

image the vibrational and electronic properties of single-walled carbon nanotubes with a spatial resolution of down to 10nm, limited only by the tip diameter [1,2]. Local perturbations along an individual nanotube, as well as energetic coupling between different nanotubes can thereby be directly observed, revealing the interaction of phonons and excitons with the nanotube structure and its environment.

- [1] A. Hartschuh et al., *Nano Lett.* 5, 2310 (2005)
 [2] N. Anderson et al., *Nano Lett.* 7, 577 (2007)

DS 18.38 Tue 14:30 Poster A

Vibrational Study of Free-Base Tetraphenylporphyrin Films
 — ●SIMONA DORINA POP, DANA MARIA ROSU, KARSTEN HINRICHS, and NORBERT ESSER — ISAS-Institute for Analytical Sciences, Department Berlin, Albert-Einstein Str. 9, D-12489, Berlin, Germany

The vibrational structure of the vacuum deposited free-base meso-tetraphenylporphyrin (H₂TPP) films on silicon substrates is investigated by infrared spectroscopic ellipsometry. The dielectric function of the H₂TPP films is determined in the mid-infrared energy range. The H₂TPP films exhibit a uniaxial structure in agreement with the results obtained by spectroscopic ellipsometry performed in the visible energy range. The orientation of the H₂TPP molecules on silicon substrates as well as the thickness dependence of the IR dielectric function are analyzed. The assignment of the observed vibrational bands is performed with the help of density functional theory method.

DS 18.39 Tue 14:30 Poster A

Application of Raman Spectroscopic Techniques in the Characterization of Nanostructured Semiconductors and Semiconductor Microstructures — ●DIMITRA PAPADIMITRIOU — National Technical University of Athens, Faculty of Applied Sciences, Department of Physics, GR-15780 Athens, Greece

Applications of Raman spectroscopic techniques in basic and applied research studies are reviewed. Emphasis is given to the characterization of structural phases, phase-transformation, and nanometric scale effects in nanostructured semiconductors by Raman and the validation of strain-stress effects in semiconductor microstructures by micro-Raman Spectroscopy. In particular: a) applications of combined Raman scattering and photoluminescence emission techniques in the determination of the pressure dependence of the energy band-gap and the transformation pressure of nanocrystalline (porous) silicon under high hydrostatic pressure are presented [1], b) applications of the Raman selection rules in the structural characterization of light emitting silicon quantum wires are discussed [2], and c) the relevance of micro-Raman techniques for the characterization of elastic strain in porous silicon microstructures is demonstrated [3].

References: [1] D. Papadimitriou, Y.S. Raptis and A.G. Nassiopoulou, *Phys. Rev. B* 58(21), 14089, (1998). [2] D. Papadimitriou and A.G. Nassiopoulou, *J. Appl. Phys.* 84(2), 1059 (1998). [3] D. Papadimitriou, C. Tsamis, A. Nassiopoulou, *Sensors and Actuators B: Chemical* 103(1-2), 356 (2004).

DS 19: Organic Interfaces (SYSA 6)

Time: Wednesday 14:30–17:30

Location: H 2013

Invited Talk

DS 19.1 Wed 14:30 H 2013

Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry — ●I. STICH^{1,2}, M. KONOPKA¹, R. TURANSKY¹, J. REICHERT³, N. L. DOLTSINIS⁴, H. FUCHS³, and D. MARX⁴ — ¹Slovak Tech. Univ. (FEI STU), Slovakia — ²Inst. of Phys., Slovak Acad. of Sci., Slovakia — ³Uni. Muenster, Germany — ⁴Ruhr-Uni. Bochum, Germany

Different methods of activation of chemical reactions are compared for organometallic nanojunctions. The study is based on density functional theory simulations. First we provide a comparison of thermal activation with mechanical activation, or mechanochemistry. Study of thiolate/copper junctions and interfaces provides evidence for vastly different reaction pathways and products. The differences are understood in terms of mechanical manipulation of coordination numbers and system fluctuations in the process of mechanical activation. Next we compare photo- and mechanochemistry. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. We study azobenzene optomechanical switch which combines photo excitation with external pulling force to manipulate optical switching properties of the azobenzene molecule anchored to gold tips by thiolate bonds. We focus on the separation between ground (S₀) and first excited (S₁) singlet states. We observe a pronounced dependence of the S₀-S₁ separation on the applied strain. Furthermore we find that ground-state mechanochemistry alone can be used to achieve switching. For instance, mechanochemistry with modest applied forces leads to cis -> trans reversion.

