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الطرق شبه التجريبية لتقييم الخصائص الحرارية والإلكترونية النظرية لأكسيد الجرمانيوم(GeO_2) ، أكسيد السيليكون(SiO_2) ، وأكسيد السيلينيوم(SeO_2)

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الملخص:

استخدمنا المحاكاة بواسطة برامج كمومية شبه تجريبية (WinMopac7.21 و Hyper Chem8.0) لدراسة جزيئات الأكاسيد العازلة غير الخطية مثل ثاني أكسيد الجرمانيوم(Germanium Dioxide – GeO_2) ، ثاني أكسيد السيليكون(Silicon Dioxide – SiO_2) ، وثاني أكسيد السيلينيوم (Selenium Dioxide – SeO_2). هدف هذا البحث هو تحقيق أفضل شكل جزيئي مع الحفاظ على أقل طاقة كلية ممكنة للجزيء. تمت دراسة الخواص الكهربائية والحرارية لجزيئات GeO_2 و SiO_2 و SeO_2. وتمت دراسة الخصائص الحرارية بالنسبة لدرجة الحرارة ضمن مدى (100 إلى 2000) كلفن .(K) كما تم فحص الطاقة الكلية كدالة للمسافة بين الذرات، بالإضافة إلى حساب الخصائص الطاقية. تم دراسة الترددات الاهتزازية، الجهد الكهروستاتيكي، كثافة الشحنة الكلية، مستوى هومو (HOMO) ومستوى لومو .(LUMO) أظهرت النتائج أن جميع المركبات المدروسة هي مواد عازلة وتمتلك فجوة طاقة كبيرة بسبب تأثير الأكسيد على الجزيئات.

الكلمات المفتاحية: ثاني أكسيد الجرمانيوم(GeO_2) ، ثاني أكسيد السيليكون(SiO_2) ، وثاني أكسيد السيلينيوم(SeO_2) ، شبه تجريبي كوانتمي(semi-empirical quantum) ، الجهد الكهروستاتيكي (electrostatic potential)، أعلى مدار جزيئي مشغول(HOMO) ، وأدنى مدار جزيئي غير مشغول (LUMO).

Semi-Empirical Methods for the Theoretical Evaluation of the Thermal and Electronic Properties of GeO_2, SiO_2 and SeO_2

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Abstract:

We use simulations with semi-empirical quantum programs (WinMopac7.21 and Hyper Chem8.0) to look into the nonlinear insulating oxide molecules Germanium Dioxide(GeO_2),Silicon Dioxide(SiO_2) and Selenium Dioxide(SeO_2). The objective

of this effort is to maximize molecular form while maintaining the lowest feasible molecular total energy. This study has investigated the electrical and thermal properties of GeO_2 , SiO_2 and SeO_2 . Thermal properties have been studied in connection with temperature in the (100 to 2000) K range. The total energy as a function of interatomic distance was investigated in addition to computing the energetic properties.Vibrational frequencies, electrostatic potential, total charge density, HOMO, and LUMO have all been studied. The findings indicated that all examined compounds are insulators with a significant energy gap attributable to the oxide's influence on the molecules.

Keywords: Germanium Dioxide(GeO_2),Silicon Dioxide(SiO_2) and Selenium Dioxide(SeO_2), semi-empirical quantum, electrostatic potential, HOMO, and LUMO

Introduction

1. Computational Information

The computational research was conducted using semi-empirical quantum programs (WinMopac v.7.21 and Hyper Chem v.8.0) and the MNDO/PM3 methodology.

The Energy gap $\mathbf{E_g}$ for every The calculation of a molecule is feasible.

using the following formula: (17 – 20)

$$\mathbf{Eg = ELUMO – EHOMO}$$

E_{HOMO} represents The energy of the molecular orbital with the maximum occupancy,

whereas E_{LUMO} The lowest vacant molecular orbital's energy.The Electron Affinity (E.A.) and Ionization Potential (I.P.) can be calculated by applying the Koopman theorem. (20 – 23) :

