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A Comprehensive Study on Physical Properties of Antiperovskite $GeNCa_3$

Ahmet İyigör*[1] and Selgin Al[2]

Abstract

A comprehensive study has been carried out in order to reveal physical properties of antiperovskite compound $GeNCa_3$ in the cubic structure. This study presents extensive properties including mechanical, electronic, vibrational and thermodynamical by means of generalised gradient approximation approach within the density functional theory. The equilibrium lattice constant and bulk modulus of the compound are obtained via energy-volume data. The mechanical stability evaluation is conducted based on Born's criteria using elastic constants. Subsequently, electronic band structures and partial and total densities of states are computed for antiperovskite $GeNCa_3$. The electronic band structure of the compound reveals a metallic character with highest contribution to the conductivity Ge 4p and Ca 3d states. Moreover, phonon distribution curve is obtained by employing the linear response technique. The results indicate a dynamically stable compound. Finally, thermodynamic properties such as entropy and specific heat value and the results are presented.

Keywords: first principle calculations, antiperovkites, phonon, elastic constants.

1. INTRODUCTION

Perovskite materials can be used in various areas such as semiconductors, fuel cells, batteries, sensors, membrane reactors, hydrogen production and so on [1, 2]. These types of materials have a formula of ABX_3 where A and B are cations, X is an anion and have unique chemical and structural properties. Moreover, they can be synthesised with a wide range of elements where large (ionic radius) cations sit in the A site and small cations sit on the B site.

The positions of cations and anions interchange in the case of antiperovskite materials. Other than that, the crystal structures of both types of materials are similar. They also have remarkable thermoelectric properties and broad band gaps which make them attractive for the research and technology purposes. Antiperovskite materials can extract waste heat and turn it into electricity making them interesting for any industrial application [3].

Because of those fascinating properties, antiperovskite materials have been taking great interest from many researchers [4-15]. The phase transitions of a couple of calcium nitrides ($MNCa_3$ with M = P, As, Sb, Bi, Ge, Sn, Pb) were studied by Chern *et al.* [6] and seen a phase transition from cubic to orthorhombic for $PNCa_3$ and $AsNCa_3$ due to small radius of P and As. A first principle computation was done by Moakafi *et al.* [8] for $SbNCa_3$ and $BiNCa_3$ cubic antiperovskite compounds and reported that these compounds are semi-conductors. The metallic nature of $XNCa_3$ (X=Ge, Sn and Pb) compounds were established by Haddadi *et al.* [15] via ab initio calculations. The physical properties of $TlNCa_3$ [16] and $AuNCa_3$ [17] and both compounds showed metallic behavior. In addition, $AsNMg_3$ and $SbNMg_3$ antiperovskites were studied experimentally and noted as ionic semiconductors [9, 18, 19]. The electronic

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investigations of $MNSr_3$ and $MNBa_3$ (M=Sb, Bi) antiperovskite compounds revealed a semi-conductor behavior [20]. The electronic and optical properties of $GeNCa_3$ were studied by Igbal *et al*. [21]. Moreover, structural and elastic properties of $GeNCa_3$ were computed using density functional theory by Haddadi *et al*. [2].

The studies of calcium nitrides depict that these kinds of materials take great interest by the scientists due to their significant properties. Moreover, the properties such as magnetic, thermoelectric and optic are strongly dependent on their electronic states. Also, phonon modes are extremely important to determine the dynamical stability of these antiperovskites. Thus, a full investigation including phonon density of states is crucial. Motivated by those reasons, this study presents a detailed investigation of cubic antiperovskite $GeNCa_3$ compound's electronic, magnetic, structural and dynamic properties in the frame of density functional theory.

2. METHOD

This study adopted first principle calculations in order to obtain extensive properties of $GeNCa_3$ [22, 23] within the Quantum-Espresso software package [24]. Perdew-Burke-Ernzerhof, generalised gradient approximation (PBE-GGA) was employed for the exchange correlation potential [25, 26]. A 70 Ry kinetic cut off energy was used to expand electronic wave functions in plane-wave basis. A 700 Ry cut off energy was employed for electronic charge density. The Brillouin zone was presented by a 10x10x10 k-points. A Methfessel-Paxton [27] smearing parameter with a width of $\sigma = 0.02$ Ry was used for the integration up to the Fermi surface in order to obtain a smooth density of states. The lattice dynamic calculations were carried out within the framework of the DFPT [28, 29]. A 4x4x4 q-point mesh was utilised to collect the phonon frequencies to get ten dynamic matrices. Fourier deconvolution was employed to this mesh to reassess these dynamical matrices at arbitrary wave vectors.

