Point native defects and p-type conductivity of ZnRh2O4: a first principles study — Oksana Volmińska1,2 and Piotr Bogusławski1,2 — 1Institute of Physics PAS, al. Lotnikow 32/46, 02-668 Warsaw, Poland — 2Institute of Physics, Kazimierz Wielki University, 85-064 Bydgoszcz, Poland

Transparent conducting oxides are the subject of active current research in the context of applications in semiconductor devices and photovoltaics. ZnRh2O4, with the band gap of about 2.2 eV, is a member of this class. It crystallizes in the spinel structure, and exhibits a p-type conductivity. Using the density functional theory within the generalized gradient approximation we calculated the electronic structure and formation energies of point native defects in ZnRh2O4 (vacancies, interstitials, and antisites). In the oxygen-rich conditions, there are two defects with formation energies lower than 1 eV, and therefore expected to occur at high concentrations, namely the zinc vacancy and the zinc antisite. Both defects are shallow acceptors that can be responsible for the observed p-type conductivity of ZnRh2O4. Formation energies of the remaining defects exceed 3 eV, and thus they are not expected to affect properties of ZnRh2O4.

Supported by EU within European Regional Development Fund through grant Innovative Economy (POIG.01.03.01-00-159/08, "InTechFun").

HL 80.1 Thu 11:45 H15

HL 80.2 Thu 12:00 H15

Importance of oxygen vacancies for the two dimensional metallic state at the surface of SrTiO3 — Juan Shen, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We analyze by means of density functional theory (DFT) the electronic structure of various oxygen-deficient (SrTiO3)x surface slabs. We find a significant surface reconstruction after introducing oxygen vacancies and we show that the charges resulting from surface-localized oxygen vacancies -independently of the oxygen concentration- redistribute in the surface region and deplete rapidly within a few layers from the surface suggesting the formation of a two-dimensional electron system (2DES). We also investigate possible oxygen-vacancy clustering effects and discuss our results in the context of recent angle-resolved photoemission spectroscopy observations of a highly metallic 2DES at the (001) vacuum-cleaved surface of SrTiO3.

HL 80.3 Thu 12:15 H15

Towards ion beam synthesis of single CdSe nanocrystal quantum dots in a SiO2 matrix — Hans Moritz Mangold1, Jörg B. Kinzel1, Helmut Karl2, Hubert J. Krenn1, and Achim Wixforth3 — 1Emmy Noether Group at Lehrstuhl Experimentalphysik I, Universität Augsburg, Augsburg, Deutschland — 2Lehrstuhl Experimentalphysik IV, Universität Augsburg, Deutschl — 3Lehrstuhl Experimentalphysik I, Universität Augsburg, Deutschland

II-VI compound semiconductor quantum dots (QDs) are a promising class of materials for applications in optical devices in the visible spectral domain. Here we show that in addition to traditional fabrication techniques such as molecular beam epitaxy or chemical synthesis, high fluence ion-beam implantation followed by a rapid thermal annealing step, can be readily applied to synthesize CdSe nanocrystals with superior optical properties within the thermal oxide on a Si wafer. In order to confine the implantation volume we employ chromium masks with arrays of nanoscale aperture openings with diameters smaller than 250 nm. We analyzed the such implanted and annealed samples by scanning electron microscopy and micro-photoluminescence spectroscopy. We observe a pronounced broadening and blue shift of the nanocrystal emission when decreasing the aperture diameter to < 1000 nm. We attribute this behavior to a reduction of the mean nanocrystal size but increase of its size distribution. For the smallest aperture sizes used we observe a pronounced shell-filling behavior characteristic for single quantum dot nanoemitters.