# Predict New Half Heusler Compound XZrZ (X=Ni, Cu and Z=C, B) Suitable for Thermoelectrical and Optical Application

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***Abstract*—**In the present work, we have studied the structural, magnetic, electronic and elastic properties of the Heusler alloys XZrZ (X = Ni, Cu, Z = C, B).For this purpose, we performed ab-initio calculations using first principle method based on (DFT), using the full potential linearized augmented plane wave (FP-LAPW), implemented in the Wien2k code. In order to determine these properties, we used the approximation of the generalized gradient (GGA) for the term of the exchange and correlation potential (XC).Both materials have a semi-conductor character; the NiZrC has a 0.18eV direct bandgap, and the CuZrB possesses a 0.27eV indirect bandgap, which helps these compounds to have a crucial figure of merit (ZT) value that is a function of temperature up to 1200K. Mainly, good thermoelectric performance requires a high Seebeck coefficient, high electrical conductivity, and low electronic thermal conductivity. Making these compounds promising candidates for thermoelectric applications. In addition, the optical dielectric function, the reflectivity, and the refractive spectra are performed.

***Index Terms*—** Half Heusler, Wien2k, Thermoelectric, Optical

## I. Introduction

The Half Heusler alloys don't cease to demonstrate their great interest in technology since the discovery of half Heusler compounds by German engineer Heusler in 1903 [1]. The domains most used of these materials: are magnetism [2], piezoelectricity [3], and spintronics [4], and they are also intriguing prospects for ecologically friendly and low-cost thermoelectric materials [5]. In recent years, numerous studies of thermoelectrical materials have revealed their great potential for thermal heat conversion into electrical energy [6]. A good thermoelectric material (TE) is preferably a narrow gap semiconductor or semi- conductor with high carrier mobility and low thermal conductivity [7]. In terms of measurable physical quantities, a ZT value equals one unit or above. Increasing the value of ZT is of great technological importance. Half-Heusler materials, with 18 and 8 valence electrons, have been studied and developed for various TE applications. Most of them should work efficiently at high temperatures (over 900 K). Recently, authors in Ref. [8] discovered that Half -Heusler materials have excellent thermoelectric properties [9,10]. The goal of this work is to provide a DFT investigation report on the stabilities, electronic, magnetic, optical, and thermal properties of the new half Heusler to determine their technological applications. The paper is ordered as follows: Sec. 2 shows all the calculated parameters and explains how they were calculated. Section 3 summarizes the results and discusses the alloy properties of these compounds. Sec. 4 summarizes the conclusions obtained as a result of the study.

The determinations of the structural, electronic, optical, and thermoelectric properties are achieved through the FP-LAPW method as implemented in WIEN2K package[11,12], considering the exchange-correlation. The unit cell is divided into two regions in the FP-LAPW method: one region is composed of non-spheres centered on each atom (muffin-tin spheres) of radius RMT, while the other region is comprised of the interstitial region between the spheres. The calculations are carried out by expanding the wave functions up to $l_{max}$ 10 within the muffin tin; yet in the interstitial region, the Fourier charge density has been expanded up to $G_{max}$ = 12 and in the Fourier series. Plane waves are limited *to* $R_{MT}.K_{max}$ = 8. The cut-off energy of —6 Ryd has been employed to separate the core and valence states and 12 × 12 × 12 k points were used for the numerical integration of the Brillouin zone. In this work, we obtained the Muffin-tin radii $(R_{MT})$ to be equal to 2.5, 2.2, 2.0 and 1.90 u.a (atomic unit) for Ni, Cu, Zr, C, and B, respectively. FurthermoreThese half heusler materials crystallize in the cubic structure with space group F4-3m(216).However, the subsequent study has demonstrated that the structure changes depending on the atomic position configuration, resulting in three different structure types: type α (4c;4b;4a), type β (4b;4a;4c), and type γ (4a;4c;4b). These materials are stable in the α phase where Zr occupied the single site 4a, Ni (Cu) occupied 4b site, and B/C occupied the 4c site.

