Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Tuesday, December 20th 2016 - 14:00
CFEL Seminar room I (Bldg. 99)

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Ab initio modeling of perovskite materials and two-dimensional organic networks

Perovskite materials with stoichiometry ABX_3 are a rich family of ionic compounds with many technological interesting properties. They can be traditional inorganic, metal per- ovskites or hybrid perovskites with one organic cation. In this talk I want to discuss some results of a special modification of the latter kind, the so-called layered perovskites. This family of structures is currently rediscovered, and we report on the geometrical and electronic structure of one promising candidate ($(C_6H_5C_2H_4NH_3)_2PbI_4$) with phenethylammonium cations on the A-site and compare the differences towards the benchmark case of three-dimensional (3D) hybrid perovskites, CH_3PbI_3. The influence of varying the cation as well as changing the dimensionality from 3D to 2D systems is discussed by comparing bulk and monolayer structures of both systems. In addition, insight into the optical behavior and the observed electron-phonon coupling will be given.

As a second topic, I would like to present some work on the multiferroic $BiFeO_3$, a material of high technological potential, which significance in electronics is currently limited by the lack of successfully p-doped modifications. Investigating a broad set of possible dopants, we clarify the doping mechanism and identify best suited target metals for substitutional cation doping.

Furthermore, we study the influence that oxygen vacancy formation has on such doped $BiFeO_3$ materials and vice versa.

Last, some interdisciplinary work on the surface assisted, controlled synthesis of two-dimensional networks via bottom-up synthesis from designed, small organic precursors will be presented. The experimentally observed electronic structure is analyzed and explained based on theoretical results, focusing on the changes induced by increasing the dimensionality from 0D monomers over 1D structures towards extended 2D networks.

Host: Angel Rubio

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