

The Effect of Hydrogen on the Magnetic Properties of ZnO: A Density Functional Tight Binding Study

Authors : M. A. Lahmer, K. Guergouri

Abstract : The ferromagnetic properties of carbon-doped ZnO (ZnO:CO) and hydrogenated carbon-doped ZnO (ZnO:CO+H) are investigated using the density functional tight binding (DFTB) method. Our results reveal that CO-doped ZnO is a ferromagnetic material with a magnetic moment of 1.3 μ_B per carbon atom. The presence of hydrogen in the material in the form of CO-H complex decreases the total magnetism of the material without suppressing ferromagnetism. However, the system in this case becomes quickly antiferromagnetic when the C-C separation distance was increased.

Keywords : ZnO, carbon, hydrogen, ferromagnetism, density functional tight binding

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