Elastic constants of compounds can be used to predict mechanical stability. The stiffness of compounds against externally applied strain can be also estimated using elastic constants. Moreover, it allows to estimate other features such as strength and melting temperature [30]. It is also possible to collect elastic constants from the slopes of the acoustic modes in the full phonon spectra [31, 32]. Small waves in the acoustic phonons correspond to sound velocities which are correlated to C_{11}, C_{12} and C_{44} as described in references [4, 33]. Subsequently, computation of elastic constants the relevant polycrystalline features such as Bulk modulus (B), Shear modulus (G), Young's modulus (E), anisotropy factor (A) and Poisson's ratio (σ) can be collected using the following standard relationships [34]:

$$B = \frac{C_{11}+2C_{12}}{3} \quad (1)$$

$$G = \frac{G_v+G_R}{2}, G_v = \frac{C_{11}-C_{12}+3C_{44}}{5}, G_R = \frac{5\,(C_{11}-C_{12})C_{44}}{3(C_{11}-C_{12})+4C_{44}} \quad (2)$$

$$E = \frac{9BG}{3B+G} \quad (3)$$

$$A = \frac{2C_{44}}{(C_{11}-C_{12})} \quad (4)$$

$$\sigma = \frac{1}{2}\left(1 - \frac{E}{3B}\right) \quad (5)$$

3. RESULTS AND DISCUSSION

3.1. Structural and Elastic Properties

The crystal structure of $GeNCa_3$ antiperovskite compound is displayed in Figure 1 where Ge atoms sit at (0,0,0) positions, N atoms sit at (1/2, 1/2, 1/2) whilst Ca atoms sit (0,1/2,1/2) positions. The total energy is computed based on the unit cell. The obtained total energy is then matched to Murnaghan's equation of state [35] to collect lattice constants (a) in the equilibrium and bulk modulus (B). The obtained lattice constants, bulk modulus and elastic constants of the compounds are presented in Table 1. As it is clearly seen from Table 1 that the computed lattice constant and bulk modulus of the antiperovskite $GeNCa_3$ in line with the existing data.

Elastic constants of a solid are knows as the quantitative numbers that can provide valuable data on mechanical and dynamical behaviour of a solid [34]. The elastic constants in this study are computed using strain-stress method at the optimised lattice. A cubic structure has three elastic constants which are defined as follows; C_{11}, C_{12} and C_{44}. The general Born criteria [36] for mechanical stability of a cubic structure is given as;

$(C_{11}+2C_{12})>0$, $C_{44}>0$, $C_{11}>0$ and $C_{11}-C_{12}>0$ (6)

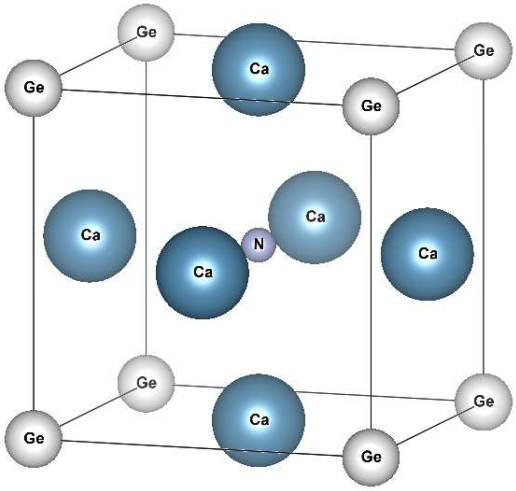

Figure 1. The calculated electronic structure of $GeNCa_3$ in the cubic structure.

