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Importance of strong-correlation on the lattice dynamics of light-actinides Th-Pa alloy[1] 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 structural, electronic, and lattice dynamics of the $Th_{1-x}Pa_x$ actinide 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 energetics is analyzed as the ground-state crystal structure is changed form fcc to bct, as well as the electronic density of states (DOS), and the phonon frequencies. Such properties have been calculated with and without strong correlations effects through the LDA+U formalism. Although the strong-correlation does not influence on a great manner the Th properties, such effects are more important as the content increases towards Pa, affecting even the definition of the ground-state crystal structure for Pa (experimentally determined as bct). The evolution of the density of states at the Fermi level ($N(E_F)$) and the phonon frequencies as a function of Pa-content are presented and discussed in detail, aiming to understand their influence on the electron-phonon coupling for the Th-Pa alloy.

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