Abstract

Magnetic properties of stable iron-based compounds (FeMnP1-xAx (A = Si, In, Se and Sn) were investigated by use of Quantum Espresso (QE) within the Density Functional Theory (DFT) formalism as a viable magnetic refrigerant. In this research work, DFT technique was the first principle theoretical approach that was employed along with the planewave pseudopotentials (ultrasoft), and the projected augmented wave (PAW) within the generalized gradient approximation (GGA) to describe the electronic structure and investigation of magnetic properties. Magnetic stability is described as the repeated magnetic performance of a material under specific conditions over the life of a magnet. In this case our reference compound, FeMnP0.67 Si0.33 was optimized and its properties were examined in both ferromagnetic (FM) and antiferromagnetic (AFM) states. Two Si atoms were later substituted with atoms of post-transitional metals in period four and five which has shown first-order magnetic transition at near room temperatures. In, Se and Sn were chosen to replace silicon since they would easily mimic the bond, their availability and nontoxic nature. The results showed that only ferromagnetic states of both host and doped compounds gave promising magnetic properties that can be applied in magnetocaloric effect phenomenon. Their band structure results indicated that they were all metals. Antiferromagnetic states showed no magnetic properties as the spin-polarized graph resulted in perfect symmetry of spin up projected density of states (PDOS) and spin down PDOS. From the thermo_pw calculations, it was realized that FeMnP0.67 In0.33 is the best candidate for near room temperature magnetic refrigeration among the studied compounds.

Keywords

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