MATERIALS RESEARCHE SOCIETY (MRS), November 25-30, 2012

Ab initio study of the effect of oxygen vacancy on magnetism in Co doped ZnO

S. LARDJANE, G. MERAD, N. FENINECHE, H. I. FAROUAN, A. BILLARD

Abstract :

The effect of oxygen vacancy (VO) on the electronic and magnetic properties of ZnCoO was studied with first principle methods based on density functional theory (DFT). Calculations were performed, on a periodic 3×3×3 wurtzite supercell of ZnO which consists of 108 atoms with two Co ions substituted for two Zn atoms, using the generalized gradient approximation with Hubbard U correction method (GGA+U). We have studied the interatomic exchange interaction with and without VO for different configurations with different magnetic atom lattice arrangements. The total energies, electronic structures and magnetic moments were calculated for each configuration.

Key Words :

Magnetic properties; spintronic; II-VI.