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CoFeNbZ (Z=l, Si and In) quaternary heusler alloys: A first principle study

Heusler alloys are intermetallic compounds made up of four interpenetrating fcc sublattices. Some of them have multifunctional nature i.e. a combination of functions (properties) within the same compound, which have technological applications. Co-based Heusler compounds gained considerable attention in the recent past due to their high Curie temperature, high spin polarization and tunable electronic structure with possible applications in spintronics. They have the general composition X_2YZ where X and Y are transition metals and Z is an sp element. Quaternary Heusler alloys (QHA) are formed when one of the X atoms is replaced by a third transition metal. In this study, the structural, electronic, magnetic and transport properties of CoFeNbZ (Z=Al, Si and In) quaternary Heusler compounds are investigated employing the full potential linearized augmented plane wave (FP-LAPW) method implemented in WIEN2k code within the density functional theory prescription. The exchange and correlation effects are treated by using generalized gradient approximation (GGA). From the electronic and magnetic properties, it is found that CoFeNbAl is a half-metal with a spin flip gap of 0.33 eV and satisfies the $M_t=Z_t-24$ Slater Pauling rule. It is known that GGA underestimates the band gaps of semiconductors and insulators. Here, the Tran and Blaha modified Becke Johnson potential (TB-mBJ) is used to obtain accurate band gaps. The spin-flip gap increases to 0.34 eV with the use of TB-mBJ and the nature of gap changes from indirect to direct. The half-metallic gap in CoFeNbAl arises due to the complex hybridization between the d-states of transition metals Co, Fe, and Nb. CoFeNbIn has metallic behavior in both spin channels. CoFeNbSi is a near half-metal with a near integer magnetic moment. The effect of hydrostatic strain on the magnetic and half-metallic properties of CoFeNbAl is determined. The transport coefficients such as the Seebeck coefficient, electrical conductivity, and thermal conductivity are computed in combination with the second principles BoltzTraP code. In the spin-up channel, electrical conductivity decreases as a function of temperature whereas it increases in the spin down the channel for CoFeNbAl. This affirms the metallic behavior in the spin-up channel and the semiconducting behavior in the spin down channel. The high spin polarization and robustness of half-metallicity against hydrostatic strain make CoFeNbAl a potential candidate for spintronic applications.

Biography

Rita John is Professor and Head, Department of Theoretical Physics, University of Madras, Chennai, India. She is Visiting Professor on Fulbright Fellowship at the Department of Physics and Astronomy, Texas Christian University, Fort Worth, Texas, USA (2014). Her area of research includes Computational/Theoretical Condensed Matter Physics. She has published over 50 papers in peer-reviewed journals. The book titled 'Solid State Physics' authored by her and published by Tata McGraw Hill publisher (2014) is used by Physics graduate students globally. She has edited and published 4 other books on advanced topics in Physics. She has also authored a book titled '*Science uncovers the signature of God*' highlighting the scientific facts recorded in the Holy Bible. She is the recipient of various awards and prizes for her academic contributions.

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