The Born stability criteria also brings a restriction for the bulk modulus of the compound. The bulk modulus of a cubic structure should take a value between C_{11} and C_{12} as follows [37];

$$C_{11} > B > C_{12} \quad (7)$$

As can be seen from Table 1 that both conditions given in equations 6 and 7 are fulfilled for $GeNCa_3$. Table 1 demonstrates that $GeNCa_3$ fulfils the mechanical stability condition, indicating that the studied antiperovskite $GeNCa_3$ is mechanically stable.

Table 1: The obtained equilibrium lattice constant *a(Å),* bulk modulus *B* (GPa) and elastic constants of $GeNCa_3$.

Material	***Ref.***	***a(Å)***	***B***	C_{11}	C_{12}	C_{44}
$GeNCa_3$	This work	4.807	56.324	109.437	29.768	40.956
	PBE-GGA [21]	4.825	53.578	-	-	-
	PBE-GGA [2]	4.787	58	102	36	43

Table 2: The computed bulk modulus *B* (GPa), shear modulus G (GPa), B/G ratio, Young's modulus E (GPa), Anisotropy factor A (GPa), Poisson's ratio σ, Cauchy Pressure ($C_{12} - C_{44}$) of $GeNCa_3$.

Material	***Ref.***	***B***	***G***	***B/G***	***E***	***A***	***σ***	$C_{12} - C_{44}$
$GeNCa_3$	This work	56.324	40.504	1.390	98.016	1.028	0.209	-11.188
	PBE-GGA [2]	58	66	0.8787	143	1.30	-	-7

Based on the calculation in this study given in Table 2 that $GeNCa_3$ shows a resistance towards a volume change under pressure due to the fact that the value of bulk modulus (*B*) is higher than the value of shear modulus (*G*) which contradicts Haddadi *et al*.'s values. Their reported bulk modulus is lower than shear modulus which maybe owing to using a different code.

Moreover, *B/G* ratio is computed in order to evaluate brittleness and ductility of $GeNCa_3$. This feature is extremely important for high temperature strength. Based on the Pugh criteria [38], if this ratio is higher than 1.75, the solid is ductile if not it is brittle. According to the ratio given in Table 2, $GeNCa_3$ is brittle. This result is in well accordance with Haddadi *et al.*[2]. In addition, the bonding characteristics of $GeNCa_3$ is examined via Poisson's ratio and Cauchy pressure. It is accepted that if the Poisson's ratio is about 0.1, the solid shows covalent bonding characteristics, if it is about 0.25, it demonstrates ionic bonding characteristics [38, 39]. For the values between 0.25 and 0.5, the central forces dominate [40]. As shown in Table 2 that the inter atomic forces of $GeNCa_3$ seem to be ionic. Cauchy pressure ($C_P = C_{12} - C_{44}$) can be used to predict angular atomic bonding characteristics of metals and compounds. On the assumption that Cauchy pressure is more positive, the solid exhibits more metallic characteristics, otherwise the solid shows angular character in the bonding [38, 41, 42].Thus, it can be said that $GeNCa_3$ is brittle with angular bonding at zero pressure.

The Young modulus and elastic anisotropy are also important physical parameters. As Young modulus of a solid increases it gets much stiffer [43]. If it is around unity (A=1), the solid is isotropic. The value of higher or lower than unity indicates anisotropy. Table 2 exhibits that $GeNCa_3$ is nearly isotropic owing to A~1.

3.2. Electronic and Phonon Properties

Electronic band structure and density of states were calculated along the high symmetry directions in the Brillouin zone in order to evaluate the electronic properties of $GeNCa_3$. Figure 2 and 3 illustrates the electronic band structure and the total and partial density of states of $GeNCa_3$. The antiperovskite $GeNCa_3$ has metallic character since there is no band gap at the Fermi energy level.

Figure 3 demonstrates the total and partial density of states of $GeNCa_3$ which provides information about orbital interactions. As can be seen from the figure that Ge 4p states contribute to the band above Fermi level whilst N 2p states contribute below Fermi level.