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https://doi.org/10.17758/EARES16.EAP1223133

## II. Results and Discussions

This chapter describes the current state of analogous studies related to the credibility of algorithms, approaches to navigation systems when driving, and other relevant topics. It then discusses the novelty and significance of the present research.

### A. Structural Properties and Stability

The structural properties are the first and most essential step in any calculation. Said determination provides us with supplementary information about the properties of the observed material. The variation of total energy as a function of volume for the two half Heusler materials using GGA-PBE approximations, which in turn characterizes our half Heusler materials, NiZrC and CuZrB is elucidated in Fig. 1. Initial inspection of this figure reveals that the three phases α, β, and γ (see Table 1) of total energy as a function of the volume of both materials mark stability in the α phases. Therefore, we use this configuration for the rest of our calculations of both compounds. However, it is note- worthy that no experimental data are available to compare with the achieved results; therefore, it is considered a detailed predictive study. The lattice parameter $a_0$, the bulk modulus $B_0$, and its derivative $B_0$', which corresponds to the minimum total energy, are determined by adjusting the total energy according to the volume, which is determinedby the Murnaghan equation [14], and the obtained structural parameters of compounds are summarized in Table 1. The estimation of the formation energy (*ΔH*) of these compounds is critical for studying their thermodynamic stability. Therefore, we calculated the formation energy per formula unit of all alloys using the following formula [15]:

$$\Delta H^{XZrZ} = E_{tot}^{XZrZ} - \left(E_X^{Bulk} + E_{Zr}^{Bulk} + E_Z^{Bulk}\right)$$

where $E_{tot}^{XZrZ}$ is the equilibrium total energy of XZrZ (X = Ni, Cu and Z = C, B) compounds, $E_X^{Bulk}, E_X^{Bulk} E_{Zr}^{Bulk} and\ E_Z^{Bulk}$ are the total energies of the isolated atoms.

TABLE I: The achieved values of lattice constant (a), bulk modulus (B), first pressure derivative (B'), volume ($V_0$) and and formation energy (ΔH) for NiZrC and CuZrB half-Heusler compounds.

| Compound | *a* (Å) | *B* (Gpa) | *B'* | $V_0$ (Å)$^3$ | *ΔH (eV)* |
|---|---|---|---|---|---|
| NiZrC | 5.33 | 1 99.72 | 4.08 | 255.84 | -0.17 |
| CuZrB | 5.52 | 152.05 | 3.47 | 285.52 | -0.22 |

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## III. Thermoelectric Properties

This study investigates the thermoelectric properties of NiZrC and CuZrB HHs via the BoltZtrap package [23]. The understanding of the thermoelectric efficiency of NiZrC and CuZrB HHs is accomplished through the evaluation of the transport parameters such as electrical conductivity, seebeck coefficient, thermal conductivity, and the figure of merit (ZT) as a function of the temperature (T in K) up to 1200K, whereas the coefficients mentioned above are visible in Fig. 5. Mainly, good thermoelectric performance requires large Seebeck coefficient, high electrical conductivity, and low electronic thermal conductivity [7]. The Seebeck coefficient S (μV/K) of NiZrC and CuZrB HHs is illustrated in Fig. 5 (a) as a function of temperature. It is also observable in the same figure that there is a linear increase from 200 K to 1200 K for NiZrC HHs, and that there is linear decrease from 200 K to 1200 K for NiZrB HHs. Besides, the Seebeck coefficient is equal to almost zero when the temperature less than 200K, however, its values are respectively 3.53 and 1.81 μV/K of NiZrC and CuZrB HHs at room temperature. Fig. 5 (b) depicts the electrical conductivity (σ/τ) of NiZrC and CuZrB HHs as a function of the temperature, this depiction reveals that the increase of temperature is met by a decrease of the electrical conductivity (σ/τ). Furthermore, the values of the electrical conductivity (σ/τ) of NiZrC and CuZrB HHs at room temperature are 3.26 and 5.83 1020 S $cm^{-1}$ $s^{-1}$, respectively. In Fig. 5 (c), the electronic thermal conductivity (κ/τ) of NiZrC and CuZrB HHs changes with the temperature up to 1200K. Fig. 5 (c) also exhibits a couple of observations: that the electronic thermal conductivity (κ/τ) increases with the increase of temperature, and that the values of the electronic thermal conductivity (κ/τ) of NiZrC and CuZrB HHs at room temperature are 0.23 and 0.19 (1015 $wk^2\ ms^{-1})^{-1}$, respectively. Finally, the figure of merit (ZT) is determined as a function of temperature (T) up to 1200K, which represented in Fig. 5 (d). The ZT values reach their maximum of 0.33 at 1200 K and 0.29 at 1200 K for NiZrC and CuZrB HHs, respectively, whereas ZT values are 0.00 up to 200 K. Moreover, it is notable that the ZT value increases when going from 0 to 1200K, and the ZT values of NiZrC are greater than those of the CuZrB. Based on these findings, it concluded that these NiZrC and CuZrB materials could be promising for thermoelectric devices.

