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RESEARCH ARTICLE

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Predicting the electronic structure, magnetism, and transport properties of new Co-based Heusler alloys

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Summary

First-principle calculations on structural, electronic, magnetic, and transport properties of novel Co_2TaSi and Co_2TaGe Heusler compounds have been accomplished successfully. The structural optimizations and cohesive energies confirm the stability of these alloys in Fm-3m phase as well as deliver the equilibrium lattice parameters. Modified Beckhe Johnson scheme predicted more efficient results than the generalized gradient approximation in defining the electronic structure and ground state properties. From the band structure analysis and density of state calculations together with spin magnetic moments, half-metallic character is anticipated with an indirect spin-down gap of 0.84 eV for Co_2TaSi and 1.04 eV for Co_2TaGe. Seebeck coefficients and electrical conductivities are calculated to envisage the possible thermoelectric response of these materials.

KEYWORDS

electronic structure, half-metallic, magnetic materials, Seebeck coefficient

1 | INTRODUCTION

The perspective of advanced materials with enhanced properties has geared up the future technological developments in the field of spin/orbital electronics. The materials community therefore witnessed the central change in innovative designing and discovering of novel materials for smart device applications. A comprehensive increase in simulation power, along with algorithmic advances and developments in quantum theory, allows well-organized and precise quantum mechanical calculations. This helps to unlock the exit of computing the overall properties of a wide range of materials that once appeared prohibitively impossible. Massive material projects are progressively built within the commitment of characterization and knowledge extraction criteria, to identify potential candidates for future-generation technologies.[1,2] It is a well-established fact that the modification of the structural or electronic distribution in transition metal alloys via the chemical component substitution/doping leads to the production of new materials with magnificent and multifunctional properties.[3] From the last few decades, the Heusler materials have been an important topic for their potential usage in novel spin-based devices, thermoelectrics, spin filters, data storage devices, and so on. To achieve this, density functional theory (DFT) has proven to be a handy tool for the researchers worldwide.[4-7]

Heusler alloys have long been in demand for their interesting physical properties like half-metallicity,[8] high spin polarization at Fermi level,[9] ferromagnetism and large curie temperatures,[10] thermoelectric performance,[11] etc. With such spell-bound properties, they have emerged as a new class of smart materials. Such alloys have been investigated much decisively for the possible application in spintronics, magnetoresistive materials, spin valve generators, and memory devices.[12-15] Recently, Co_2TaX (X = Al, Ga, In) have been predicted to be half-metallic

