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First principles study of the electron-phonon coupling on the light-actinides Ac-Th alloy: effect of spin-orbit coupling[1] OMAR DE LA PEÑA SEAMAN, ROMEO DE COSS-MARTINEZ, PAOLA GONZALEZ-CASTELAZO, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the electronic, lattice dynamics, and electron-phonon (e-ph) properties of the $Ac_{1-x}Th_x$ actinide alloy. This system have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The electronic density of states (DOS), the full-phonon dispersion as well as the Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling (λ) parameter have been calculated with and without the inclusion of spin-orbit coupling (SOC). For Ac the observed effects of SOC on $\alpha^2F(\omega)$ are very minor. However, as Th-content increases on the alloy the SOC influence is more important. Such evolution has its roots on a continuous increase of density of states at the Fermi level ($N(E_F)$) difference between schemes, as well as a steady hardening of the SOC full phonon dispersion. The evolution of λ as a function of Th-content for both schemes is presented and discussed on the light of SOC effects on the electronic and vibrational properties.

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