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Lattice dynamics, mechanical stability and electronic structure of Fe-based Heusler semiconductors

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The structural and mechanical stability of Fe_2TaAl and Fe_2TaGa alloys along with the electronic properties are explored with the help of density functional theory. On applying different approximations, the enhancement of semiconducting gap follows the trend as GGA < mBJ < GGA + U. The maximum forbidden gaps observed by GGA + U method are $E_g = 1.80$ eV for Fe_2TaAl and 1.30 eV for Fe_2TaGa. The elastic parameters are simulated to determine the strength and ductile nature of these materials. The phonon calculations determine the dynamical stability of all these materials because of the absence of any negative frequencies. Basic understandings of structural, elastic, mechanical and phonon properties of these alloys are studied first time in this report.

Significant momentum in the study of intermetallic Heusler alloys has increased over the last decade as these systems exhibit numerous extraordinary capabilities in exposing the desired properties, extending from robust spin-polarization, half-metallic magnetism, magnetoresistance, shape memory effect, spin gapless semiconductor to giant magnetocaloric effect, phase transitions and thermoelectric effect[1–7]. The technological applications exploiting these properties have been achieved successfully. Spintronic and thermoelectric applications are the offshoots of half-metallic ferromagnetism (being castoff in spin injectors[8], spin filters[9], magnetic tunnel junctions[10], spin valves[11], random access memories[12]) and spin gapless attributes to the Seebeck effect useful for thermoelectric devices[13]. Within these dimensions, the materials with compatible lattice structure, high spin polarization and high Curie temperature are anticipated in practical spintronic applications. Magnetoelectronic devices mostly depend on the disproportionate number of majority and minority spin carriers, as exhibited ideally by half-metallic materials i.e. 100% spin polarization at the Fermi level. Such materials display the concoction properties of semiconductor and metal. Additional motive to delegate Heusler alloys in these applications is that these systems have the same crystallographic structure with different functional characteristics and some of them are even very close in electronic structure and composition[14,15]. Since the discovery of the NiMnSb Heusler alloy in 1983[16], a sequence of experimental as well as theoretical efforts (first principles simulations) were attempted to predict novel semiconductor or half-metallic systems. Among such compounds, transition metal based Heuslers have been widely investigated by material scientists worldwide. Predominantly, the Fe based Heusler structures constitute a vast family with semiconducting or half-metallic band profiles. For example, Fe_2YSi (Y=Cr, Mn, Fe, Co, Ni) alloys were experimentally synthesized and predicted to be half-metallic alloys[17]. Fe_2TiAl was reported to have thermoelectric applications[18]. Other materials like, Fe_2TiSi, Fe_2TiGe and Fe_2ZrSi[19], FeMnSi[20], FeVRuSi[21] and many more to report here have been investigated for their magnetic, semiconducting or mechanical properties. Using first-principle calculations, Fe_2YZ (Y=V, Ti, Nb, Zr, Ta, Hf and Z=Al, Ga, In, Sn, Ge, Si) Heusler compounds with room temperature power factors 4 to 5 times larger than classical thermoelectrics were reported recently by *Bilc et al.*[22]. However, a little information is available on the electronic structure, mechanical stability, phonon dynamics and bonding characteristics of Fe_2TaAl and Fe_2TaGa alloys. In addition, the untouched lattice dynamical parameters and phonon properties are necessary to understand the intriguing physical properties and hence in this work, we tried to investigate their structural and mechanical stability, electronic and lattice dynamical properties in detail.

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