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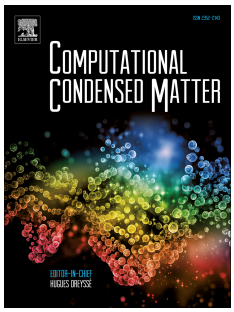

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Ferromagnetism induced by Cr, V single and double impurities doped BN from Ab-initio and Monte Carlo study

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Abstract

Using the Ab initio calculations and Monte Carlo (MC) simulations, we investigate the electronic and magnetic properties of cubic BN compound doped and co-doped with Chrome (Cr) and Vanadium (V) atoms. The calculated band electronic structure and density of states (DOS) of doped BN with single and double impurities can induce localized edge states around Fermi level, leading from semiconductor to half-metal transition. Thereafter, the stability of ferromagnetic (FM) ordering and disordered local magnetic moment (DLM) configurations has been explored. The interesting Curie temperature (T_c), magnetization and Susceptibility results for the various concentrations of Chrome (Cr) and Vanadium (V) co-doped (doped) BN suggest a vast exploitation attention in spintronics applications.

Keywords: Ab initio calculations; Monte Carlo simulations; KKR-CPA; Curie temperature.