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First principles study of Al and C-doped MgB_2: evolution of two gaps and critical temperature OMAR DE LA PEÑA-SEAMAN, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, ROLF HEID, KLAUS-PETER BOHNEN, Institut fuer Festkoerperphysik, Forschungszentrum Karlsruhe, Germany — We have studied the electron-phonon and superconducting properties of the $Mg_{1-x}Al_xB_2$ and $MgB_{2(1-x)}C_{2x}$ alloys within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloys. For both systems, the Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated in the two band model (σ,π) for several concentrations until $x(\mathrm{Al}) = 0.55$ and $x(\mathrm{C}) = 0.175$. Using the calculated $\alpha^2_{ij}F(\omega)$ and a diagonal expression for the Coulomb pseudopotential matrix, μ^*, we solved numerically the Eliashberg gap equations in the two band model without interband scattering. We reproduce the experimental decreasing behavior of $\Delta_\sigma(x)$, $\Delta_\pi(x)$, and $T_c(x)$ for both alloy systems. The role of the interband scattering in the observed behavior of the superconducting gaps and T_c in the Al- and C-MgB_2 alloys is discussed. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

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