CPP 43: New Materials

Time: Friday 10:30–12:15 Location: ZEU 114

CPP 43.1 Fri 10:30 ZEU 114

Electronic Properties of Conjugated Fullerenes using O-, NH-, or CH_2-Groups as Bridges — •Markus Reinmöller[1,2], Uwe Ritter[1], Erich Runge[2], and Wichard J. D. Beenken[2] — [1]Technische Universität Ilmenau, Institut für Physik, FG Chemie, Deutschland — [2]Technische Universität Ilmenau, Institut für Physik, FG Theoretische Physik I, Deutschland

We performed quantum-chemical calculations by DFT methods on C_{60} molecules connected by several conjugated bridges formed by –O– , –NH–, or $-CH_2-$ groups. For the optimized structure, we obtain regularly an inter-fullerene-bond (C–C) near the bridging group. Both together form furane-, pyrrole-, or cyclopentane-rings. These molecules were compared with oligo-fullerenes directly connected by two C–C bonds, i.e., where the bridge is cyclobutadien-like. All fullerenes conjugated in the described way exhibit highest occupied molecular orbitals (HOMOs) that are anti-binding regarding the π-system on the bridge. The lowest unoccupied molecular orbital (LUMO) is non-binding in this respect; whereas some unoccupied MOs higher in energy are found to be binding over the bridges and consequently delocalized over the whole chain. These states are of some interest for effective band-like electron transport in conjugated fullerenes. Therefore, we determined the energetics of the localized and delocalized MOs in dependence of the number of conjugated C_{60} molecules to examine the structure of an evolving conduction-band. Furthermore, we studied the optically excited states by time-dependent DFT in order to get some insights about possible photo-conduction.

CPP 43.2 Fri 10:45 ZEU 114

Resonant Raman Scattering on Chemically Functionalized Carbon Nanotubes — •Reinhard Meinke[1], Matthias Müller[1], Janina Maultzsch[1], Benjamin Gebhardt[2], Christian Thomsen[1], and Andreas Hirsch[2] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Zentralinstitut für Neue Materialien und Prozesstechnik, Universität Erlangen-Nürnberg, Germany

We present resonant Raman scattering on carbon nanotubes functionalized to various degrees of functionalization. From the resonance profiles of the radial breathing mode (RBM) we assign the chiral indices of the tubes [1] in order to study the reactivity as a function of tube species and diameter as has been observed for several reactants [2,3].

[1] J. Maultzsch et al., Phys. Rev. B 72, 205438 (2005). [2] M. Strano et al., Science 301, 1519 (2003). [3] M. Müller et al., phys. stat. sol. (b), 245, 1957 (2008).

CPP 43.3 Fri 11:00 ZEU 114

Towards understanding of C60-based nanowire growth with anomalous anisotropy — •Ilia Solov'yov[1], Junfeng Geng[2], Andrey Solov'yov[1], and Brian Johnson[2] — [1]Frankfurt Institute for Advanced Studies, Goethe University, Frankfurt am Main, Germany — [2]Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

The growth of one-dimensional (1D) nanocrystals is an important research topic in crystal engineering for nanotechnology. In a recent study, we demonstrated that exceptionally long fullerene nanowires, with a length-to-width aspect ratio as large as ˜3000, can be grown from 1,2,4-trimethylbenzene solution of C60.

We perform a thorough theoretical and experimental analysis, aimed to explain the exceptionally large aspect ratio of C60-based nanowires. By accounting for different interactions in the system we have calculated the structure of the unit cell and determined the role of the fullerene and of the solvent molecules in the crystallization process of the nanowire. We have calculated the adhesion energy of C60 molecules to the nanowire surface and demonstrated that it is related to the anisotropy of the crystal.

To get a more in-depth understanding of the nanowire growth mechanism we have also considered the influence of electron polarization on the anisotropy of the C60-based nanowires and studied the possible polymerization reactions in the system, which likely occur between the C60 and the solvent molecules in the nanowire.

CPP 43.4 Fri 11:15 ZEU 114

Intercalated fullerene polymers and Raman spectroscopy - Vibrations and more? — •Markus Reinmöller[1], Thomas Wågberg[2], and Bertil Sundqvist[2] — [1]Ilmenau University of Technology, Institute for Physics, Department of Chemistry, Ilmenau, Germany — [2]Umeå University, Institute for Physics, Department of Nanophysics and Material Science, Umeå, Sweden

We have synthesised very homogeneous samples from two-dimensional intercalated fullerene polymers in the chemical compositions of Li4C60 and Na4C60. On both samples we performed Raman measurements with a He-Ne-laser from 300 K to 480 K.

In the temperature studies we analysed the temperature dependence of selected Raman active modes. The results can be compared to values from several other fullerene polymers [1]. A qualitative evaluation of the heat transport properties can be accomplished by a variation of the laser light intensity. From our analysis we deduced the temperature dependence of characteristic modes and explain differences between the materials by the unequal bonding types [2].

In our Raman studies of Li4C60 at elevated temperatures we find two different regimes. From the transition of these regions the initiation of depolymerisation can be estimated.

