Optical and magnetic properties of some XMnSb and Co$_2$YZ Compounds: \textit{ab initio} calculations

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In present work, our research is mainly focused on the electronic structures, optical, and magnetic properties of XMnSb (X = Ni, Cu, Pd), Co$_2$YZ (Y = Ti; Z = Si, Ge, Sn), and Co$_2$YZ (Y = Mn; Z = Al, Ga, Si) Heusler compounds by using \textit{ab initio} calculations within the generalized gradient approximation. The calculations are performed by using the Vienna \textit{ab initio} simulation package based on the density functional theory. The band structure of these Heusler alloys for majority spin and minority spin were calculated and the majority spin states cross the Fermi level and thus have the metallic character, while the minority spin states open the band gaps around the Fermi level and thus have the narrow-band semiconducting nature. We also find that these Heusler compounds have the indirect band gaps in the minority spin channel. The real and imaginary parts of dielectric functions and hence the optical functions such as energy-loss function, the effective number of valance electrons and the effective optical dielectric constant for XMnSb and Co$_2$YZ compounds were also calculated. In addition, we also show the variations of the total magnetic moment per f.u. and minority spin gap width of these compounds with optimized lattice constants: minority spin gap width decreases with increasing the lattice constants.

1 Introduction The Heusler compounds is a ferromagnetic metal compounds based on a Heusler phase. They have interesting electronic and magnetic properties. Because of these properties, the Heusler compounds have attracted for the design of single-spin electron sources and spin injectors in the field of magneto-electronics and related technological applications [1, 2, 3]. The half-Heusler phases XYZ, comprising three interpenetrating fcc lattices, constitute an important class of materials with particular regard to their magnetic properties [4]. Ternary Heusler and half-Heusler compounds have the chemical formula X$_2$YZ or XYZ, where X and Y are transition or rare earth metals and Z a heavy element. In some cases, Y is replaced by a rare earth element [5]. Half-Heusler compounds XYZ, also called semi-Heusler compounds, crystallize in the MgAgAs-type structure (see Table 1), in the space group F-43 m [4].

NiMnSb, CuMnSb, and PdMnSb are member of the family of Heusler compounds. Otto et al. have investigated of the crystal structure the microstructure and the magnetic properties of the inter-metallic compounds NiMnSb and CuMnSb [6]. They have reported that magnetic properties show an effective paramagnetic moment which differs from the value corresponding to the saturation moment at 0 K. This effect is attributed to a decrease of the conduction electron spin polarisation at high temperature. PdMnSb compound is synthesized by Webster and Ziebeck [7]. In the present work, by means of a DFT approach we examined the series of Heusler alloys XMnSb and Co$_2$YZ assuming they crystallize in the typical C1$_1$ and L2$_1$ structures. For all these compounds we derived structural, mechanical, electronic, optical properties. Consequently, the primary purpose of this work is to provide some
2 Methodology  
The ab initio calculation based on DFT was used with the aid of the VASP [8, 9, 10] program. The exchange and correlation potentials were Perdew-Burke-Ernzerhof method [11] based on generalized gradient approximation (GGA). The plane wave cutoff energy in the wave vector K space was 500 eV. We have performed Brillouin-Zone integration by using 9 × 9 × 9 gamma centered special Monkhorst-Pack k-points [12]. The investigated properties of XMnSb and Co2YZ are calculated using the primitive cells (Z = 1). When the total energy was stabilized within 10⁻⁶ eV, the force acting on each atom of the cell after optimization was less than 0.001 eV Å⁻¹, the residual stresses of the cell was less than 0.001 GPa and the tolerance offset was less than 10⁻⁵. Therefore, it can be said that, XMnSb and Co2YZ compounds for considered structure are mechanically stable.

Isotropic bulk moduli, shear moduli, Young’s moduli, Poison’s ratios, B/G ratios, and Debye temperatures are calculated by using Voigt-Reuss-Hill approach [23, 24, 25]. The results are tabulated in Table S1 (in Supporting Information). It shows that the calculated values of bulk moduli, shear moduli, Young’s moduli of Co2YZ are higher than XMnSb. We note that the B/G values are all higher than 1.75. Therefore, the studied systems in all forms can be classified as ductile materials [26]. Our calculated values of Poison’s ratio vary from 0.27 to 0.40 for these compounds. Thus, indicating strong metallic contribution in the intraatomic bonding for these compounds.

3 Results and discussion
3.1 Crystal structures  
We have examined XMnSb and Co2YZ compounds with the half-Heusler and Heusler structure, respectively. First, a structural optimization was performed for these compounds to determine whether the experimental lattice parameter minimizes the total energy. The calculated equilibrium lattice constant, total energy, ground state volume, and total magnetic moments values are given Table 2. It was found that the optimized lattice parameter and magnetic moments from the calculation agrees very well with experimental values [6, 7]. Co2MnSi has the highest magnetic moment and Co2TiSn has the lowest one. We also show the variations of the total magnetic moment per f.u. and minority spin gap width of these compounds with optimized lattice constants: minority spin gap width decreases with increasing the lattice constants.

