HL 33: New materials

Time: Wednesday 16:45–17:45 Location: H15

HL 33.1 Wed 16:45 H15

Study of the Ba giant dipole resonance in Ba_8Si_{46} with non-resonant inelastic x-ray scattering — •Sternemann Henning[1], Sternemann Christian[1], Tse John S.[2], Desgreniers Serge[3], Vankó György[4], Schacht Andreas[1], Soininen Juha Aleksi[5], and Tolan Metin[1] — [1]Dept. Phys. / DELTA, University of Dortmund, D-44221 Dortmund — [2]Dept. Phys. & Engn. Phys., University of Saskatchewan, Canada — [3]Dept. Phys., University of Ottawa, Canada — [4]ESRF, Grenoble, France — [5]Div. X-ray Physics, Dept. Physical Sciences, University of Helsinki, Finland

Atomic Ba shows a giant dipole resonance arising from collective $4d$ electron motion above the energetic threshold of the $N_{IV,V}$ edges. We will present the first experimental observation of the Ba resonance in the complex silicon clathrate network of Ba_8Si_{46}. The measurements were done at different momentum transfers using non-resonant inelastic x-ray scattering. The giant resonance spectra were modeled within the time-dependent local density approximation using a real-space multiple-scattering approach. The resulting spectra show very good agreement with the experiment. Separate calculations for $Ba@Si_{20}$ and $Ba@Si_{24}$ demonstrate the sensitivity of the resonance concerning the local environment of the Ba atom. Thus, a combined study of absorption edges and the fine-structure of the giant resonance by means of non-resonant inelastic x-ray scattering yields the possibility to study electronic and structural changes in pressure-induced phase transitions of the clathrate simultanously. The experimental setup for such studies will also be presented.

HL 33.2 Wed 17:00 H15

Interstitial Mn in Si: half-metallic heterostructures studied by density-functional theory — Hua Wu[1,2], •Peter Kratzer[3], and Matthias Scheffler[2] — [1]II. Physikalisches Institut, Universität zu Köln, D-50973 Köln, Germany — [2]Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany — [3]Fachbereich Physik, Universität Duisburg-Essen, D- 47048 Duisburg, Germany

Adding magnetic functionality to the most common semiconductor, Si, is in its infancy. So far, research on Mn-doped Si has concentrated on substitutional Mn (Mn_{sub}) as done for Mn-doped GaAs and Ge, although Mn_{sub} impurities in Si are energetically less stable than interstitial Mn (Mn_{int}). In this work, we investigate the role of Mn_{int} impurities for ferromagnetism in Si, and propose a novel type of heterostructures with Mn_{int} δ-doping. Using density-functional theory within the generalized gradient approximation, we show that Si-based heterostructures with 1/4 layer δ-doping of Mn_{int} are half-metallic. For Mn_{int} concentrations of 1/2 or 1 layer, the δ-doped heterostructures still display a high spin-polarization of conduction electrons, about 85% and 60%, respectively. The proposed heterostructures are more stable than previously assumed δ-layers of Mn_{sub}. Contrary to widespread belief, the present study demonstrates that interstitial Mn can be utilized to tune the magnetic properties of Si, and thus provides a new clue for Si-based spintronics materials.

HL 33.3 Wed 17:15 H15

Coupling Phenomena of Surface Plasmons — •Stephan Schwieger, Erich Runge, and Parinda Vasa — Technische Universität Ilmenau, Institut für Physik, Fachgebiet Theoretische Physik I, Postfach 100565, 98684 Ilmenau

Surface plasmons on an array of nanometer-sized metal wires, which is embedded in a multilayer system, are studied numerically. We investigate the coupling of different plasmonic modes as well as the coupling of plasmonic modes with light. These couplings influence fundamental properties of the excited surface plasmons as e.g. theire life time and details of their dispersion relation. We discuss the dependence of these couplings on the geometry of the nano-wire arrays as well as on the dielectric proporties of the adjescent layers.

HL 33.4 Wed 17:30 H15

Strukturelle und thermoelektrische Eigenschaften von epitaktischen IV-VI-MBE-Schichten legiert mit Zinn — •Jan König[1], Joachim Nurnus[2], Armin Lambrecht[1] und Harald Böttner[1] — [1]Fraunhofer Institut für Physikalische Messtechnik, Heidenhofstr. 8, 79110 Freiburg, Deutschland — [2]Micropelt GmbH, Emmy-Noether-Staße 2, 79110 Freiburg, Deutschland

IV-VI Halbleiterverbindungen sind bekannte Materialien mit hervorragenden thermoelektrischen Eigenschaften bei Temperaturen um 700K. Durch die Verwendung von Mischkristallen können die thermoelektrischen Eigenschaften durch eine Reduzierung der thermischen Leitfähigkeit mittels Legierungsstreuung optimiert werden. Außerdem kann durch Mischkristalle die Bandlücke für die thermoelektrische Anwendungstemperatur hin optimert werden. Dieses Konzept wird seit vielen Jahren an Massivmaterialien erprobt. Jedoch bestehen nur sehr wenige Daten über Dünnschichthalbleiter. Daher wurden mittels MBE mit Zinn legierte IV-VI-Schichten hergestellt. Es wird über die strukturellen (SEM-, EDX- und FT-IR Untersuchungen) und die thermoelektrischen Eigenschaften (Seebeck-Koeffizient- und Hall-Effekt-Messungen für Ladungsträgerkonzentration, Beweglichkeit und elektrische Leitfähigkeit) dieser Schichten berichtet. Zusammen mit der Bestimmung der thermischen Leitfähigkeit parallel zu Schichtebene wurde eine komplette thermoelektrische Qualifizierung erreicht.