ABSTRACT

The structural, electronic and mechanical properties of Re doped $FeMnP_{0.67}A_{0.33}$ (A= Ga and Ge) were examined by use of density functional theory (DFT) within the generalized gradient approximations as demonstrated in Quantum ESPRESSO code. The optimized structural parameters as well as derived lattice parameters are in consistent with other computational and achievable experimental results. The computed independent elastic constants confirm the mechanical stability of the investigated materials. The computed Poisson's and Pugh's ratios as well as Cauchy pressure, verify that $FeMn_{0.67}Re_{0.33}P_{0.67}Ga_{0.33}$ is the most ductile among the studied compounds. The calculated values of bulk modulus, shear modulus and Young's modulus confirm high values of bond strength, hardness and stiffness of the investigated materials respectively. Therefore, the four compounds considered may be appropriate for industrial applications. The results report that $FeMn_{0.67}Re_{0.33}P_{0.67}Ga_{0.33}$ compound is more ductile and mechanically stable compared to other investigated compounds. This is the first qualitative computational prediction of the elastic properties of $FeMnP_{0.67}Ge_{0.33}$, $FeMnP_{0.67}Ga_{0.33}$, $FeMn_{0.67}Re_{0.33}P_{0.67}Ge_{0.33}$ and $FeMn_{0.67}Re_{0.33}P_{0.67}Ga_{0.33}$ compounds and this awaits experimental ratification. The calculated electronic density of states confirms that the Re_2*p* states are located in the conduction band (CB) in the unite cell while Re_3*d* dominate the CB in the supercell. Results from the doped compounds could not be compared with experimental or computational findings because to the best of our knowledge, this has not been done.

Keywords: DFT, doping, ductility, electronic density of states, mechanical stability, and elastic constants.