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Native point defects and conductivity of $ZnRh_2O_4$: a GGA + U study[1] PIOTR BOGUSLAWSKI, OKSANA VOLNIANSKA, Institute of Physics PAS, Warsaw — $ZnRh_2O_4$ spinel belongs to the family of transparent conducting oxides, which are promising for applications in optoelectronic technology. To assess essential material properties, we analysed energy levels and formation energies of native point defects, i.e., vacancies (V), interstitials, and cation antisites in $ZnRh_2O_4$. Calculations were based on generalized gradient approximation (GGA) to the Density Functional Theory supplemented by the +U corrections. The value of U was treated as a free parameter, which allowed for the systematic study of the U-induced changes of the electronic structure. The experimental band gap of $ZnRh_2O_4$ is reproduced only when the +U term is imposed on both d(Rh) and p(O) orbitals, and the pronounced distortions of the oxygen sublattice are included. Zn:Rh is the dominant acceptor that can be responsible for the observed p-type conductivity in $ZnRh_2O_4$. The low formation energy of Zn:Rh can make the intentional n-doping difficult. In the O-rich conditions, the second important acceptor is V:Zn. The two dominant donors in Zn-rich and O-rich conditions are V:O and Rh:Zn, respectively. Growth conditions leading to the lowest concentrations of native defects were identified.

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