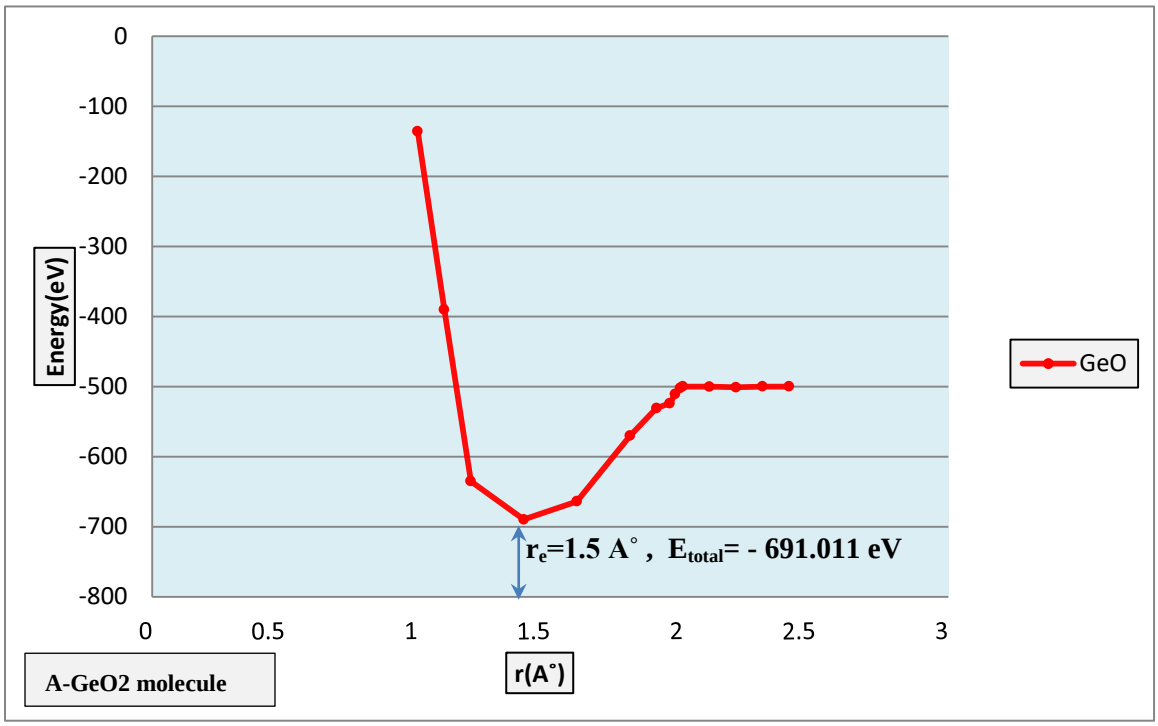
$$I.P = - E_{HOMO}$$

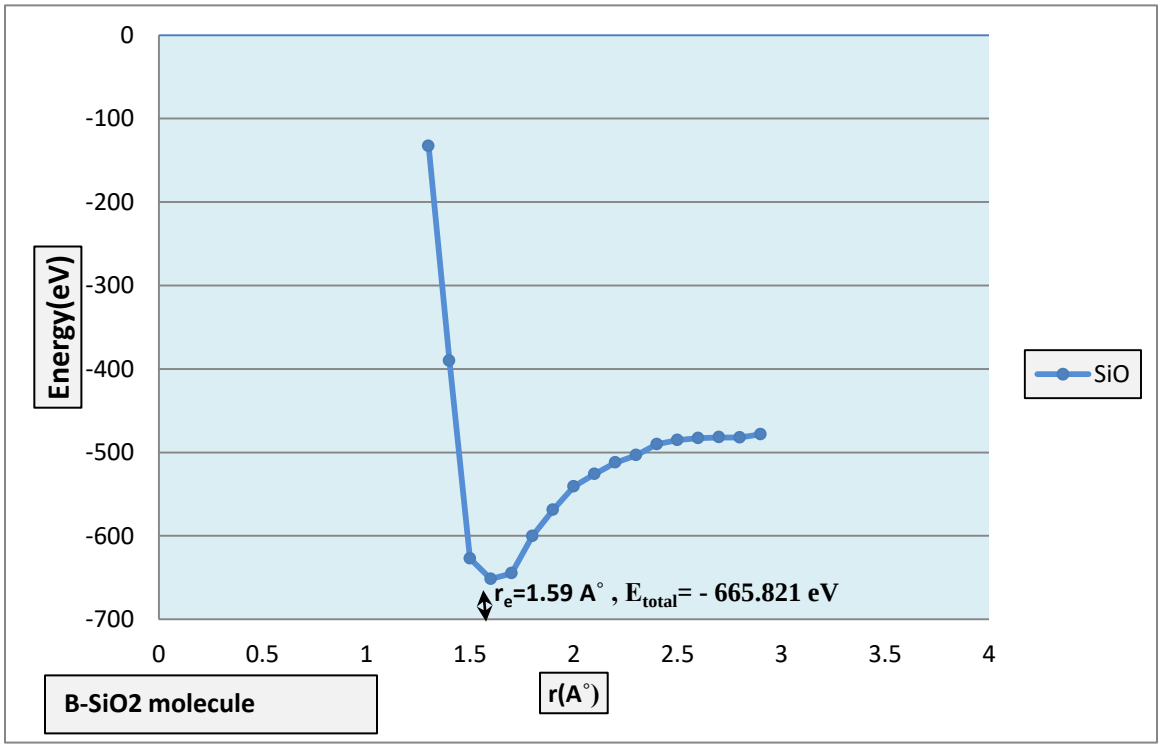
$$E.A = - E_{LUMO}$$

The structure of molecules with a low free energy was optimized using the MNDO/PM3 method to calculate total energy, binding energy, Ionization potential, electron affinity, and electrical energy, electrical characteristics like total charge density, molecule electrostatic potential, HOMO, and LUMO energies, and thermal characteristics like heat of formation, enthalpy, heat of capacity, and entropy

Results and Discussion

The interatomic distance, or bond length, is plotted against the total energy of all the molecules under investigation (Germanium Dioxide-GeO_2,Silicon Dioxide-SiO_2 and Selenium Dioxide - SeO_2) in Figure (1:A,B,C). The total energy is found to decrease with increasing interatomic distance until it reaches the lowest total energy at a specific distance called the equilibrium distance. The (nucleus-nucleus) repulsion causes atoms' kinetic energy to increase, which raises the total energy above the equilibrium distance. As the interatomic distance grows, Until the connection in the molecule breaks and it separates into individual atoms, the restored force gradually diminishes. The equilibrium separations, OF The (Germanium Dioxide molecule)(Ge=O), (Silicon Dioxide molecule) (Si=O), and (Selenium Dioxide molecule)(Se=O) bonds were (1.5, 1.59, and 1.3)A°, respectively, as shown in Figure 1. The lowest total energy values, which were(-691.011, -665.821, and -621.741) eV, respectively, were correlated with these values.


0
-100
-200
-300
-400
-500
-600
-700
-800
Energy(eV)
0
0.5
1
1.5
2
2.5
3
r(A°)
re=1.5 A° , Etotal= - 691.011 eV
GeO
A-GeO2 molecule


0
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Energy(eV)
0
0.5
1
1.5
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4
r(A°)
re=1.59 A° , Etotal= - 665.821 eV
SiO
B-SiO2 molecule

