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First principles study of the electronic structure and phonon properties for Al and C-doped MgB_2 O. DE LA PEÑA-SEAMAN, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, R. HEID, K.-P. BOHNEN, Institut fuer Festkoerperphysik, Forschungszentrum Karlsruhe, Germany — We have studied the structural, electronic and lattice dynamic properties of the superconducting alloys Al and C-doped MgB_2 within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. For both systems the structural parameters were determined on the following ranges, $0 \leq x \leq 1$ for $Mg_{1-x}Al_xB_2$ and $0 \leq x \leq 0.4$ for $MgB_{2(1-x)}C_{2x}$, finding a very good agreement between the calculated structural parameters and experimental data. The complete phonon dispersion curves were calculated for selected Al and C-concentrations. The calculated phonon bands for MgB_2 using the LDA and GGA approximations are compared in detail with the experimental data available in the literature. The evolution of the full-dispersion curves are analyzed as a function of Al and C-concentration, specially the E_{2g}-phonon mode frequency. In agreement with the experimental observed behavior, we find strong renormalization of the E_{2g}-mode for both Al and C-doped MgB_2. Additionally, we found a strong reduction of the E_{2g}-band dispersion with the filling of the σ-band. This research was supported by CONACYT, México under Grant No. 43830-F.

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