# FIRST PRINCIPLES STUDY OF ELASTIC AND THERMODYNAMIC PROPERTIES OF MgXSi (X = Mg, Sr)

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#### Abstract

In this paper, an application of the first principles investigation of elastic and thermal properties of MgXSi (X=Mg, Sr) compounds was conducted. The density functional theory (DFT) with pseudo-potential plane-waves approach using Projector Augmented Wave (PAW) method for the exchange and correlation potential was employed. Elastic constants and elastic compliances of MgXSi as well as the vibrational free energies, entropy, constant volume specific heat capacities were computed and presented. Our results show that elastic constants of Mg2Si agree with previous theoretical results and compare favourably with experimental data. Elastic constants and compliances of MgSrSi are presented and discussed. Elastic constant,  $C_{11}$  of 166.8GPa was recorded at the Debye temperature of 341.9K for MgSrSi. At 300K, Constant Volume specific heat capacity,  $C_v$  for Mg2Si and MgSrSi were measured to be 62.8 J/K/(N mol) and 70 J/K/(N mol) respectively.

Keywords: Elastic constants; first-principle; heat capacity; MgXSi; Elastic compliances.

#### 1. Introduction

Desire for less toxic, naturally abundant and cost-effective materials has led to continuous investigations of Magnesium based alloys and compounds due to their potentials for use in several technological applications such as; thermoelectric, photo-voltaic, piezoelectric and infrared photonics. [1-3]. Mechanical alloy of Tin (Sn) into Magnesium silicide (Mg<sub>2</sub>Si) have been reported to exhibits better comprehensive properties and thermoelectric properties than Mg<sub>2</sub>Si. Difficulties in the experimental set up includes differences in temperatures of constituent's elements and contamination in material processing. Magnesium silicide is one of the silicidesthat is more prominent in solid state application because of its compatibility with Silicon, which is a based material for solid state devices and electronics. This material has high thermal stability as well as desirable oxidization resistance properties which makes fit as a green material for semiconductor applications. It is a semiconductor with narrow band gap, which has been used at a wavelength range of 1.2 to 1.8 micrometers as an infrared detector [4-6]. Doping and alloying have been used to enhance properties of semiconductors for optimum applications in optoelectronics and energy generations [7-8]. Elastic properties of the Mg<sub>2</sub>Si structure under pressure have been reported by Zhang et al., their calculated elastic constants are stable at minimal pressure range of 0 to 7GPa under Born stability conditions. at low pressures [4]. Experimental measurement of the compressive-to-phase transformation characteristics of Mg<sub>2</sub>Si at room temperature was reported by Hao et al. [10]. Some literatures only report elastic constants and young modulus without leaving out other elastic properties in their work. In this paper, we present a first-principles calculations of elastic properties and some thermodynamic properties of MgXSi (X = Mg, Sr) in antifluorite face-centered cubic (FCC) structure. The elastic constants, elastic compliances and specific heat capacities at constant volume, Cv and the Debye temperatures  $\theta_D$  of Mg<sub>2</sub>Si and MgSrSi are computed and discussed. The results are compared with available experimental and theoretical results.

#### 2. The Calculation Model and Method

The computation is based on the density functional theory (DFT) [11] using the Projected Augmented Wave (PAW) PBE functional which defines the exchange-correction energy.First-principles computations were carried in this work. The PBE-

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PAW pseudo-potential were used to describe the ionic core and valence electrons interactions. The pseudo-potentials used in materials modeling are Mg.pbe-spn-kjpaw\_psl.1.0.0.UPF, Si.pbe-n-kjpaw\_psl.1.0.0.UPF and Sr.pbe-spnkjpaw\_psl.1.0.0.UPF with configurations ([Ne] 3s2.0 3p0), ([Ne] 3s2 3p2 3d-1) and ([Kr] 5s2 5p0 4d-1) for Magnesium, Silicon and Strontium respectively. Brillouin zone sampling was performed by using the Monkhorst–Pack scheme [12] with a k-point grid of 8 x 8 x 8. Geometry optimization was considered to be performed when all components of all forces are smaller than 0.1 micro Ry.The plane wave cut-off energy was relaxed to 90 Ry. Relaxation of the atomic structures were carried out using the Broyden-Fletcher-Goldfarb-Shanno method[13].All computations were carried out with thermo\_pw [14] implementation on the Quantum Espresso (QE) code [15-16]. Elastic properties computed were further post processed and analysed using the ELATE code[17].