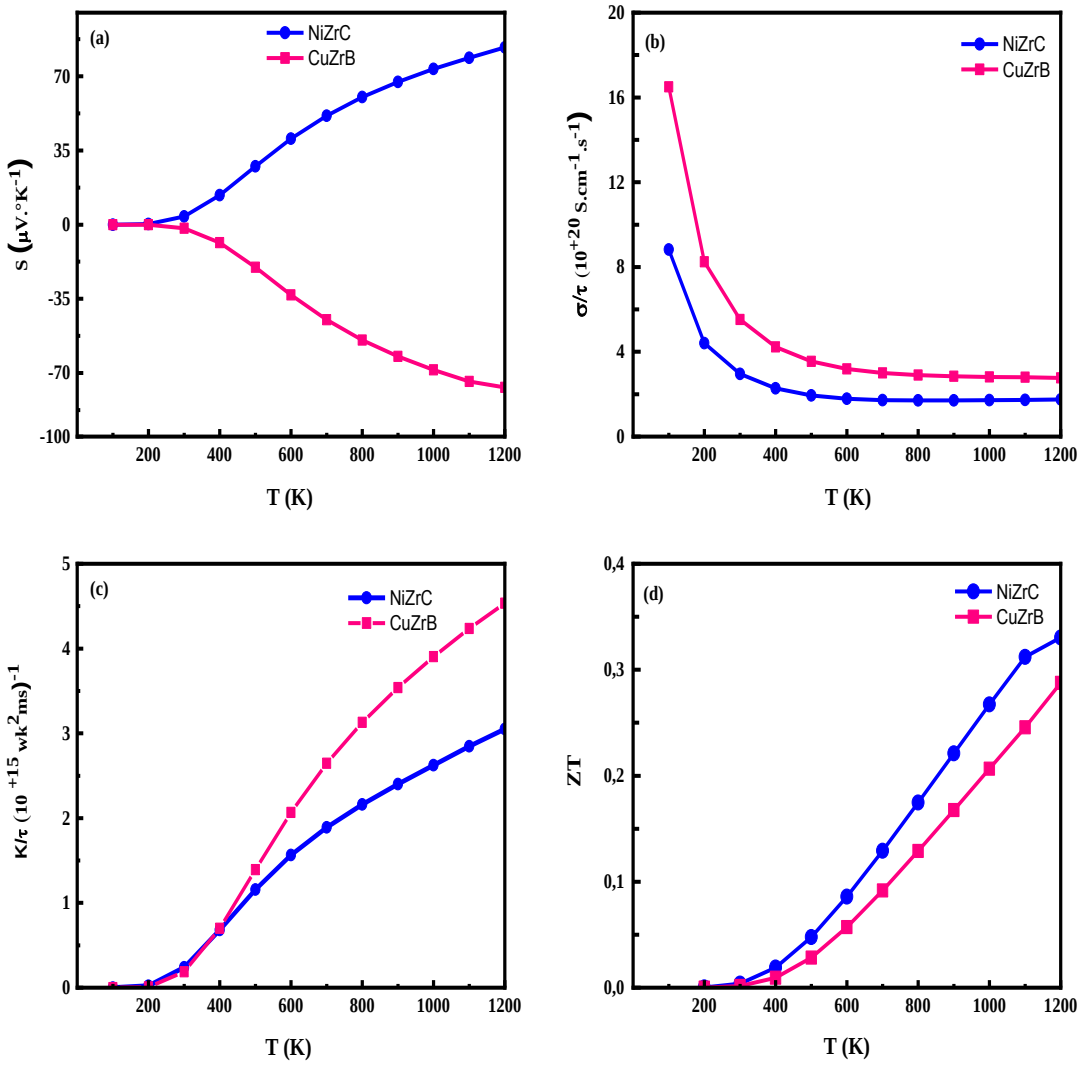


Fig. 5. Seebeck coefficient (a), electric conductivity (b), thermal conductivity (c) and the figure of merit ZT (d) as a function of temperature for NiZrC and CuZrB half-Heusler compounds

## IV. Optical properties

To understand the electronic system, we will discuss in this section the study of optical properties of both compounds. The optical properties calculations were performed up to 10 eV and used 1200 k-points with the considered broadening value being 0.04 eV. A more detailed description of optical computation can be found in Ref. [24]. In Fig. 6 (a), the inspection of the spectrum of the real part ε1(ω) of NiZrC and CuZrB HHs reveals that ε1(0) is the static dielectric constant equal 23.05 and 27.30, respectively. The minimum negative summits of ε1(ω) for the NiZrC and CuZrB HHs are noted at values 6.88 and 8.95eV, respectively. On the other hand, the initial negative values for ε1(ω) of the NiZrC and CuZrB HHs are noted at values 4.38 and 5.92eV, respectively, where the incident photons are completely reflected in the energy range of negative values of ε1(ω). It is noticeable that ε1(ω) turn into constant from 8.0 eV. In Fig. 6 (a) the imaginary part ε2(ω) of NiZrC and CuZrB HHs illustrates the threshold energy at 0.18 and 0.22eV, respectively. The optical transition between VBM and CBM of NiZrC and CuZrB HHs is neatly attached to the optical band gap, which is the threshold of the first peak of imaginary part ε2(ω) [25,26]. Furthermore, the great peaks of imaginary part ε2(ω) of NiZrC and CuZrB HHs are located less than 2 eV. The variations of the refractive index n(ω) for NiZrC and CuZrB HHs are provided