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A theoretical study on native point defects and dopants in cuprous oxide WEICHAO WANG, DANGXIN WU, QIMING ZHANG, Department of Physics, University of Texas at Arlington, MENG TAO, Department of EE, University of Texas at Arlington — We have performed a first-principle study on the electronic structures, atomic configurations, and formation energies of native point defects in cuprous oxide, i.e. vacancies(V_{Cu}, V_O), interstitials (Cu_i, O_i) and antisite defects (Cu_O, O_{Cu}) by using Density Function Theory based VASP package with PAW potentials. We have carefully studied the formation of native point defects under different chemical environments and Fermi level positions. We have also calculated the electronic structures of dopants such as F, Cl, N, Ca and Mg in the cuprous oxide crystal. Their formation at different chemical environments and Fermi level positions will be presented as well.

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