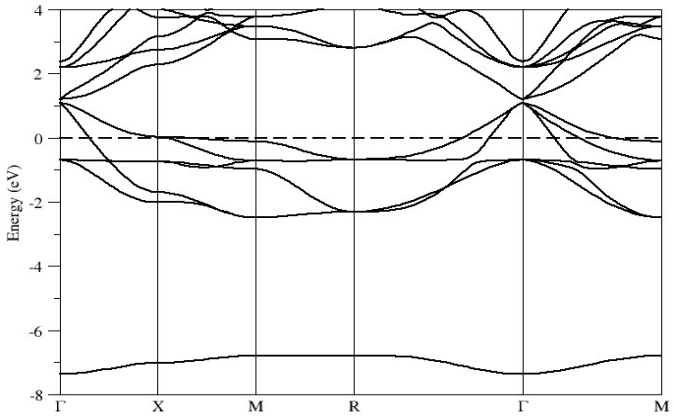

Figure 2. The calculated electronic structure of $GeNCa_3$ in the cubic structure.

$GeNCa_3$ antiperovskite compound has 15 phonon modes; twelve of them is optical and three of them is acoustical. The phonon modes of $GeNCa_3$ are positive as shown in Figure 4. The phonon modes are degenerate along the Γ-X and R-Γ high symmetry directions and reduce 10 phonon modes. Along the M-R high symmetry directions the phonon modes also reduce to 11 due to symmetry. Ge atoms vibrate in the acoustic region (transverse and longitudinal acoustical) since it has larger mass than other atoms. In the mid frequency region, the optical modes are due to vibrations of Ca atoms (9 modes) and the phonon modes in the high frequency region are due to N atoms vibrations (3 modes). It can be predicted that this compound has low thermal conductivity since lower frequency optical modes and acoustic modes cut each other [44]. The gap between Ca optical phonon modes and N optical phonon modes is 0.233 THz. This gap is formed because of the mass difference between Ca and N atoms. The optical phonon frequencies at the zone centre are; 3.350 THz, 4.439 THz, 7.518 THz and 10.445 THz. The phonon modes indicate that $GeNCa_3$ is dynamically stable. Unfortunately, there is no available data to compare phonon modes of $GeNCa_3$ in literature. Phonon dispersion curves and phonon density of states are obtained for the first time in this study and added to the literature.

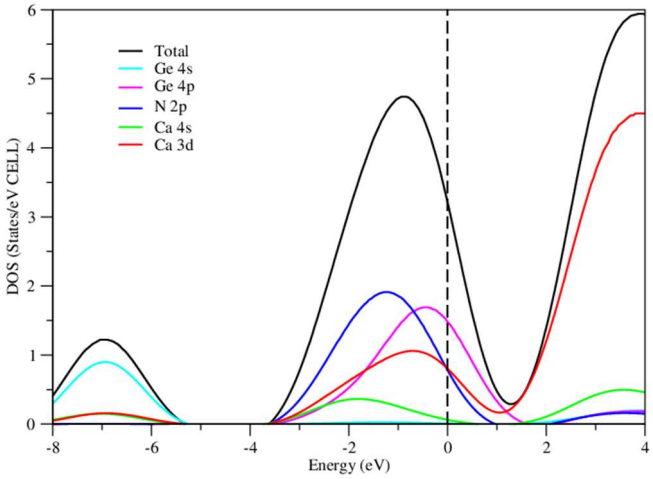

Figure 3. The calculated total and partial density of states of $GeNCa_3$ in the cubic structure.

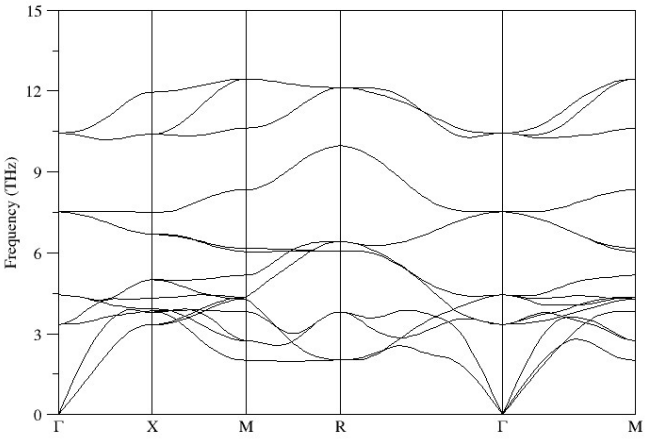

Figure 4. The phonon dispersion curves of $GeNCa_3$ in the cubic structure.