#### **3 Results and Discussion**

Results base on the computations are presented in this section for thermodynamical and elastic properties. The results are discussed and compared with other results from theory and experiments.

#### **3.2 Thermodynamic Properties**

The Helmholtz free energy within the quasi-harmonic approximation (QHA) which is fundamental to computing thermodynamical properties is given as [9,18, 19]

$$F(V,T) = U_{stat}(V) + k_B T \sum_{q\lambda} ln\left(2sinh\left[\frac{\hbar\omega_{q\lambda}(V)}{2k_B T}\right]\right) + F_{el}(V,T)$$
(1)

where  $U_{stat}(V)$  is the static internal energy at volume V and  $k_B T \sum_{q\lambda} ln\left(2sinh\left[\frac{\hbar\omega_{q\lambda}(V)}{2k_BT}\right]\right) + F_{el}(V,T)$  represent the vibrational free energy.  $\hbar$  is the reduced Planck constant, and  $\hbar\omega_{q\lambda}(V)$  is the frequency of the phonon with wave vector q and polarization  $\lambda$ , evaluated at constant volume V.  $F_{el}(V,T)$  is the thermal electronic contribution to free energy. Usually, it is assumed that the electronic contribution to total free energy can be negligible. The vibrational specific heat  $C_V$  at constant volume in the is given as

$$C_{V}^{vib} = \sum_{q\lambda} k_{B} \left(\frac{\hbar \omega_{q\lambda}(V)}{2k_{BT}}\right)^{2} \cosh^{2} \left(\frac{\hbar \omega_{q\lambda}(V)}{2k_{BT}}\right)^{2}$$
The electronic specific heat can be obtained from
(2)

$$C_V^{el} = T \left(\frac{\partial S_{el}}{\partial T}\right)_V \tag{3}$$

and the total specific heat at constant volume is then  $C_V = C_V^{ph} + C_V^{el}$ . The specific heat at a constant pressure,  $C_p$ , is different from the specific heat at a constant volume,  $C_V$  due to anharmonicity.  $C_V$  goes to a constant which is given by classical equipartition law:  $C_V = 3Nk_B$  where N is the number of atoms in the system and  $k_B$  is the Boltzmann's constant. The knowledge of heat capacity of a substance provides crucial information on its vibrational properties and applications [18].

The heat capacity at constant volume,  $C_V$  inclines towards the Petit and Dulong boundary at higher temperature,  $C_V$  is proportional to  $T^3$  [9,20]. The volume thermal expansion coefficient is given as

4)

(5)

$$\propto (T) = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)$$

while the linear thermal expansion is given as [21]

$$\epsilon(T) = \left(\frac{a(T) - a(T_c)}{a(T_c)}\right)$$

where  $a(T_c)$  is the equilibrium lattice constant and  $a(T) = [V(T)]^{1/3}$  at  $T_c = 300K$ . Vibrational contribution to the entropy of the system is given as [9]

$$S_{vib} = -k_B \sum_{q\lambda} \left[ \ln \left( 2sinh \frac{\hbar \omega_{q\lambda}(V)}{2k_B T} \right) - \frac{\hbar \omega_{q\lambda}(V)}{2k_B T} coth \left( \frac{\hbar \omega_{q\lambda}(V)}{2k_B T} \right) \right]$$
(6)

