

Abstract

Hexagonal Fe₂P-type magnetocaloric materials have been attracting a lot of research interest lately as a result of their promising application in magnetic refrigeration. These materials work under repeated magnetic and thermal cycles which results to large local strains in the polycrystalline samples and so they need to be mechanically stable across the phase transition. Hence, there is a need to conduct extensive investigations in order to obtain materials which may have better performance in magnetic refrigeration. In this study the elastic properties of FeMnP_{1-x}A_x (A= Si, Se, Sn, In, x = 0.33) were investigated using first principles density functional theory within the generalized gradient approximations as expressed in Quantum Espresso code. The work conclusively shows that FeMnP_{0.66}In_{0.33} has the highest Poisson's ratio, Pugh's and machinability index hence most ductile of the selected materials. Moreover, it had the highest anisotropic ratio further proving that of the four compounds, it is the most suitable for sustainable operation as a magnetocaloric refrigerant.