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The electron-phonon coupling and superconductivity for light-actinides on fcc structure: a first principles study[1] OMAR DE LA PEÑA-SEAMAN, PAOLA GONZÁLEZ-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 structure, lattice dynamical properties, electron-phonon (e-ph) coupling and superconducting properties of the light-actinides (Ac, Th, Pa, U) on fcc structure. These systems have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method. The electronic density of states (DOS), 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). The observed effects of SOC on $\alpha^2F(\omega)$ for the light-actindes under study have its roots on the changes of two quatities: the full phonon dispersion and the e-ph coupling matrix elements. The observed influence of these two ingredients is different depending of the actinide, and it is analyzed together with the contribution of the different states on the DOS at the Fermi level. The superconducting critical temperature (T_c) has been analyzed solving numerically the Eliashberg gap equations on the strong-coupling regime with the information provided from $\alpha^2F(\omega)$ for the entire series, analyzing the superconducting behavior of the light-actinides.

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