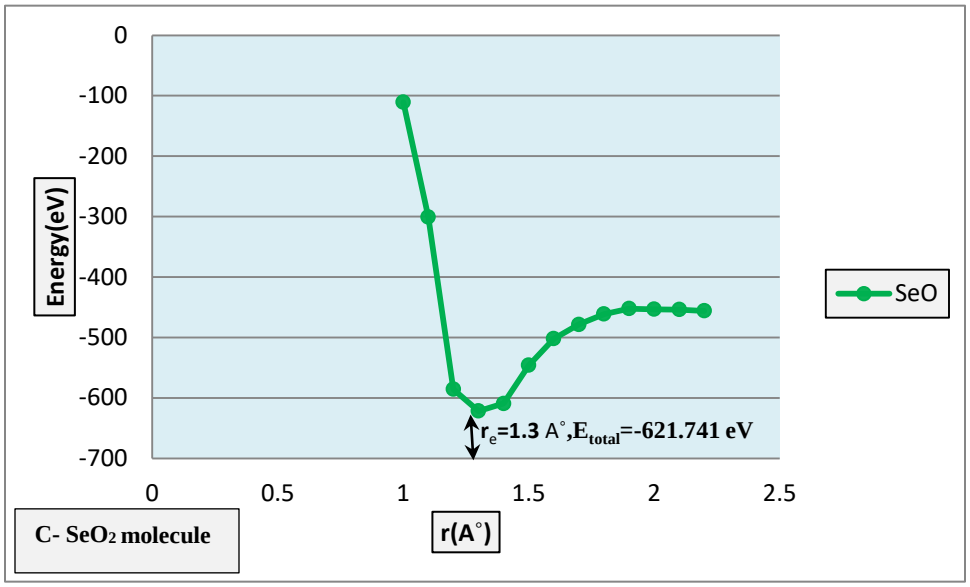

Fig. 1: Total energies of (**A-GeO_2 , B-SiO_2 and C- SeO_2**) molecules respectively with variation of interatomic distance

The energetic properties of each of the molecules under investigation, including their electric energy, ionization potential, binding energy, total energy, and electron affinity,

were computed and recorded at the equilibrium distance in Table 1. Furthermore, all of the molecules under study had their vibrational frequencies determined with intensity and symmetry for each frequency, as indicated in Table 2. According to The vibratory movements in Fig. 2 illustrate the three vibration modes that exist according to the rule (3N-6) for nonlinear molecules [24].

Table 1: Properties of the energy Germanium Dioxide ,Silicon Dioxide and Selenium Dioxide molecules

Qualities	Germanium Dioxide	Silicon Dioxide	Selenium Dioxide
Total energy – eV	-682.2131	-668.9326	-790.4411
Binding energy – eV	-10.9975	-9.8501	-7.9978
Electronic energy– eV	-1135.3947	-1116.9858	-1321.2307
Ionization Potential– eV	11.54393	9.064424	11.48217
Electron Affinity – eV	1.527	1.124	2.427

Table 2: Germanium Dioxide ,Silicon Dioxide and Selenium Dioxide molecules' vibrational frequencies with intensity and symmetry.

Molecule	Number of Vib.	Wave number (cm^{-1})	Intensity (km/mol)	Symmetry
Germanium Dioxide	first	664.3166	24.988	1A1
	second	739.5211	7.979	1B2
	third	1062.7320	13.987	2A1
Silicon Dioxide	first	270.5325	14.441	1A1
	second	665.5431	0.743	2A1
	third	682.8087	12.595	1B2
Selenium Dioxide	first	781.0988	16.934	1A1
	second	898.1123	11.093	1B2
	third	1301.654	16.007	2A1