3.3. Thermodynamic Properties

The thermodynamic properties are collected within the quasi-harmonic approximation for different

temperatures from the energy-volume relation. The entropy change of $GeNCa_3$ with temperature is calculated and presented in Figure 5. As Figure 5 clearly exhibits that the entropy of $GeNCa_3$ increases with temperature, meaning that free energy of $GeNCa_3$ decreases.

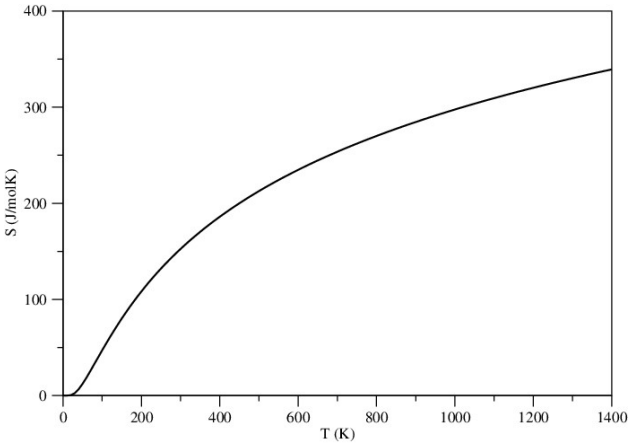

Figure 5. Entropy (S) change versus temperature of $GeNCa_3$ in the cubic structure.

The variations of thermal expansion coefficients at a constant volume and pressure versus temperature are displayed in Figure 6 and 7, respectively. As it is clearly seen from the figures that thermal coefficients of $GeNCa_3$ rapidly increase up to 300 K. After this point, it increases gradually and becomes flat. At higher temperatures, both specific heat capacities reach the Dulong-Petit limit.

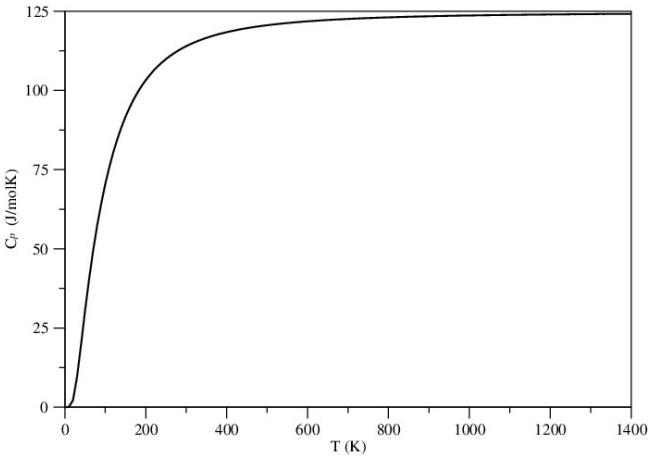

Figure 6. The temperature dependence of the specific heat capacities at constant pressure (C_p) of $GeNCa_3$ in the cubic structure.

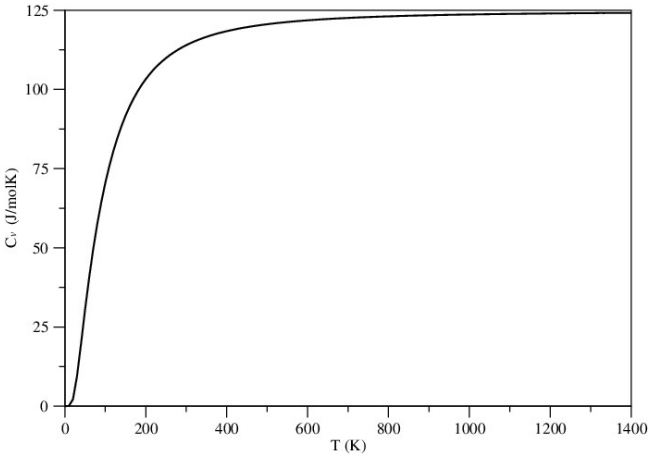

Figure 7. The temperature dependence of the specific heat capacities at constant volume (C_V) of $GeNCa_3$ in the cubic structure.

