structure-selected, neutral diamondoids ranging in size from 0.5 to 1 nm have been determined by means of PES, XAS, and optical absorption measurements. All data were taken from high purity samples in the gas phase revealing optical gap and band edges with near theoretical purity. We find that the optical properties of the perfectly size- and shape-selected nanocrystals exhibit strong shape dependence unlike band edges or ionization potentials which have also been determined. The observed isomeric dependencies of the optical gap will be discussed and first experimental data on the influence of targeted surface modification (e.g. thiols, alcohols) will be presented.

HL 11.3 Mon 11:30 EW 202

Molecular doping and pseudo Landau levels in graphene — ●TIM WEHLING and ALEXANDER LICHTENSTEIN — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

Controlling graphene's density of states near the Fermi level is crucial for future applications based on this material. Two mechanisms related to this goal will be addressed, here. Firstly, we present a joint experimental and ab-initio theoretical investigation of adsorbate induced doping of graphene. A general relation between the doping strength and whether or not adsorbates are open- or closed- shell systems is demonstrated with the NO_2 -system: The single, open shell NO_2 molecule is found to be a strong acceptor, whereas its closed shell dimer N_2O_4 causes only weak doping. This effect is pronounced by graphene's peculiar density of states (DOS), which is ideal for chemical sensor applications. We explain the recently observed [Schedin et. al., Nat. Mater 6, 652 (2007)] NO_2 single molecule detection.

In addition, we present first principles calculations on midgap states in corrugated graphene: Rippling induces pseudomagnetic fields leading to the formation of flat bands near the Fermi level — so-called pseudo-Landau levels. Especially, the chiral zero-energy pseudo-Landau level gives rise to specific real space signatures like full sublattice polarization and related sublattice stripes observable in any experiment probing the local electronic structure.

In collaboration with A. Balatsky (LANL), A. Geim (U. Manchester), M. Katsnelson (U. Nijmegen) and K. Novoselov (U. Manchester).

HL 11.4 Mon 11:45 EW 202

Synthesis and investigation of iron-filled carbon nanotubes as probes for magnetic force microscopy — ●UHLAND WEISSKER, THOMAS MÜHL, ALBRECHT LEONHARDT, CHRISTINE TÄSCHNER, SIEGFRIED MENZEL, FRANZISKA WOLNY, CHRISTIAN MÜLLER, and BERND BÜCHNER — Leibniz Institute for Solid State and Material Research IFW, Dresden

Magnetic force microscopy is a powerful method for imaging magnetic stray fields of magnetic surfaces with high spatial resolution. For magnetic force microscopy a conventional atomic force microscopy tapping mode cantilever is coated with a magnetic layer that interacts with the sample stray field. Using this kind of probes the rather complicated pyramid shape of the probe influences the measurement results. Because of that, a straightforward quantitative interpretation of MFM data is hardly possible. On the other hand, quasi one-dimensional ferromagnetic wire-shaped probes should allow quantitative stray field measurements.

One promising solution is the use of iron-filled carbon nanotubes as scanning tip. The filled nanotubes offer a high aspect ratio, good mechanical properties and are magnetic. We report a chemical vapour deposition method (CVD) for fabrication of in-situ filled carbon nanotubes, which exhibit a long continuous iron-filling of several microns. The nanotube structure is investigated by SEM and TEM, whereas the filling is examined by AGM, XRD and EELS.

HL 11.5 Mon 12:00 EW 202

Scratching Multilayer Graphene with an Atomic Force Microscope — ●PATRICK BARTHOLD, THOMAS LÜDTKE, and ROLF J. HAUG — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover

The atomic force microscope (AFM) is a well known tool used for structuring devices on different materials. Besides others, one way is to scratch the surface and thus create insulating lines. We used this technique on thin graphite films. In situ measurements of the resistance while the sample was mounted and electrically contacted in the AFM show an astonishing reversible change in the resistance when the sample was scratched with a diamond coated tip. After moving the tip several times across the sample the resistance changes permanently. We contribute the reversible effect to induced and then moving defects in the graphite, whereas the irreversible change indicates that different layers have been cut through.

HL 11.6 Mon 12:15 EW 202

Ab initio calculation of the lattice dynamics of graphene nanoribbons — ●ROLAND GILLEN, MARCEL MOHR, JANINA MAULTZSCH, and CHRISTIAN THOMSEN — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

During the past decades, graphite-related materials of nanoscale, such as fullerenes and nanotubes, have been subject to scientific interest. Their remarkable optical and electronic properties make them promising for use in future nanotechnology. Recently, another type of nanoscale materials, narrow stripes of graphene (single layer graphite) have been fabricated and were investigated regarding their electrical transport properties. Those graphene nanoribbons are, depending on the direction of their edges, classified into armchair (AGNR), zig-zag (ZGNR) and chiral nanoribbons (CGNR). They correspond to "unrolled" carbon nanotubes, i.e. the model system used in zone-folding calculations of carbon nanotube properties. We use DFT calculations to obtain the band structure and phonon dispersion of various AGNR and ZGNR. Group theory was applied to classify the resulting phonon modes. We show that most of the phonon modes can be interpreted as "overtones" of a few fundamental modes. These overtone frequencies can be understood from zone folding the phonon dispersion of graphene. Shape and size dependences of the phonon frequencies of the nanoribbons are found. Similarities between nanoribbons and carbon nanotubes will be discussed.

HL 11.7 Mon 12:30 EW 202

Phonon symmetries of carbon picotubes — ●NILS ROSENKRANZ¹, MARÍA MACHÓN¹, RAINER HERGES², and CHRISTIAN THOMSEN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — ²Institut für Organis-

che Chemie, Christian-Albrechts-Universität Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

Picotubes are ring-shaped hydrocarbons closely related to very short carbon nanotubes. They seem to be a promising starting point for the specific synthesis of nanotubes, which is one of the great goals in nanotube research. We identified the symmetries of all main modes in the Raman spectrum of semitrimer picotubes by performing polarization-dependent Raman measurements on crystalline samples. Furthermore, the semitrimer molecule has been subject to ab initio calculations, the results of which agree excellently to the experimental data. By comparing experiment and theory, we can assign phonon eigenvectors to all main Raman peaks.

HL 11.8 Mon 12:45 EW 202

The intermediate frequency modes in the carbon nanotube Raman spectra — •MARTIN WEISS¹, HAGEN TELG¹, JANINA MAULTZSCH¹, VIERA SKÁKALOVÁ², and CHRISTIAN THOMSEN¹ — ¹Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Max Planck Institut for Solid

State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

The carbon nanotube Raman spectrum as it is commonly referred to consists of three features, the radial breathing mode (RBM), the high energy modes and the defect induced D mode. These modes are used to gain information on the diameter distribution, the presence of metallic tubes, the defect density and even the precise chiral indices (n_1, n_2) of the tubes in a nanotube sample. However, apart from these three modes the nanotube Raman spectrum contains features in the intermediate frequency range of which the scattering mechanism is not yet consistently understood. These modes in part result from second-order scattering and resemble the phonon density of states. Therefore, they can give information on the phonon dispersion of nanotubes and on Raman inactive modes. We performed resonant Raman measurements of the intermediate frequency modes (IFM) located between ~ 400 and ~ 1000 cm^{-1} . By comparing the resonance conditions of the IFMs and RBMs we assign the IFMs to certain groups of nanotubes (n_1, n_2) . Furthermore we discuss the dependence of the IFMs on excitation energy and their lineshapes with respect to the calculated phonon density of states.