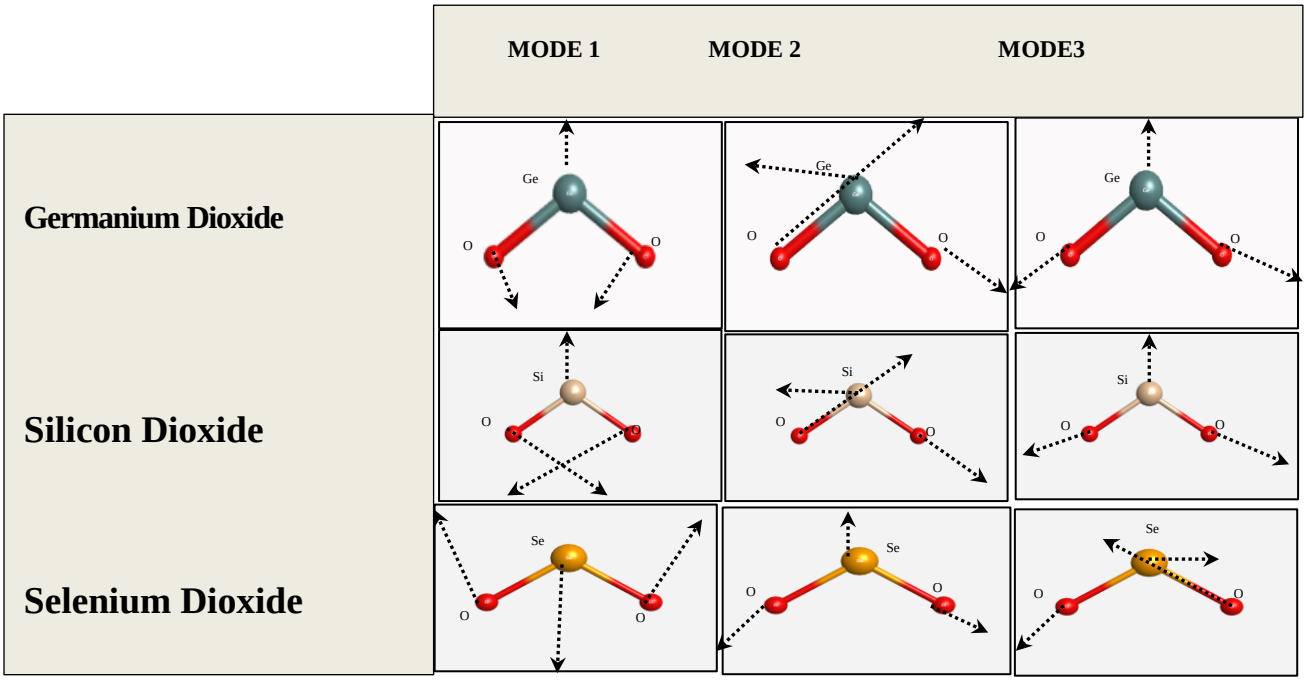

Fig. 2: GeO2, SiO2, and SeO2 molecules' vibrational mode

The Thermal characteristics of the Germanium Dioxide ,Silicon Dioxide and Selenium Dioxide molecules' are shown in Table 3 and were computed at room temperature using the MNDO/PM3 method and the WinMopac 7.21 application. The way that the thermal characteristics (entropy, enthalpy, capacity, and heat of

formation) behave in relation to temperature in the (100-2000)K range was examined, as depicted in Figures 3, 4, 5, and 6. The relationship between temperature and the Heat of Formation, as demonstrated by the linear relationship between the two variables in Figure 3.

The linear relationship between enthalpy and temperature change—in which rising temperatures lead to rising enthalpy levels—is depicted in Figure 4. The direct proportionality between temperature and heat of capacity is shown in Figure 5, where it is observed that at high temperatures, the curve drifts towards stability. Additionally, as Fig. 6 illustrates, entropy shows a linear trend with temperature variation.

Table 3: Thermal characteristics of Germanium Dioxide, Silicon Dioxide, and **Silicon Dioxide** molecules at room temperature

Thermal properties	Germanium Dioxide	Silicon Dioxide	Selenium Dioxide
Heat of Formation (Kcal/mol)	-73.449	-60.298	-61.547
Enthalpy (cal/mol)	2776.088	4832.72	2611.21
Heat of capacity (cal/K.mol)	11.543	11.879	10.721
Entropy (cal/K.mol)	64.77	83.046	64.981

