Ab initio study of ZnCoO diluted magnetic semiconductor and its magnetic properties

Auteur: Lardjane, S.; Merad, G.; Fenineche, N.; Billard, A.; Faraoun, H. I.

Abstract/Résumé : Transition metal-doped wide band gap semiconductors, such as ZnO, attract much attention due to the theoretical prediction that ZnO is a room temperature ferromagnetic semiconductor [1,2]. Very controversial experimental and theoretical papers have been published to discuss the origin of ferromagnetic ordering and the relevance of the Curie temperature (T-C) of Co-doped ZnO [3-5]. In order to get better insight, electronic structure of CoxZn1-xO magnetic semiconductor was investigated via first principle calculations. The generalised gradient approximations (GGA) and the GGA with Hubbard U correction (GGA + U) in the framework of density functional theory (DFT) have been used. Calculations are done for different doping concentrations to discuss the contribution of different atoms in magnetic moments and magnetic coupling. (C) 2012 Elsevier B.V. All rights reserved.

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