Raman spectroscopy is a powerful tool and we show that it can be used in an indirect and maybe uncommon way to learn more about materials.

[1] A. V. Talyzin et al., Sol. State Comm., 140 (2006) 178.

[2] S. Margadonna et al., J. Am. Chem. Soc., 126 (2004) 15032.

CPP 43.5 Fri 11:30 ZEU 114

Designed Polymer-Metal nanocomposites: On the use of colloidal polymer templates — •Stephan V. Roth[1], Gerd Herzog[1,2], Adeline Buffet[1], Sebastien Couet[1], Rainer Gehrke[1], Ralf Röhlsberger[1], Andre Rothkirch[1], Kai Schlage[1], Wilfried Wurth[2], Gunar Kaune[3], Volker Körstgens[3], Robert Meier[3], Ezzeldin Metwalli[3], and Peter Müller-Buschbaum[3] — [1]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Inst. f. Exp.Phys., Univ. Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — [3]TU München, Physik-Department Lehrstuhl E13, James-Franck-Str. 1, D-85747 Garching, Germany

Polymer-metal nanocomposites are important materials for data storage, optical and electronic technologies. In combination with the wide variety of nanostructures offered by polymer materials in thin film technology, new routes for tailoring such nanocomposite devices are possible. Especially the use of colloidal nanoparticles is very attractive for magnetic data storage by ordering the colloidal nanoparticles. In our route to produce new colloidal polymer-metal nanocomposites, we combine the advantages of ordering colloidal thin films, polymer material characteristics and sputter deposition, leading to order on multiple length scales, from metal nanoparticle to large-scale domains. To understand the build-up of these multiple length scales, we use microbeam grazing incidence small angle x-ray scattering. We investigate IN-SITU the growth kinetics of magnetic and non-magnetic metals on colloidal polystyrene thin films as a function of the template treatment and present the resulting different growth regimes.

CPP 43.6 Fri 11:45 ZEU 114

A Novel Lipid-Polyelectrolyte Composite Structure on Polyelectrolyte Multilayer Coated Colloidal Particles — •Edwin Donath[1], Irina Estrela-Lopis[1], Luis Cuellar[1], Martin Fischlechner[2], and Sergio Moya[3] — [1]Institute of Medical Physics and Biophysics, 04107 Leipzig, Härtelstrasse 16/18, Germany — [2]Nanoscience Centre, Cambridge, United Kingdom — [3]CICBIOMAGUNE, San Sebastian, Spiain

Polyelectrolyte multilayers from poly(diallyl dimethyl ammonium chloride) PDADMAC and poly (styrene sulfonate) were formed on silica particles. Then unilamellar lipid vesicles containing mixtures of acidic and zwitterionic lipids were added to the multilayer coated particles. While with other multilayer coatings not containing PDADMAC this resulted usually in the deposition of a lipid bilayer, we observed in the presence of PDADMAC a unique structural transition of the multilayer induced by the interaction with and the subsequent adsorption of lipids into the multilayer. The resulting structure showed a 3D-distribution of circular inhomogeneities on scales ranging from nanometers to microns. These inhomogeneities were identified by a different softness probed with AFM. Otherwise the surface was surprisingly smooth. FTIR linvestigations revealed the special properties of water near the quarternary ammonium groups which was subsequently replaced by lipids. We believe, this is beside electrostatic interaction one of the driving forces for the very strong interaction. The composite polyelectrolyte film on the particles shows unique transport properties and may find interesting applications as a novel material.

CPP 43.7 Fri 12:00 ZEU 114

Multi-responsive hybrid colloids based on gold nanorods and poly-(NIPAM-co-allyl-acetic acid) microgels: temperature- and pH-tunable plasmon resonance — MATTHIAS KARG[1], ENRIQUE CARBÓ-ARGIBAY[2], ISABEL PASTORIZA-SANTOS[2], JORGE PÉREZ-JUSTE[2], LUIS LIZ-MARZÁN[2], and •THOMAS HELLWEG[1] — [1]Universität Bayreuth, Physikalische Chemie I, Universitätsstrasse 30, 95447 Bayreuth, Germany — [2]Universidade de Vigo, Departamento de Quimica Fisica, 36310 Vigo, Spain

This work describes the reversible changes of the optical properties of multiresponsive organic/inorganic hybrid particle colloids, which consist of a thermoresponsive poly-(NIPAM-co-allylacetic acid) microgel core and gold nanorods adsorbed to their surface. These composites combine the interesting optical properties of the rod-shaped gold particles – exhibiting two distinct pronounced plasmon modes – with the sensitivity of the microgel toward external stimuli, such as temperature or solution pH. We show here that the collapse of the microgel core, induced by changes in either temperature or pH, enhances the electronic interactions between gold nanorods on the gel surface, as a result of the subsequent increase of packing density derived from the reduced surface of the collapsed microgel [1]. These interactions lead to remarkable redshifts of the longitudinal plasmon resonance, which can be as large as 50 nm.

[1]. Karg, I. Pastoriza-Santos, J. Perez-Juste, T. Hellweg, L. M. Liz-Marzan, Nanorod-coated PNIPAM microgels: Thermoresponsive optical properties. Small 2007, 3, 1222.