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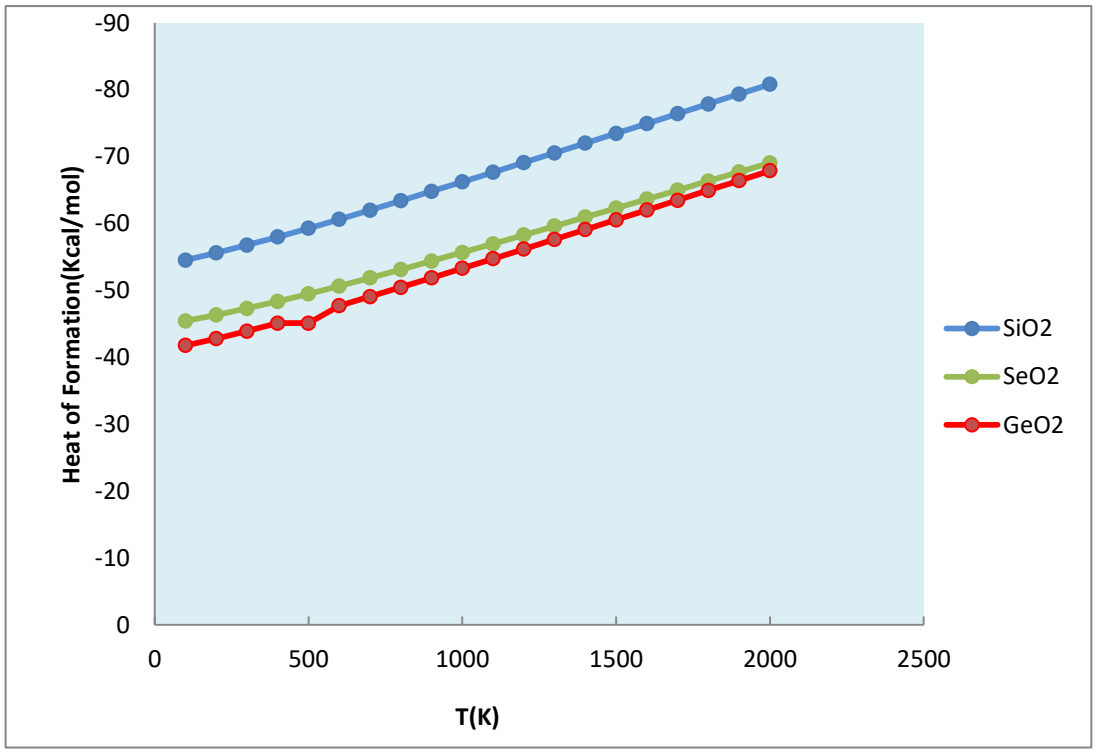

