

MM 14: Materials for Storage and Conversion of Energy IV

Time: Monday 16:45–18:00

Location: C 264

MM 14.1 Mon 16:45 C 264

Pressure Induced Oscillating Band-gap Variation in KBaTeSbO6 : Towards Transparent Solar Cell — ●MANASA GATTAVADI BASAVARAJAPPA¹, DIWAKAR SINGH², and SUDIP CHAKRABORTY¹ — ¹Harish-Chandra Research Institute, Chhatnag Road, Jhansi, Prayagraj, India 211019 — ²University of Duisburg-Essen, Essen, North Rhine-Westphalia, Germany

Recently, double oxide perovskites have emerged as a group of promising materials for wide range of applications due to their unique electronic and optical properties. There has been substantial studies establishing the fact that employment of external stimuli such as pressure on these materials may lead to drastic change in their properties, further enhancing their usefulness.

In this work, we have studied various pressure-induced structural, electronic and optical properties in an extended double oxide perovskite, KBaTeSbO6. Our study reveals the occurrence of band-gap tuning via blue shift followed by a red shift in KBaTeSbO6 with external pressure. This transition leads to modified electronic properties. We observed distinct structural changes under pressure such as lattice compression, distortion and phase transition. Our results indicate that the pressure-induced changes in band structure and lattice parameters directly affects the optical properties, resulting in altered absorption and reflection spectra. In order to validate the realisation of the material, we have also studied the formation and thermodynamic stability of the material under various pressure.

MM 14.2 Mon 17:00 C 264

Unveiling the Electronic and Structural Properties of Phosphonium- Based Perovskites: A First Principle Study Using Density Functional Theory — ●ARIJEET SARANGI and SUDIP CHAKRABORTY — Harish-Chandra Research Institute, Chhatnag Road, Jhansi, Prayagraj, India 211019

Phosphonium-based perovskites have emerged as promising materials for various electronic and optoelectronic applications due to their unique electronic and structural properties. In this study, we present a comprehensive investigation into the electronic and structural characteristics of phosphonium-based perovskites, aiming to shed light on their potential for enhancing device performance. Through DFT calculations, we explore the crystal structure, band gap engineering, charge transport, and optical properties of these materials. Our results provide valuable insights into the electronic band structure, density of states, and effective mass of charge carriers in phosphonium-based perovskites, enabling a deeper understanding of their optoelectronic behavior. Additionally, we explore the influence of defects and doping on the electronic properties and discuss their impact on device performance. Our findings provide valuable insights into the fundamental understanding of phosphonium-based perovskites, paving the way for their application in thin film solar cells, optoelectronic devices, and other emerging technologies. This study contributes to the ongoing research efforts towards harnessing the full potential of phosphonium-based perovskites and advancing the field of perovskite materials for sustainable energy solutions.

MM 14.3 Mon 17:15 C 264

Investigation of varied doping mechanism on the thermoelectric properties of pyrite FeS₂ — ●ANUSTUP MUKHERJEE and ALASKA SUBEDI — CPHT, Ecole Polytechnique. Institut Polytechnique de Paris, Palaiseau, France - 91120

Pyrite FeS₂ is an earth-abundant, nontoxic sulphide mineral with semiconducting behaviour. Hence, it has been investigated for various energy applications, including thermoelectrics using experiments and theoretical studies. Large values of thermopower have been observed at room-temperature. However, there exists a discrepancy in the magnitude and sign of thermopower reported in the literature depending on the nature of sample. Co-doped FeS₂ samples show similar varia-

tions in the magnitude of room-temperature thermopower. Therefore, it is of immense importance to examine the intrinsic thermopower of self- and Co-doped FeS₂ systems. We have investigated the electronic structure, magnetism and thermoelectric transport properties of these systems using first-principles calculations. We have implemented three different doping schemes, namely explicit Co-substitution, jellium doping and electron addition within the rigid band approximation (RBA) picture to understand electron doping in FeS₂. The former two doping schemes take structural modification and charge screening into consideration which is absent in the simpler RBA method. The thermopower is overestimated within the RBA picture, however the room-temperature thermopower observed is under 50 μ V/K for all the doping schemes, suggesting that electron doped FeS₂ is not a good candidate for thermoelectric applications.

MM 14.4 Mon 17:30 C 264

Ab-initio study of doping in silicon carbide — ●ZAHRA RAJABZADEH and LORENZ ROMANER — Department of Materials Science, Montanuniversität Leoben, Roseggerstraße 12, 8700 Leoben, Austria.

The wide band gap semiconductor SiC is an outstanding material for high-power electronics, e.g. for inverter applications in electric cars.. Although SiC is generally doped with elements such as N or Al, the fundamental properties of these point defects are still not understood.

We use density functional theory (DFT) calculations to investigate the impact of dopants on SiC properties focusing on the most relevant polytypes 3C, 6H, 4H and 2H. Calculations are carried out with the Vienna Ab- initio Simulation Package (VASP). We employ the PBE exchange-correlation functional with and without van der Waals (vdW) corrections as well as the HSE06 hybrid functional. First, we present results where a nitrogen or aluminum atoms are placed inside the crystal structure for different polytypes and the formation energy for different dopants are discussed. Then we will discuss binding energy for (N, Al) co-doping configurations. Furthermore, we explore concentration effects which allow studying the impact of non-stoichiometry on the formation energies. The results for all defects are analyzed also in terms of the electronic structure including band gaps and projected density of electronic states. Finally, we discuss nitrogen solubility to understand how much nitrogen can dissolved in SiC.

MM 14.5 Mon 17:45 C 264

A direct observation of the influence of nitrogen-doping on ion dynamics for electric double layer capacitor performance — ●HENRY R. N. B. ENNINFUL^{1,3}, MARIUS HERMESDORF², DESIRÉE LEISTENSCHNEIDER², MARTIN OSCHATZ², ALEX FORSE³, and RUSTEM VALIULLIN¹ — ¹Universität Leipzig — ²Friedrich-Schiller-Universität Jena — ³University of Cambridge, UK

Substantial improvements in the design of Electric Double Layer Capacitors (EDLC) have led to increased performance in both power and energy densities. To obtain comparable energy densities to those of batteries, electrode materials functionalized with nitrogen have been produced to yield very high specific capacitances and energy densities.

The mechanisms that underlie the improved capacitances due to electrode-electrolyte surface interactions is still rarely understood. This work sheds light on ion transport and mobility at the pore surface and within the pore interior. We show that for carbon electrodes synthesized from cellulose and potassium carbonate, increased melamine content leads to a sacrifice of the pore surface area and volume, resulting in reduced specific capacitances. Furthermore, the substitution of melamine with urea in the same ratio produces reduced nitrogen content in the resulting material. The effect thereof, is an attendant reduction in specific capacitance regardless of the comparable surface area. Lastly, we show that electrodes with a certain threshold of nitrogen content are able to store ions from a pure water *electrolyte*. The phenomena resulting in the produced performances are explained and future prospects in this work are shown.