4. CONCLUSION

The antiperovskite compound $GeNCa_3$`s physical properties are examined using first principle calculations. Various constants such as lattice constant, bulk modulus, elastic constants and shear modulus are collected. The evaluation of lattice constants in terms of mechanical stability shows that $GeNCa_3$ is mechanically stable since it fulfils the well-known mechanical stability criteria. The analysis of bonding characteristics suggests that $GeNCa_3$ antiperovskite compound has dominant ionic bonding. According to B/G ratio and Pugh's criteria, the antiperovskite $GeNCa_3$ is a brittle material. The electronic band structure of $GeNCa_3$ illustrates that $GeNCa_3$ is metallic in nature. The biggest contributions to the conductivity are due to Ge 4p and Ca 3d states. The dynamical stability of the compounds has also examined by computing the phonon modes. The positive frequency of phonon modes suggest that $GeNCa_3$ is dynamically stable. Thermodynamic properties such heat capacities and entropy have also calculated and evaluated. The heat capacities of $GeNCa_3$ at a constant volume and pressure reach the Dulog-Petit limit at around 500 K. This work is undertaken a systematic investigation to reveal all properties of GeNCa3 antiperovskite compound including phonon and presented new data for future investigations and applications.

References

[1] E. C. C. d. Souza and R. Muccillo, "Properties and Applications of Perovskite Proton Conductors", *Materials Research*, 13, pp. 385-394, 2010.

[2] K. Haddadi, A. Bouhemadou, L. Louail and Y. Medkour, "Structural, Elastic and Electronic Properties of $XNCa_3$ (X= Ge, Sn and Pb) Compounds", *Solid State Communications*, 149, 15-16, pp. 619-624, 2009.

[3] M. Bilal, S. Jalali-Asadabadi, R. Ahmad and I. Ahmad, "Electronic Properties of Antiperovskite Materials from State-of-the-Art Density Functional Theory", *Journal of Chemistry*, 2015, pp. 11, 2015.

[4] R. Sharma, S. Dwivedi and Y. Sharma, "Hydrides of Ypd_3: Electronic Structure and Dynamic Stability", *International Journal of Hydrogen Energy*, 40, 2, pp. 1071-1082, 2015.

[5] S. Iqbal, G. Murtaza, R. Khenata, A. Mahmood, A. Yar*, et al.*, "Electronic and Optical Properties of Ca_3Mn (M = Ge, Sn, Pb, P, as, Sb and Bi) Antiperovskite Compounds", *Journal of Electronic Materials*, 45, 8, pp. 4188-4196, 2016.

[6] M. Y. Chern, D. A. Vennos and F. J. Disalvo, "Synthesis, Structure, and Properties of Anti-Perovskite Nitrides Ca_3Mn, M=P, as, Sb, Bi, Ge, Sn, and Pb", *Journal of Solid State Chemistry*, 96, 2, pp. 415-425, 1992.

[7] D. Cherrad, D. Maouche, L. Louail and M. Maamache, "Ab Initio Comparative Study of the Structural, Elastic and Electronic Properties of $SnAMn_3$(A=N,C) Antiperovskite Cubic Compounds", *Solid State Communications*, 150, 15, pp. 782-787, 2010.

[8] M. Moakafi, R. Khenata, A. Bouhemadou, F. Semari, A. H. Reshak*, et al.*, "Elastic, Electronic and Optical Properties of Cubic Antiperovskites SbNCa3 and $BiNCa_3$", *Computational Materials Science*, 46, 4, pp. 1051-1057, 2009.

[9] A. Bouhemadou and R. Khenata, "Ab Initio Study of the Structural, Elastic, Electronic and Optical Properties of the Antiperovskite $SbNMg_3$", *Computational Materials Science*, 39, 4, pp. 803-807, 2007.

[10] M. Bilal, Saifullah, I. Ahmad, S. Jalali-Asadabadi, R. Ahmad*, et al.*, "Dft and Post-Dft Studies of Metallic MxY_3-Type Compounds for Low Temperature Te Applications", *Solid State Communications*, 243, Supplement C, pp. 28-35, 2016.