in Fig. 6 (b). The values of static refractive n(0) of HHs are estimated to be 4.71 and 4.98, respectively, and these values are perfectly appropriate with the relation n(0) = (ε(0))1/2. Indeed, the maximum values of the refractive index n(ω) are the values corresponding to the energies 0.83 eV and 1.25 eV for NiZrC and CuZrB HHs, respectively. Afterwards, these values the n(ω) decrease with the increase of energy. In Fig. 6 (c) delineates changes in terms of the reflectivity R(ω) of NiZrC and CuZrB HHs with photon energy. The reflectivity R(ω) are 43.25% and 46.32% at zero value of NiZrC and CuZrB HHs, respectively. Besides, it is

observable that the highest R(ω) values of NiZrC and CuZrB HHs are 58.64% (10 eV) and 54.03% (10 eV), respectively, and that there are fourteen peaks. The achieved results suggest that NiZrC and CuZrB HHs behaves similarly to a semiconductor. Fig. 6 (d) displays the absorption coefficients α(ω) of NiZrC and CuZrB HHs. It is also noticed that the absorption threshold ranges from energy values 0.18 and 0.22eV of NiZrC and CuZrB HHs, respectively. Conversely, there is a considerable band absorption (up to 10 eV), which is at the expense of the inter band transitions of NiZrC and CuZrB HHs. Additionally, the maximum values of α(ω) are 208.17 104 cm− 1 (10 eV) and 193.89 104 cm− 1 (10 eV) of NiZrC and CuZrB HHs, respectively. Indeed, these peaks are within the ultra-violet region, which is beyond the visible light region. Finally, it is also noteworthy that there are ten peaks for α(ω) located up to 10 eV. However, the achieved results of α(ω) suggest that the NiZrC and CuZrB HHs could be beneficial in optoelectronic applications.

