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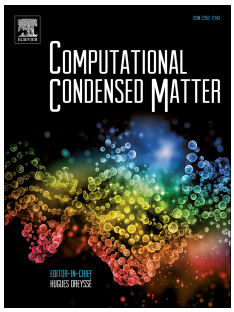

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First principle calculations with SIC correction of Fe-doped CuO compound

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ABSTRACT

In this work, the electronic properties of Fe-doped CuO ($Cu_{1-x}Fe_xO$) thin films are studied by using a standard density functional theory (DFT). This approach is based on the ab-initio calculations under the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA). We carried out our investigations in the framework of the general gradient approximation (GGA) and self-interaction-corrected (SIC). The density-of-states (DOSs) in the energy diagrams are presented and discussed. The computed electronic properties of the studied compound ($Cu_{1-x}Fe_xO$) confirm the half-metalicity nature of this material. In addition, the absorption spectra of the studied compound within the Generalized Gradient Approximation GGA, as proposed by Perdew–Burke–Ernzerhof (PBE) and GGA-PBE -SIC approximations are examined. When compared with the pure CuO, the Fermi-levels of doped structures ($Cu_{1-x}Fe_xO$) are found to move to the higher energy directions. To complete this study, the effect of Fe-doping method in CuO has transformed the material to half-metallic one. We found a high wide impurity band in two cases of approximations LDA and SIC methods.

Keywords: *Ab-initio calculation; Fe-doped CuO; KKR-CPA; GGA; SIC correction; Half-metalicity.*