Insight to heat capacity of a materials is helpful in understanding the vibrational properties of materials as well as their area of applications. The temperature, T dependent thermodynamic properties for MgXSi (X = Mg, Sr) computed are presented in Figures 1 – 4. The figures show the thermodynamics properties for the two variant materials; Mg<sub>2</sub>Si and MgSrSi computed at temperature range of 0 to 800K. Figure 1 shows the Debye Vibrational Energy as a function of Temperature for Mg<sub>2</sub>Si and MgSrSi.At 0 K, the Debye Vibrational Energies of 15.8 kJ/(N mol) and 10.0 kJ/(N mol) were measured while at the maximum temperature of 800 K, 61.8 kJ/(N mol) and 60 kJ/(N mol) were measured respectively for Mg<sub>2</sub>Si and MgSrSi. Calculated values for Vibrational energies at 300K for Mg<sub>2</sub>Si and MgSrSi are 26.7 kJ/(N mol) and 23.5 kJ/(N mol) respectively. In figure 2, the computed Vibrational Free Energy if presented as function of Temperatures 0K, 300K and 800K, the measured vibrational free energies are 15.8 kJ/(N mol), - 0.9 kJ/(N mol) and -39.5 kJ/(N mol) for Mg<sub>2</sub>Si and 10 kJ/(N mol), -4.9 kJ/(N mol) and -70.1 kJ/(N mol) for MgSrSi.

Figure 3 shows the entropy computed for Mg<sub>2</sub>Si and MgSrSi variants, the entropy for the two variants rises gradually from

around 27K for MgSrSi and 45K for Mg2Si. The entropies of Mg2Si peaked at 124.1 J/K/(N mol) while that of MgSrSi reached its peak at 164 J/K/(N mol) at the same temperature of 800K. At 300K, MgSrSi has better entropy values of 90.2 J/K/(N mol) as against 57.1 J/K/(N mol) for Mg<sub>2</sub>Siat the same temperature. Entropy, which is a quantitative measure of disorder or randomness within a system is an important property in thermodynamics of material. in a system.

Constant Volume specific heat capacity,  $C_{\nu}$  of Mg<sub>2</sub>Si and MgSrSi computed as a function of temperature is presented in figure 4, at low temperature,  $C_v$  obeys  $T^3$  law. Specific heat capacity was zero for Mg<sub>2</sub>Si and MgSrSi until they approached 26K and 20K respectively. Computed C<sub>v</sub> for Mg<sub>2</sub>Si and MgSrSi for at 300K is 62.8 J/K/(N mol) and 70 J/K/(N mol).



Figure 1: Debye Vibrational Energy for MgXSi (X=Mg, Sr).

Figure 3: Calculated Entropy for MgXSi (X=Mg, Sr).



Mg<sub>2</sub>Si AgSrSi ŝ (K) -10 -20 -30 -40 -50 -60 Debye -70 100 200 300 400 500 600 700 т (к)

Figure 2: Debye Vibrational Free Energy for MgXSi (X=Mg, Sr).



Figure 4: Calculated Heat Capacity for MgXSi (X=Mg, Sr).

#### **3.2 Elastic Properties**

For small deformation, each component of the stress tensor,  $\sigma$  is directly proportional the strain tensor,  $\varepsilon$  and vice versa as given below [22].

applied to the elasticity ( $c_{ijkl} = c_{klij}$  and compliance $s_{ijkl} = s_{klij}$  tensors, thereby reducing the number of independent components to 21.

 $\sigma_{ij} = c_{ijkl} \varepsilon_{kl}$ (8) $\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$ where i, j, k and l could be 1, 2, or 3.  $c_{ijkl}$  represents the components of elasticity tensor while  $s_{ijkl}$  represents the components of the elastic compliance tensor. The equation presents a fourth order tensor with  $3^4 = 81$  independent components. These components are reduced to 36 components since  $\sigma_{ij} = \sigma_{ji}$  and  $\varepsilon_{ij} = \varepsilon_{ji}$ . Since deformation process is considered to be reversible, the symmetry may be