3.2 Mechanical properties  
The estimated independent elastic constants are tabulated in Table 3. To our knowledge, there are no experimental or theoretical data available for elastic constants except Co2MnSi. The calculated elastic constants satisfy Born criteria [20, 21, 22]. Therefore, it can be said that, XMnSb and Co2YZ compounds for considered structure are mechanically stable.
minority spin (spin-down) were calculated. The calculated band structures and total density of states are shown in Fig. 1 for Co$_2$TiZ ($Z$ = Si, Ge, Sn) compound (see Figs. S1 and 2 for XMnSb ($X$ = Ni, Cu, Pd) and Co$_2$MnZ ($Z$ = Al, Ga, Si) compounds in Supporting information). It is seen that for these compounds, the majority spin states cross the Fermi level and thus have the metallic and semimetallic characters, while the minority spin states open the band gaps around the Fermi level and thus have the narrow-band semiconducting nature.

3.4 Optical properties

We have first calculated the real and imaginary part of $\varepsilon'(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ complex dielectric function using the Kramers–Kroning relations [27]. The optical constant such as energy-loss function, the effective number of valance electrons and the effective optical dielectric constant have been calculated with the help of the real and imaginary part of dielectric function for these compounds. The obtained results showed manner similar to our recent works [28].

The energy values of $\varepsilon_1$ that decreasing $(d\varepsilon_1)/(d\varepsilon < 0)$ and increasing $(d\varepsilon_1)/(d\varepsilon > 0)$ are zero are 2.18 and 15.84 eV for Co$_2$MnAl compound, 6.60 and 20.92 eV for Co$_2$MnSi compound, and 2.28 and 22.00 eV for Co$_2$MnGa compound. These values that the $\varepsilon_1$ are zero are points reduced of the reflections, and show that the polarization disappears. The maximum peak values of $\varepsilon_2$ are 1.13, 2.28, and 7.28 eV for Co$_2$MnAl compound, 2.45, 8.40, and 11.10 eV for Co$_2$MnSi compound, and 1.30, 6.30, and 9.17 eV for Co$_2$MnGa compound. These values show how much the electromagnetic wave polarizes the system, and corresponds to the electronic transitions from the valance band to the conduction band. Furthermore, 0–1.3 eV, 0–0.6 eV, and 0–0.7 eV energy region for Co$_2$MnSi, Co$_2$MnAl, and Co$_2$MnGa compounds, respectively is the region where dispersion and transparency are low. This energy region corresponds to the region beginning of the transition between the bands. The 1.4–10 eV energy region for these compounds is the region where the transitions between the bands are very intense. The 2–10 eV energy region has reduced transitions between the bands. The energy region above 12 eV also corresponds to the collective vibration of valance electrons. This energy region defined as plasma oscillations is described by the energy loss function ($L$). The sharp maxima in the energy-loss function are associated with the existence of plasma oscillations (as an example see Fig. 2).

The optical data for XMnSb show that in the limit of infrared or visible region of the spectrum that has been studied the values of the real part of the dielectric constant lie near zero (as for Co$_2$YZ). This means that the negative contribution from the accelerating mechanism of absorption is quite small and is compensated by the positive contribution from the real and virtual interband transitions of electrons. Such a behavior of the $\varepsilon_1$ function indicates the low concentration of conduction electrons in XMnSb. The presence of a Drude component in the dielectric functions of X$_2$YZ ($L_2$ phase) permitted us to determine the parameters of free electrons-plasma frequency of conduction electrons $E_{pl} = 18.3$ eV and the effective number of free electrons $N_{eff} = 2.4 \times 10^{22}$ cm$^{-3}$. The low values of $N_{eff}$ indicate the formation of a pseudogap in the energy band spectrum of Co$_2$YZ. In the case of XYZ, the zero values of $\varepsilon_1$ prevent making corresponding estimates for $N_{eff}$. However, it is reasonable to explain the observed behavior of the dielectric

![Figure 1](https://example.com/figure1.png)

**Figure 1** Electronic band structure and total density of states of the Co$_2$TiZ ($Z$ = Si, Ge, Sn) compounds. Solid and dashed lines refer the spin-up and spin-down states, respectively. Find the figures for XMnSb and Co$_2$MnZ ($Z$ = Al, Ga, Si) compound in Supporting information (Figs. S1 and 2).
properties of XMnSb by the formation of a deeper pseudogap in the density of states as compared to Co$_2$YZ. Our results concerning the low-energy interband absorption indicate a weak “growing-in” of the gap in the density of states, which was predicted theoretically for the C1$_b$ phase of XMnSb. Thus, we can conclude that there occurs a loss of the half-metallic character of the energy band spectrum of XMnSb in the case of the vacancy-containing phase with the structure of the L2$_1$ type.

4 Conclusions In this work, we have investigated structural, mechanical, magnetic, electronic, and optical properties of some Co$_2$YZ and XMnSb Heusler alloys. The estimated lattice parameters are agreement with experimental data. The results of elastic constants reveal all compounds are mechanically stable. The traditional B/G ratio indicates that considered compounds possess ductile nature. The electronic structure calculations show that the majority spin states cross the Fermi level and thus have the metallic character, while the minority spin states open the band gaps around the Fermi level and thus have the narrow-band semiconducting nature. We also find that these Heusler compounds have the indirect band gaps $E_{g}$ in the minority spin channel. Finally, optical properties were studied. The relations of the optical properties to the interband transitions were also discussed.

Supporting Information Additional supporting information may be found in the online version of this article at the publisher’s web-site.

References