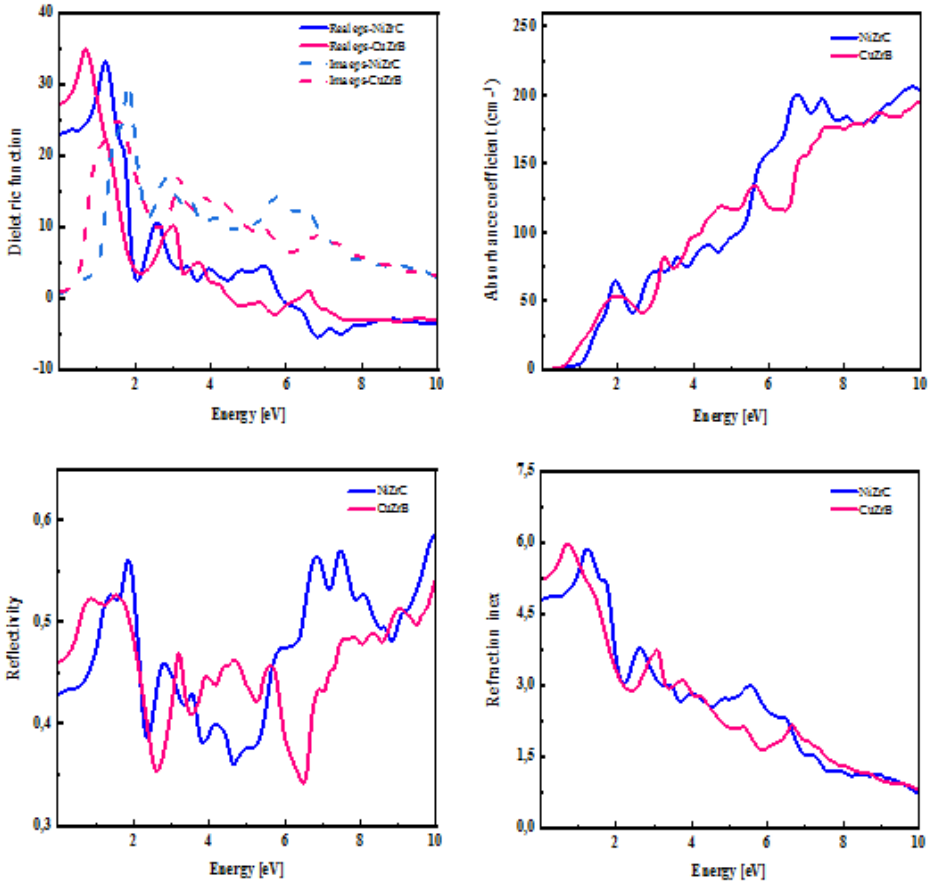


Fig. 6. Real and imaginary parts of the dielectric function (a), refraction index (b), reflectivity (c) and absorption coefficient (d) for NiZrC and CuZrB halfHeusler compounds

## V. Conclusions

The investigated structural, electronic, thermoelectric, and optical properties of a new half-Heusler alloy XZrZ (X = Ni, Cu, Z = C, B) show that both materials exhibit a semiconductor behavior, with 0.185 eV direct bandgap and 0.72 eV indirect bandgap for NiZrC and CuZrB, respectively. The negative value of formation energy, phonon dispersion, and elastic constants calculations confirms the chemical stability of both materials. The investigated thermoelectric properties using the Boltz TraP code implemented in the Wien2k program provided a good indication of both materials’ performance in the thermoelectric devices due to their low thermal conductivity, high Seebeck coefficient, and high electrical conductivity. The obtained results indicate that the halfHeusler XZrZ (X = Ni, Cu, Z = C, B) can be considered a source of lowtemperature energy to produce electricity and could be applicable for thermoelectric fields. In addition, these alloys exhibit high absorption coefficients in the ultraviolet domain of light. We can deduce that this compound may be required for optical application within the field of semiconductors in the optoelectronics industries, including solar and photovoltaic cells.

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