

## HL 47: New Materials: mainly thermoelectric and nanomechanical Properties

Time: Wednesday 16:00–17:15

Location: H14

HL 47.1 Wed 16:00 H14

**Coulomb gap variable range hopping in graphitized polymer surfaces** — ●YURI KOVAL, IRINA LAZAREVA, and PAUL MÜLLER — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

Polymer surfaces were graphitized by low-energy ion irradiation. We show that the conductance of the graphitized surfaces gradually increases with the energy of ions and the temperature of irradiation. At rather modest ion energies ( $\sim 1000$  eV) and irradiation temperatures ( $\sim 400^\circ\text{C}$ ) the transition to a metallic state was observed. We investigated electric transport on the insulating side of metal-insulator transition (MIT). Temperature dependences of conductance and current-voltage characteristics (IVs) at low temperatures were measured and analyzed. We found that electric transport in the graphitized surfaces can be described by 2D Coulomb gap variable range hopping. Similar to low-temperature results in crystalline 2D systems, the pre-factor is temperature independent and has a unique value  $e^2/h$ . In the activationless regime of hopping, the pre-factor of IVs has a significantly smaller but also unique value  $\sim e^2/5h$ . We show that the localization length is constant for all samples. The dielectric constant gradually increases approaching MIT from the insulating side. Due to an extremely high bare density of states, the Coulomb gap persists up to high temperatures. We explain this by a strong inhomogeneity of density of states in the graphitized surfaces.

HL 47.2 Wed 16:15 H14

**Type-I clathrate compounds as thermoelectric materials** — ●CHRISTOPHE CANDOLFI, UMUT AYDEMIR, NIELS OESCHLER, MICHAEL BAITINGER, YURI GRIN, and FRANK STEGLICH — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

In the last decade, huge efforts were devoted to improve the thermoelectric properties of intermetallic clathrates. Their crystal structures are composed of face-condensed polyhedral cages in which metal cations are situated. Cage compounds represent a promising class of material for thermoelectric applications at high temperatures since they usually feature a low thermal conductivity and chemical stability up to 900 K. By changing the chemical composition, the charge carrier concentration can be tuned with the aim at achieving high thermoelectric figure of merits. Here, we present and discuss how this can be realized in some type-I clathrates in the system  $\text{Ba}_8\text{M}_x\text{Ge}_{46-y}$  (where M is a transition metal) both in the high and low temperature ranges (2 - 700 K).

HL 47.3 Wed 16:30 H14

**Thermoelectric properties and electronic structure of  $\text{NiTsn}$  ( $T = \text{Ti, Zr, Hf}$ ) Heusler compounds.** — ●S. OUARDI<sup>1</sup>, G. H. FECHER<sup>1</sup>, B. BALKE<sup>1</sup>, G. STRYGANYUK<sup>1</sup>, C. FELSER<sup>1</sup>, and E. IKENAGA<sup>2</sup> — <sup>1</sup>Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — <sup>2</sup>Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan

Heusler compounds with 1:1:1 composition attracted attention as potential candidates for thermoelectric applications. Complex  $C1_b$  compounds such as  $\text{NiTiSn}$  are promising n-type thermoelectrical materials. In the present study we have used stoichiometric doping of such compounds to investigate its influence on the transport properties. Our

work focuses on a systematic investigation of pure  $\text{NiTsn}$  systems and the substituted derivatives  $\text{NiT}_{1-x}\text{T}'_x\text{Sn}$  ( $T, T' = \text{Ti, Zr, and Hf}$ ). The  $C1_b$  structure was verified for all compounds by powder X-ray diffraction. The effect of electron- or hole- doping was studied by electrical conductivity, Seebeck coefficient, and thermal conductivity measurement in the temperature range from 2 K to 300 K using a physical properties measurement system (PPMS). The electronic structure - in particular of the valence band - was studied by photoelectron spectroscopy excited by hard X-ray synchrotron radiation at BL-47XU of SPring-8 (Japan). All experimental findings are well supported by first principle calculations of the electronic structure.

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HL 47.4 Wed 16:45 H14

**Modeling Nanomechanical Quality Factors** — ●QUIRIN UNTERREITHMEIER, THOMAS FAUST, and JÖRG KOTTHAUS — Fakultät für Physik and Center for NanoScience (Cens), Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany

The study of nanomechanical resonant motion is a rapidly advancing field of science with prospects in fundamental science and application. For many aspects, a low mechanical friction (or equally high quality factor) is advantageous. However, the dominant damping mechanism is yet to be known. We present studies on silicon nitride resonators under high tensile stress having high mechanical quality factors. Applying a damping model based on continuum mechanics that assumes a homogeneous friction throughout volume of the resonator, we are able to quantitatively model the quality factors observed in the (room-temperature) experiments.

HL 47.5 Wed 17:00 H14

**Crossover between Type II and Type I Alignment in Layered Hybrid Assemblies of CdSe and CdTe Nanocrystals** — ●ANDREAS PÖSCHL<sup>1</sup>, DIETER GROSS<sup>1</sup>, CHRISTIAN MAUSER<sup>1</sup>, ANDREI SUSH<sup>2</sup>, ANDREY ROGACH<sup>2</sup>, ENRICO DA COMO<sup>1</sup>, and JOCHEN FELDMANN<sup>1</sup> — <sup>1</sup>Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität, München, Germany — <sup>2</sup>Department of Physics and Materials Science, City University of Hong Kong, Kowloon, Hong Kong

Semiconductor nanocrystals (NCs) feature variable band gaps controlled by the quantum confinement. Reducing the size of the NCs increases the band gap. This effect is used to tune layered assemblies of CdSe and CdTe NCs between charge separation and energy transfer processes. Considering the bulk energy levels, CdSe and CdTe exhibit a type II interfaces alignment. Previously, we have shown that assemblies of large CdSe NCs and CdTe NCs provide charge separation processes, investigated by photoluminescence (PL) quenching. In this work the size of the CdSe NCs is varied. Increasing the band gap of the CdSe NCs from 2.4 to 2.7 eV yields a transition from type II to type I interface with CdTe NCs of 2.1 eV band gap. Because of the unfavorable alignment for charge transfer, energy transfer processes from the CdSe to the CdTe NCs are observed by PL spectroscopy. The use of smaller CdTe NCs with 2.2 eV band gap restores the type II alignment. These optical investigations demonstrate a facile method to probe the crossover from type II to type I in NCs assemblies and therefore the relative band alignment.