Elastic constants and compliance are given as c and s, as shown in cartesian notation.  $\sigma_{11} = c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{13}\varepsilon_{33} + c_{14}\varepsilon_{23} + c_{15}\varepsilon_{31} + c_{16}\varepsilon_{12}$  $\sigma_{22} = c_{21}\varepsilon_{11} + c_{22}\varepsilon_{22} + c_{23}\varepsilon_{33} + c_{24}\varepsilon_{23} + c_{25}\varepsilon_{31} + c_{26}\varepsilon_{12}$  $\sigma_{33} = c_{31}\varepsilon_{11} + c_{32}\varepsilon_{22} + c_{33}\varepsilon_{33} + c_{34}\varepsilon_{23} + c_{35}\varepsilon_{31} + c_{36}\varepsilon_{12}$ (9)  $\sigma_{23} = c_{41}\varepsilon_{11} + c_{42}\varepsilon_{22} + c_{43}\varepsilon_{33} + c_{44}\varepsilon_{23} + c_{45}\varepsilon_{31} + c_{46}\varepsilon_{12}$  $\sigma_{31} = c_{51}\epsilon_{11} + c_{52}\epsilon_{22} + c_{53}\epsilon_{33} + c_{54}\epsilon_{23} + c_{55}\epsilon_{31} + c_{56}\epsilon_{12}$  $\sigma_{12} = c_{61}\varepsilon_{11} + c_{62}\varepsilon_{22} + c_{63}\varepsilon_{33} + c_{64}\varepsilon_{23} + c_{65}\varepsilon_{31} + c_{66}\varepsilon_{12}$  $\varepsilon_{22} = s_{21}\sigma_{11} + s_{22}\sigma_{22} + s_{23}\sigma_{33} + s_{24}\sigma_{23} + s_{25}\sigma_{31} + s_{26}\sigma_{12}$ (10) $\varepsilon_{33} = s_{31}\sigma_{11} + s_{32}\sigma_{22} + s_{33}\sigma_{33} + s_{34}\sigma_{23} + s_{35}\sigma_{31} + s_{36}\sigma_{12}$  $\varepsilon_{23} = s_{41}\sigma_{11} + s_{42}\sigma_{22} + s_{43}\sigma_{33} + s_{44}\sigma_{23} + s_{45}\sigma_{31} + s_{46}\sigma_{12}$  $\varepsilon_{31} = s_{51}\sigma_{11} + s_{52}\sigma_{22} + s_{53}\sigma_{33} + s_{54}\sigma_{23} + s_{55}\sigma_{31} + s_{56}\sigma_{12}$  $\varepsilon_{12} = s_{61}\sigma_{11} + s_{62}\sigma_{22} + s_{63}\sigma_{33} + s_{64}\sigma_{23} + s_{65}\sigma_{31} + s_{66}\sigma_{12}$ 

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(7)

The elastic constants, c and compliances, s are given in matrices form which shows inversion between elastic constants c and the compliances s;

	c11	C12	C13	C14	C15	c16		<b>s</b> 11	<i>s</i> <sub>12</sub>	\$13	<i>s</i> <sub>14</sub>	<i>s</i> <sub>15</sub>	\$16		
	C12	C22	C 23	C 24	C25	c 26		\$12	\$22	\$23	\$24	\$25	\$26	(	(11)
$(c_{})_{=}$	C13	C 23	C33	C34	C35	C 36	and $(s_{ij}) =$	\$13	\$23	\$33	\$34	\$35	\$36		(11)
(~y)	C14	C24	C 34	C 44	C45	C46	und (og)	\$14	\$24	\$34	\$44	\$45	\$46		
	C15	C 25	C35	C 45	C 55	C 56		\$15	\$25	\$35	\$45	\$ 55	\$56		
	C16	C26	C 36	C46	C56	C66)		\$16	\$26	\$36	\$46	\$56	s 66)		

