ABSTRACT

This work has applied density functional theory (DFT) based calculations to investigate the structural and vibrational properties of $FeMnP_{1-x}A_x$ (A= Si, Se, Sn and In, x = 0.33) within the first-principles pseudopotential technique. The exchange correlation potentials were treated within generalized gradient approximation (GGA), in the Quantum ESPRESSO code. The Perdew, Burke, Ernzerhof (PBE) functional as implemented in Vanderbilt's ultra-soft pseudo potential (USPP) was used for all the calculations. Vibrational properties were calculated using phonopy code with 1 × 1 × 2 supercell of the conventional unit cell. Thermodynamic properties were predicted using the phonon density of states. The dependence of lattice thermal conductivity on temperature was determined using Debye theory. The optimized structural parameters and corresponding graphical values fit within available experimental data and other theoretical reports. There were no imaginary phonon modes in the phonon dispersion curves revealing that these materials are dynamically stable for magnetic refrigeration.

Keywords: Fe_2P-type materials magnetic refrigeration density functional theory phonons quantum ESPRESSO thermodynamic