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Electronic structure of scandium-doped MgB_2 OMAR DE LA PEÑA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico., STEFANO AGRESTINI, ANTONIO BIANCONI, Department of Physics, University of Roma, Italy. — Recently has been reported the synthesis of a new superconducting alloy based on MgB_2, where Mg is partially substituted with Sc. In order to analyze the effect of Sc doping on the structural and superconducting properties of $Mg_{1-x}Sc_xB_2$, we have performed a detailed study of the electronic structure for this new diboride. The calculations have been done using the first-principles LAPW method, within the supercell approach for modeling the doping. In this work we report results for the electronic band structure, Fermi surface, and density of states. The effect of the Sc-d orbitals on the structural and electronic properties of $Mg_{1-x}Sc_xB_2$ is analyzed. Increasing the Sc concentration (x) the σ-band is gradually filled, because Sc have one valence electron more than Mg. Interestingly, the analysis of the band structure shows that even for ScB_2 the top of the σ-band remain above the Fermi level, nevertheless the σ-band presents high dispersion and has an important contribution of d states. In this way, in addition to the band filling effect, Sc doping gradually reduces the two-dimensional character of the σ- band in $Mg_{1-x}Sc_xB_2$ as a result of increasing the sp(B)-d(Sc) hybridization. This research was partially supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grant. No. 43830-F

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