Table 1 presents the elastic properties of computed for Mg<sub>2</sub>Si and MgSrSi in comparison with experimental data and other theoretical results. Computed lattice parameter for Mg<sub>2</sub>Si compares favourably with experimental lattice constant of 0.6338 nm as well as other theoretical results. Computed elastic constant, C<sub>11</sub> is 116.0 GPa which compares well with other theoretical results. Percentage error of computed elastic constant and the experimental work is around 7.9%. Computed elastic constant for MgSrSi is 166.8GPa which is higher than that the based material Mg2Si. Resistance of materials to elastic deformation under load is measured as Young's Modulus. Stiff materials have higher Young's modulus than flexible materials. The computed Young's modulus for Mg<sub>2</sub>Si is higher than that of MgSrSi, thereby making a MgSrSi a more flexible material than Mg<sub>2</sub>Si. Computed compliances for Mg<sub>2</sub>Si and MgSrSi is presented in table 2. Further post processing and analysis of the stiffness matrix for Mg<sub>2</sub>Si and MgSrSi as shown in Table 3 using the online platform for Elastic tensor analysis called ELATE [26]. Average properties, Eigenvalues of the stiffness matrix and Variations of the elastic moduli for Mg<sub>2</sub>Si and MgSrSi are presented in tables 4 – 6 based on post processing done with ELATE. The two-dimensional (2D) and three-dimensional (3D) projections of Spatial dependence of Young's Modulusfor Mg<sub>2</sub>Si and MgSrSi are presented in figure 5. The figure shows clear distinction in the projections for Mg<sub>2</sub>Si and MgSrSi both in 2D and 3D projections.Figure 6 shows the 2D and 3D projections of Spatial dependence of linear compressibility for Mg2Si and MgSrSi.2D and 3D Projection of Spatial dependence of shear modulus are presented in figure 7 for Mg2Si and MgSrSi while the same is presented for Spatial dependence of Poisson's ratio in figure 8.

		MgSrSi					
Properties	This Work	Exp	eriment	Theoretic	This Work		
	THIS WOLK	[23]	[24]	[1]	[25]	THIS WOLK	
Lattice Constant (nm)	0.6341	0.6338	-	0.676	0.6378	0.6361	
C11 (GPa)	116.0	126	-	118.82	113.5	166.8	
C12 (GPa)	22.6	26	-	22.27	22.8	67.2	
C44 (GPa)	45.0	48.5	-	44.96	43.2	20.9	
$S = (C_{11} - C_{12})/2C_{44}$	1.04	1.03	-	1.07	1.05	2.38	
Bulk Modulus B (GPa)	53.7	59	-	54.45	53.1	100.3	
Young's Modulus E(GPa)	106.7	-	116.9	111.79	-	81.5	
shear modulus G(GPa)	45.6	-	48.92	46.25	-	29.9	
Poisson ratio v	0.17	-	0.195	0.15	-	0.36	
Average Debye sound velocity (m/s)	5287.752	-	-	-	-	3192.67	
Debye temperature (K)	566.3	-	583	-	-	341.9	

Tahle	1.	Com	nuted	elastic	nror	nerties	for	Mas	li and	MoSrSi	i in co	mnarison	with	other	results
Lable	1.	COM	puteu	elasue	րւսի	Jet ties	101	TATAZC	л ани	ungoroi	ппс	)111pai 15011	with	other	results.

#### Table 2: Computed compliances for Mg<sub>2</sub>Si and MgSrSi.

Properties	Mg <sub>2</sub> Si	MgSrSi
S <sub>11</sub> (1/Mbar)	0.92	0.77
S <sub>12</sub> (1/Mbar)	-0.15	-0.22
S <sub>44</sub> (1/Mbar)	2.22	4.77