F ig.3: B ehavior of Heat of Formation with temperature

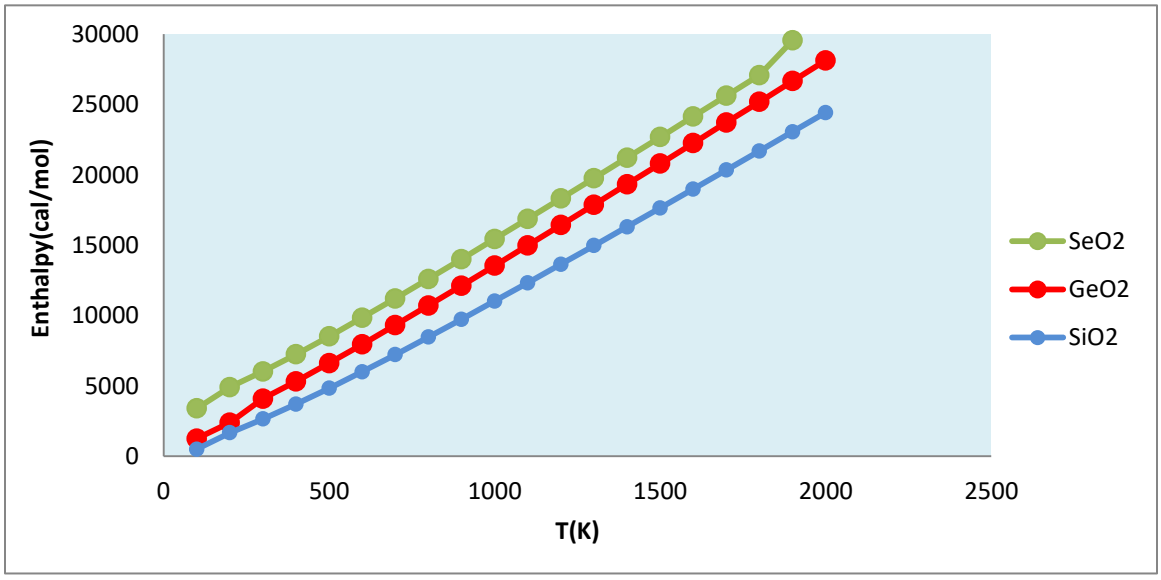

Fig.4: Behavior of Enthalpy with temperature

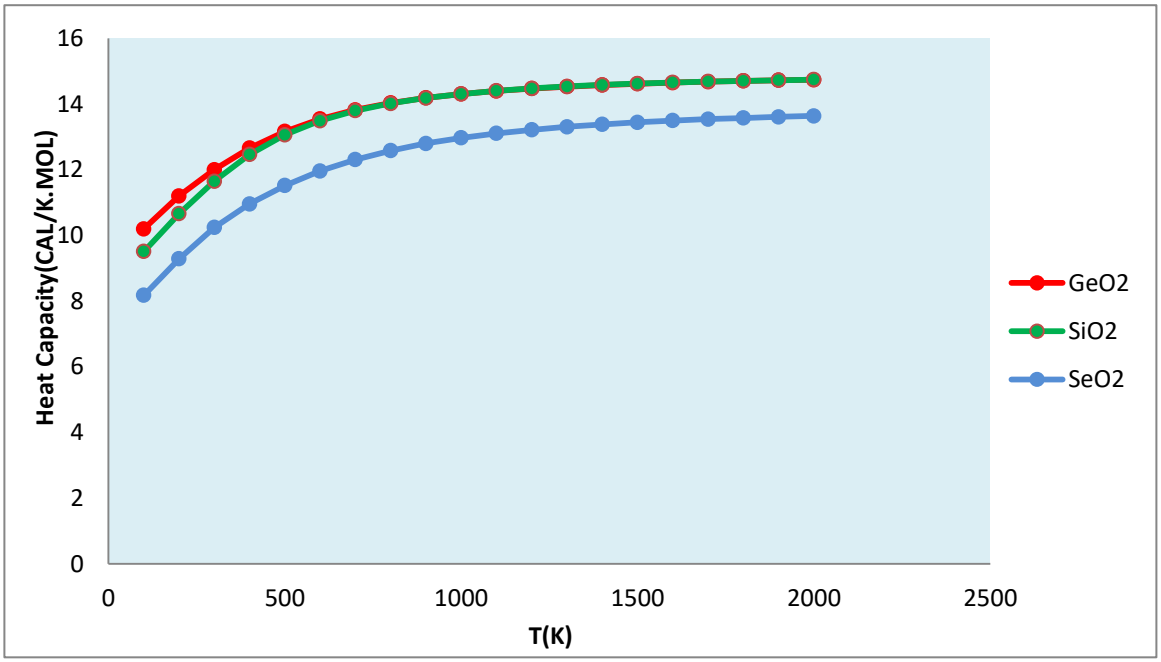

Fig.5: Behavior of Heat of Capacity with temperatur

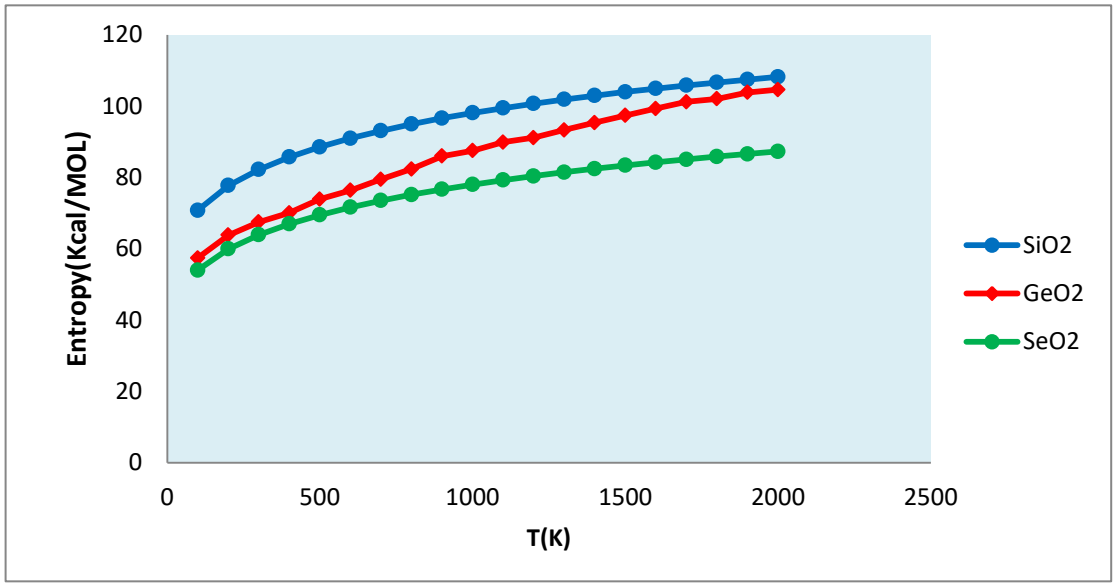

Fig.6:Entropy's Temperature-Related Behavior

The Hyperchem program's calculation of the energy values of the electrons' occupied and empty orbitals with a declaration of the symmetry molecules was one of its primary functions (HOMO - LUMO). After the molecule reached the equilibrium distance, or its ideal position, Fig. 7 displays a schematic of the