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Lattice dynamics and electron-phonon coupling on $Mn_{1-x}Fe_xSi$: effect of magnetism[1] PAOLA GONZALEZ CASTELAZO, OMAR DE LA PEA SEAMAN, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute for Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the electronic, lattice dynamics, and electron-phonon (e-ph) coupling properties of the $Mn_{1-x}Fe_xSi$ alloy. This system have been analyzed within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. In particular, the electronic density of states (DOS), the full-phonon dispersion, as well as the electron-phonon coupling (λ) and the phonon linewidth (γ) have been calculated with and without the inclusion of spin polarization. While for FeSi is very well known that the effects of magnetism on the lattice dynamics are observed trough the phonon linewidths for specific regions on the zone boundary, on MnSi such detail analysis has not been addressed so far. Thus, the evolution of phonon frequencies and linewidths as a function of Fe-content are presented and discussed in detail, paying special attention the effect of spin-polarization on such properties for the magnetic region on the phase diagram $x < 0.16$.

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Paola Gonzalez Castelazo
Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP)

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