0.7071 -0.0002

0.7071

0.7071

-0.0005

-0.7071

Axis

Second axis

0.7071

-0.7071

0.0002

1.0000

-0.0002

#### Table 3: Stiffness matrix (GPa) for Mg<sub>2</sub>Si and MgSrSi

Input to I	ELATE (GPa)	
Mg <sub>2</sub> Si		
115.96	22.589 22.589 0 0	0
22.589	115.96 22.589 0 0	0
22.589	22.589 115.96 0 0	0
0	0 0 44.932 0 0	)
0	0 0 0 44.932 0	)
0	0 0 0 0 44.932	2
MgSrSi		
166.78	67.163 67.163 0 0	0
67.163	166.78 67.163 0 0	0
67.163	67.163 166.78 0 0	0
0	0 0 20.95 0 0	
0	0 0 0 20.95 0	
0	0 0 0 0 20.95	

#### **Table 4: Average properties**

0.5774

0.5773 -0.5774

Axis

0.0000

0.00001.0000 0.9659

0.0000

0.2588

Averaging scheme			Bulk mo	dulus	Young's modulus			Shear modulus		Poisson's ratio		
					Mg <sub>2</sub> Si							
Voigt			$K_{\rm V} = 53.714~{\rm GPa}$	Pa $E_{\rm V} = 106.69 \; {\rm GPa}$			$G_{V} = 45.634 \text{ GPa}$			0.16896		
Reuss			$K_{\rm R} = 53.714  \rm GPa$	E	= 106.66 GPa		$G_{\mathbf{R}} =$	45.618 GPa	$v_{\rm R} = 0$	0.16905		
Hill			$K_{\rm H} = 53.714 {\rm GPa}$	E <sub>H</sub>	I = 106.67 GPa		$G_{\mathrm{H}} =$	45.626 GPa	$v_{\rm H} = 0$	0.169		
					MgSrSi							
Voigt			$K_{\rm V} = 100.37 \; {\rm GPa}$	и — Е <sub>Л</sub>	<sub>7</sub> = 87.986 GPa		$G_{V} =$	32.494 GPa	$v_{\mathbf{V}} = 0$	0.3539		
Reuss			$K_{\rm R} = 100.37  {\rm GPa}$	E	= 75.017 GPa		$G_{\mathbf{R}} =$	27.27 GPa	$v_{\mathbf{R}} = 0$	0.37543		
Hill			$K_{\rm H} = 100.37 {\rm GPa}$	E <sub>H</sub>	I = 81.552 GPa		$G_{\mathrm{H}} =$	29.882 GPa	$v_{\rm H} = 0$	0.36458		
Table 5: Eig	envalues	of th	e stiffness ma	atrix								
λ <sub>1</sub>			$\lambda_2$	λ3	λ3			λ <sub>5</sub>		<sup>λ</sup> 6		
					Mg2Si					-		
44.932 GPa	4	14.932	2 GPa	44.932 GPa 93.37		76 GPa	GPa 93.376 GPa		161.14 GPa			1
					MgSrSi				I			
20.95 GPa 20.95 GPa		GPa	20.95 GPa 99.617			GPa 99.617 GPa			.11 GPa		1	
Table 6: Var	iations o	of the	elastic modu	li								ı 
	,	Young'	s modulus	Linear compressibility		Shear		modulus	Poisson's ratio			
	$E_{j}$	min	E <sub>max</sub>	β <sub>min</sub>	β <sub>max</sub>		, min	G <sub>max</sub>	v <sub>min</sub>	v <sub>max</sub>		
			-		]	Mg <sub>2</sub> Si						
Value	105.41	05.41 GPa 108.6 GPa		6.2057 TPa <sup>-1</sup> 6.2057 TPa <sup>-1</sup>		1 44.932	GPa	46.688 GPa	0.15941	0.18163	Valu	ıe
Anisotropy	1.03	3		1.0000		1.039			1.1394		Anis	sotropy
Axis	0.5774 0.0000 0.5774 0.0000 0.5773 1.0000		0.0000 0.0000 1.0000	0.0000 0.0000 1.0000	0.5000 0.0000 0.8660	0.0000 0.0000 1.0000	) ) )	0.7071 -0.0002 0.7071	0.7071 0.0000 0.7071	0.7071 -0.0000 -0.7071	Axis	ŝ
						0.9397 0.3420 -0.000	) 0	0.7071 -0.0006 -0.7071	0.0000 1.0000 -0.0000	-0.7071 0.0002 -0.7071	Seco	ond axis
	•				Ň	IgSrSi				•		
Value	58.762	GPa	128.22 GPa	3.3211 TPa <sup>-1</sup>	3.3211 TPa	1 20.95	GPa	49.809 GPa	0.15219	0.62209	Valu	ie
Anisotropy	2.182	2.182		1.0000	I			•	4.0877		Anis	otropy

