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Electronic and magnetic properties of Cu-doped ZnO ANDREIA LUISA DA ROSA, LUNMEI HUANG, RAJEEV AHUJA, Uppsala University, Dept. of Physics, Box 530, SE-75121, Uppsala, Sweden — Diluted magnetic semiconductors have attracted attention in the past years, since they open the possibility for new devices with integrated magnetic, electronic and optical functionality. Among possible candidates ZnO is especially attractive, since it is a wide band gap material and is also piezoelectric. On the other hand, Cu and its oxides are non-magnetic, so magnetism coming from Cu clusters or precipitates can be ruled out. Although some experimental results confirm room temperature ferromagnetism in Cu-doped ZnO, other works have reported its absence. In this work we use first-principles calculations to study Cu-doped ZnO for various Cu concentrations. The total energy differences were computed for parallel and antiparallel arrangements of the Cu spins to determine whether Cu-doped ZnO has a ferromagnetic or anti-ferromagnetic ground state. We found that Cu-doped ZnO has a ferromagnetic ground state for all calculated concentrations. We also found that the exchange coupling between the Cu atoms is short ranged. We suggest that the strong hybridization between the Cu-3d and O-2p states is responsible for mediating the ferromagnetic interaction between the Cu atoms.

Andreia Luisa da Rosa
Uppsala University, Dept. of Physics, Box 530, SE-75121, Uppsala, Sweden

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