DS 19.2 Wed 15:00 H 2013

Self-Assembled Monolayers of Azo-based molecular switches — ●ANDREI SHAPORENKO¹, MARK ELBING², ALFRED BLASZCZYK², VIOLETTA FERRI³, CHRISTIAN GRAVE³, GIUSEPPINA PACE⁴, CARSTEN VON HÄNSICH², MARCEL MAYOR^{2,5}, PAOLO SAMORÌ⁴, MARIA ANITA RAMPI³, and ●MICHAEL ZHARNIKOV¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany — ²Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, D-76021 Karlsruhe, Germany — ³Dipartimento di Chimica, Università di Ferrara, I-44100 Ferrara, Italy — ⁴Institut de Science et d'Ingénierie Supramoléculaires / CNRS UMR 7006 -Université Louis Pasteur, F-67000 Strasbourg, France — ⁵Department of Chemistry, University of Basel, CH-4056 Basel, Switzerland

Two conjugated rod-like aromatic azo-compounds differing by molecular conformation (planar vs. twisted) and required free volume (upon assembly) have been synthesized. While the first compound forms

tightly packed self-assembled monolayers (SAMs) on coinage metal substrates with a high degree of ordering, the second one packs more loosely giving less ordered films. However, independent of the package density, both compounds show very high yields of photoisomerization in SAMs, which are close to 100%. This result questions the common belief that isomerization in SAMs of azo-compounds can only be achieved efficiently, when enough free volume is available in the monolayer. We conclude that azo units incorporated in rigid molecular rods can be of potential interest in molecular electronic devices for applications such as switchable devices and high density data storage.

DS 19.3 Wed 15:15 H 2013

Structural and optical properties of self-organized surface structures on rubrene single crystals — ●RAINER STÖHR¹, GARETH BEIRNE², PETER MICHLER², JÖRG WRACHTRUP¹, and JENS PFLAUM¹ — ¹Physikalisches Institut, Univ. Stuttgart, Germany — ²IHFG, Univ. Stuttgart, Germany

On the surface of rubrene single crystals high hole mobilities up to 15 cm²/Vs have been observed making this material interesting for organic device applications. However, the optical properties of rubrene single crystals are yet barely analysed.

We present first structural and optical studies on sublimation grown rubrene single crystals with self-organized pyramidal microstructures on the (001) surfaces. From OMBD growth at various conditions we conclude on the stabilization mechanisms of these crystallographically aligned structures.

Measuring the time- and locally-resolved micro-photoluminescence at various positions on the structured rubrene (001) surface, four peaks could be identified in the wavelength range between 500nm and 900nm. The generated microstructures on the crystal surface enhanced the peak intensities by up to an order of magnitude. A clear dependence between structure size and enhancement could be shown. The results are carefully discussed by assigning these peaks to various exciton species with respect to studies currently reported in literature [1].

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- [1] H. Najafov *et al.*, *PRL* 96, 056604 (2006)

DS 19.4 Wed 15:30 H 2013

Monitoring the crystallization process of nano-confined organic molecules — ●SILVIA MILITA¹, CHIARA DIONIGI², FRANCESCO BORGATTI², WILLIAM PORZIO³, ADINA LAZAR², ROBERTO FELICI⁴, DIDIER WERMILLE⁴, and FABIO BISCARINI² — ¹CNR -IMM, Via Gobetti 101, I-40129 Bologna, Italy — ²CNR -ISMN, Via Gobetti 101, I-40129