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0.0000

0.00001.0000

1.0000

0.0002

-0.5624

0.7330 0.3827 0.7071 -0.0003

0.7071

0.7071

-0.0005

-0.7071



Figure 5: 2D and 3D Projection of Spatial dependence of Young's Modulus for Mg<sub>2</sub>Si and MgSrSi Transactions of the Nigerian Association of Mathematical Physics Volume 13, (October - December, 2020), 9–20



Figure 6: 2D and 3D Projection of Spatial dependence of linear compressibility for Mg<sub>2</sub>Si and MgSrSi



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Figure 8: 2D and 3D Projection of Spatial dependence of Poisson's ratio for Wig2Si and WigSrSi

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# 4. Conclusion

The elastic and thermal properties of metallic alloys are important characteristics that inform as well as direct their applicability in the design of modern projects ranging from photonics to thermionics, to production of cutting tools and automobile parts. Owing to the foregoing this study evaluated by way of computational modeling the elastic and thermal properties of MgXSi (X=Mg, Sr) compounds employing the projector augmented wave (PAW) variant of pseudo-potential plane-waves approach, for the exchange and correlation potential. Elastic constants and elastic compliances of MgXSi as well as the vibrational free energies, entropy, constant volume specific heat capacities were computed. This study recorded anelastic constant,  $C_{11}$  of 166.8GPa at the Debye temperature of 341.9K for MgSrSi. At 300K, the constant volume specific heat capacity,  $C_{\nu}$  for Mg<sub>2</sub>Si and MgSrSi were 62.8 J/K/(N mol) and 70 J/K/(N mol) respectively.From the results, it is concluded that the elastic constants of Mg<sub>2</sub>Si is quite consistent with theoretical results already recorded on the subject and compares favourably with experimental data. It is submitted that the elastic and thermodynamic of MgXSi(X=Mg,Sr) has been successfully computed. Thus, It may be concluded that at a fixed volume, the thermodynamic or heat capacity of MgXSirises with temperature even at low temperatures.

# ACKNOWLEDGEMENT

## A Eulogy to anEminent Professor: Prof.John O.A. Idiodi

Unarguably some scholars are born and some are made. Permit me to rightly accord the 'born' perspective to my erudite scholar and mentor who I could unequivocally attest to the fact that my meeting with him in 2011 marked the beginning of my odyssey to fulfilling my life's destiny as ordained by God.

Our beloved Prof! You are not just a scholar for there are millions of scholars the world over, but you have unambiguously and meritoriously distinguished yourself from the millions of scholars. You have proved that a scholar can be a true mentor, a father, an advocate, a friend, confidant, and a colleague all at the same time. You are indeed a rare gem and posterity will ever attest to the positive influence you enshrined on the hearts and future of many of us who were opportune to pass through your mentorship.

Our Dear Professor, you will always remain revered and evergreen in our heart of hearts. You came! You saw! You conquered and won. Your meritorious and untainted service shall ever glow beyond the academic skies. We are convinced you are not tired, but as the chapter 3 and verse number 1 of the bible book of Ecclesiastes rightly averred: "To everything there is a season, and a time to every purpose under heaven..." Your service to humankind has outlasted many seasons but my Prof, it is our belief that your retirement from active service is a substantive evidence that cannot be controverted anywhere.

My Prof. I cannot possibly fathom all that you did but our collective prayer for you is this: May the good Lord bless you, strengthen you, cause his face to shine upon you, and add to you many more happier years in Jesus name. Amen.– Dr. A.S. Olayinka

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