[11] S. Lin, Y. Huang, J. Lin, P. Tong, W. Song*, et al.*, "Role of Chemical Doping on the Enhancement of Thermoelectric Performance in Metal-Based Thermoelectric System $SnCCo_3$", *Journal of Alloys and Compounds*, 688, Part A, pp. 565-570, 2016.

[12] R. Iqbal, M. Bilal, S. Jalali-Asadabadi, H. A. RahnamayeAliabad and I. Ahmad, "Theoretical Investigation of Thermoelectric and Elastic Properties of Intermetallic Compounds ScTm (Tm = Cu, Ag, Au and Pd)", *International Journal of Modern Physics B*, 0, 0, pp. 1850004,

[13] K. Haddadi, A. Bouhemadou and L. Louail, "Structural, Elastic and Electronic Properties of the Hexagonal Anti-Perovskites $SbNBa_3$ and $BiNBa_3$", *Computational Materials Science*, 48, 4, pp. 711-718, 2010.

[14] M. Bilal, I. Ahmad, S. J. Asadabadi, R. Ahmad and M. Maqbool, "Thermoelectric Properties of Metallic Antiperovskites Axd3 (a=Ge, Sn, Pb, Al, Zn, Ga; X=N, C; D=Ca, Fe, Co)", *Electronic Materials Letters*, 11, 3, pp. 466-480, 2015.

[15] K. Haddadi, A. Bouhemadou, L. Louail and Y. Medkour, "Structural, Elastic and Electronic Properties of $XnCa_3$ (X = Ge, Sn and Pb) Compounds", *Solid State Communications*, 149, 15, pp. 619-624, 2009.

[16] R. Niewa, W. Schnelle and F. Wagner, "Synthesis, Crystal Structure, and Physical Properties of (Ca_3N) Tl", *Zeitschrift fur Anorganische und Allgemeine Chemie*, 627, 3, pp. 365-370, 2001.

[17] J. Jäger, D. Stahl, P. C. Schmidt and R. Kniep, "Ca_3aun: Ein Calciumauridsubnitrid", *Angewandte Chemie*, 105, 5, pp. 738-739, 1993.

[18] C. Okoye, "First-Principles Optical Calculations of Asnmg 3 and $SbNMg_3$", *Materials Science and Engineering: B*, 130, 1, pp. 101-107, 2006.

[19] I. Shein and A. Ivanovskii, "Electronic Band Structure and Chemical Bonding in the New Antiperovskites $AsNMg_3$ and $SbNMg_3$", *Journal of Solid State Chemistry*, 177, 1, pp. 61-64, 2004.

[20] F. Gäbler, M. Kirchner, W. Schnelle, U. Schwarz, M. Schmitt*, et al.*, "(Sr_3N)E and (Ba_3N)E (E= Sb, Bi): Synthesis, Crystal Structures, and Physical Properties", *Zeitschrift fur Anorganische und Allgemeine Chemie*, 630, 13-14, pp. 2292-2298, 2004.

[21] S. Iqbal, G. Murtaza, R. Khenata, A. Mahmood, A. Yar*, et al.*, "Electronic and Optical Properties of Ca_3Mn (M= Ge, Sn, Pb, P, as, Sb and Bi) Antiperovskite Compounds", *Journal of Electronic Materials*, 45, 8, pp. 4188-4196, 2016.

[22] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas", *Physical Review*, 136, 3B, pp. B864-B871, 1964.

[23] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects", *Physical Review*, 140, 4A, pp. A1133-A1138, 1965.

[24] G. Paolo, B. Stefano, B. Nicola, C. Matteo, C. Roberto*, et al.*, "Quantum Espresso: A Modular and Open-Source Software Project for Quantum Simulations of Materials", *Journal of Physics: Condensed Matter*, 21, 39, pp. 395502, 2009.

[25] J. P. Perdew, K. Burke and M. Ernzerhof, "Generalized Gradient Approximation Made Simple", *Physical Review Letters*, 77, 18, pp. 3865-3868, 1996.

[26] S. Al, N. Arıkan, M. Özduran and A. İyigör, "Computational Investigations of Mechanical and Dynamical Properties of Gold-Based Compounds (X_3Au, X= Ti, Zr and V)", *Chinese Journal of Physics*, pp. 2018.

