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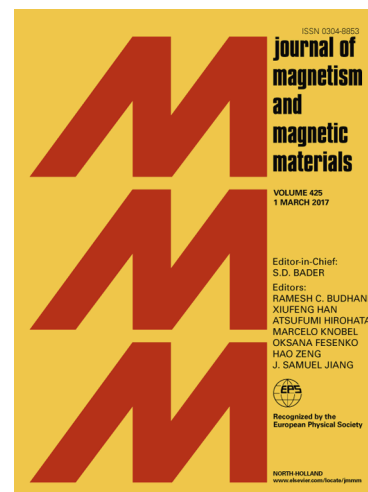
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Point defects induced magnetism in CdO monolayer: A theoretical study

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Abstract

We studied the influence of various point defects such as vacancy, antisite and impurities at different ionic sites in CdO monolayer through the electronic and magnetic properties using density functional theory. Vacancy defect such as Cd, O, Cd/O, antisite defects Cd ↔ O and extrinsic B, C, and N impurity elements are considered in CdO monolayer. The thermodynamic stability of pristine CdO monolayer is studied using phonon band dispersion and that of CdO monolayer with defect is studied in terms of the formation energy. The oxygen vacancy defect O_v introduces the indirect band gap of 1.4eV while Cd/ O_v showed the metallic behavior. Further, Cd_v and Cd/ O_v vacancy defects showed the onset of ferromagnetism with 2.0 μ_B and 1.21 μ_B magnetic moment, respectively. In contrast, the direct band gap nature of CdO monolayer is persistent against antisite defects and also no magnetic behavior is observed. The extrinsic B and C doped CdO monolayer showed half-metallic behavior, whereas N doped CdO monolayer showed semiconducting nature. These extrinsic dopants showed the onset of ferromagnetic ordering with 0.98 μ_B , 1.99 μ_B and 0.99 μ_B magnetic moments for B_O, C_O, and N_O defects in CdO monolayer.

Keywords: Oxide semiconductor; CdO; monolayer; defects; magnetism; nonmetal.

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