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Title: Structural and electronic properties of MgxCd1-xO: A first-principles study

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First-principles calculations are performed to study structural and electronic properties of MgxCd1-xO alloys within the framework of density functional theory implementing CRYSTAL code. The MgxCd1-xO alloys with x=0.25,0.5 and 0.75 are constructed following the supercell approach considering the rocksalt structure. Coupling total energy calculations with Murnaghan equation of state, the structural parameters are obtained under equilibrium conditions. The computed lattice constants are found to follow Vegards?s law. The bulk modulus increases from CdO to MgO. We perform calculations to evaluate cohesive energy of the alloys. To compute electronic band gap, electronic band structure calculations for the three compositions of alloys are performed. All alloys have direct band gap. The evolution of electronic density of states in alloys is also discussed.