[27] M. Methfessel and A. T. Paxton, "High-Precision Sampling for Brillouin-Zone Integration in Metals", *Physical Review B*, 40, 6, pp. 3616-3621, 1989.

[28] S. Baroni, P. Giannozzi and A. Testa, "Green's-Function Approach to Linear Response in Solids", *Physical Review Letters*, 58, 18, pp. 1861-1864, 1987.

[29] S. Baroni, S. de Gironcoli, A. Dal Corso and P. Giannozzi, "Phonons and Related Crystal Properties from Density-Functional Perturbation Theory", *Reviews of Modern Physics*, 73, 2, pp. 515-562, 2001.

[30] N. Arıkan, O. Örnek, Z. Charifi, H. Baaziz, Ş. Uğur*, et al.*, "A First-Principle Study of Os-Based Compounds: Electronic Structure and Vibrational Properties", *Journal of Physics and Chemistry of Solids*, 96-97, pp. 121-127, 2016.

[31] A. İyigör, M. Özduran, M. Ünsal, O. Örnek and N. Arıkan, "Ab-Initio Study of the Structural, Electronic, Elastic and Vibrational Properties of HfX (X= Rh, Ru and Tc)", *Philosophical Magazine Letters*, 97, 3, pp. 110-117, 2017.

[32] I. Shein, K. Shein and A. Ivanovskii, "Elastic and Electronic Properties and Stability of $Srtho_3$, $SrZrO_3$ and ThO_2 from First Principles", *Journal of Nuclear Materials*, 361, 1, pp. 69-77, 2007.

[33] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys*. 1958: Courier Corporation.

[34] S. Al, N. Arikan, S. Demir and A. Iyigör, "Lattice Dynamic Properties of Rh_2XAl (X= Fe and Y) Alloys", *Physica B: Condensed Matter*, 531, pp. 16-20, 2018.

[35] F. D. Murnaghan, "The Compressibility of Media under Extreme Pressures", *Proceedings of the National Academy of Sciences of the United States of America*, 30, 9, pp. 244-247, 1944.

[36] M. Born and K. Huang, *Theory of Crystal Lattices, Clarendon*. 1956, Oxford.

[37] S. Al and A. İyigör, "A Theoretical Study of Structural, Electronic and Elastic Properties of the Antiperovskite $SnNCa_3$", *Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi*, pp. DOI: 10.19113/sdufbed. 37948-Online Yayınlanma: 19115.19105. 12018, 2018.

[38] S. F. Pugh, "Xcii. Relations between the Elastic Moduli and the Plastic Properties of Polycrystalline Pure Metals", *Philosophical Magazine and Journal of Science*, 45, 367, pp. 823-843, 1954.

[39] J. Haines, J. Leger and G. Bocquillon, "Synthesis and Design of Superhard Materials", *Annual Review of Materials Research*, 31, 1, pp. 1-23, 2001.

[40] N. Liu, X. Y. Wang and Y. L. Wan, "First Principle Calculations of Elastic and Thermodynamic Properties of Ir_3Nb and Ir_3V with L1(2) Structure under High Pressure", *Intermetallics*, 66, pp. 103-110, 2015.

[41] D. G. Pettifor, "Theoretical Predictions of Structure and Related Properties of Intermetallics", *Materials Science and Technology*, 8, 4, pp. 345-349, 1992.

[42] R. Johnson, "Analytic Nearest-Neighbor Model for Fcc Metals", *Physical Review B*, 37, 8, pp. 3924, 1988.

[43] S. Al, N. Arikan and A. Iyigör, "Investigations of Structural, Elastic, Electronic and Thermodynamic Properties of X_2TiAl Alloys: A Computational Study", *Zeitschrift für Naturforschung A*, 73, 9, pp. 859-867, 2018.

[44] G. Surucu, "Investigation of Structural, Electronic, Anisotropic Elastic, and Lattice Dynamical Properties of Max Phases Borides: An Ab-Initio Study on Hypothetical M_2AB (M = Ti, Zr, Hf; A = Al, Ga, In) Compounds", *Materials Chemistry and Physics*, 203, pp. 106-117, 2018.