energy gap for each of the molecules being examined. Energy gap values of 8.97, 10.83, and 6.53 eV are noteworthy for germanium dioxide, silicon dioxide, and selenium dioxide, respectively. For the HOMO-LUMO molecules (1P1G-2P1U, 1P1G-2P2U, and 1S1G-2P1U), these values represent the corresponding symmetry values.

Figures 8, 9, and 10 display the GeO2, SiO2, and SeO2 molecules' electrostatic potential, HOMO, LUMO,and total charge density.

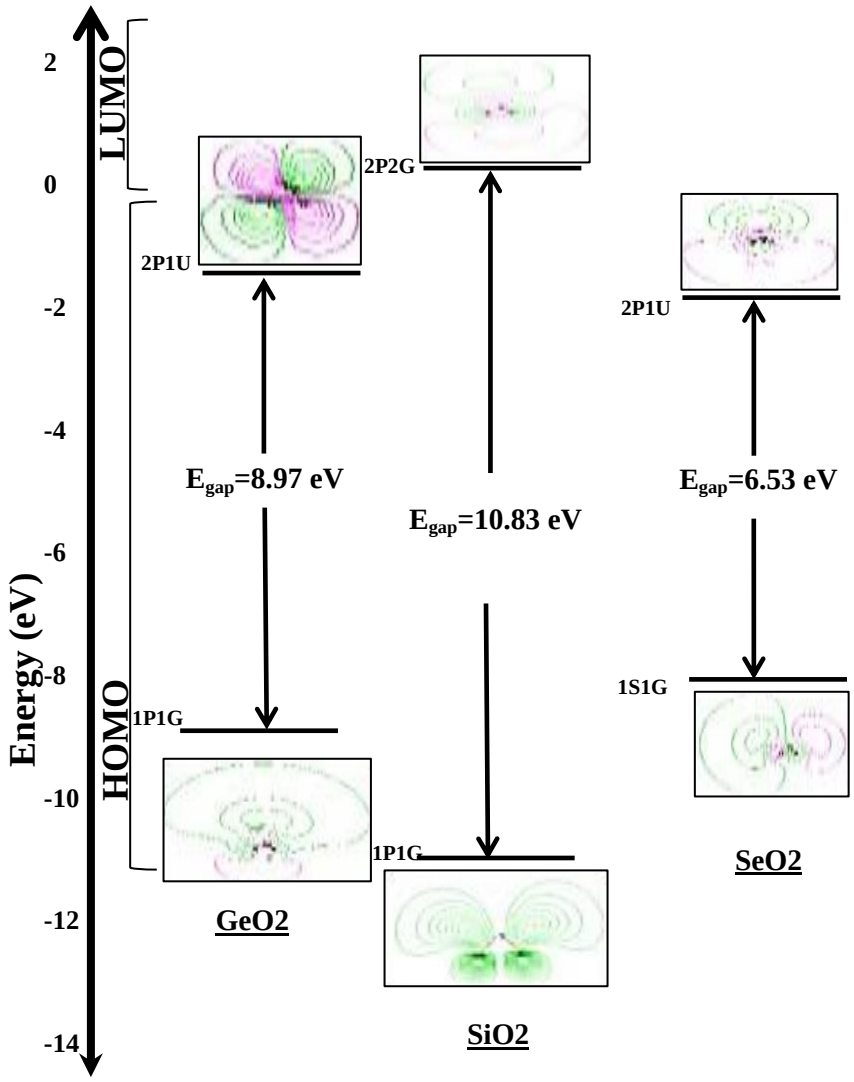

Fig.7 : GeO2, SiO2, and SeO2 molecular energy gap

GeO_2 molecule **SiO_2molecule** **SeO_2molecule**

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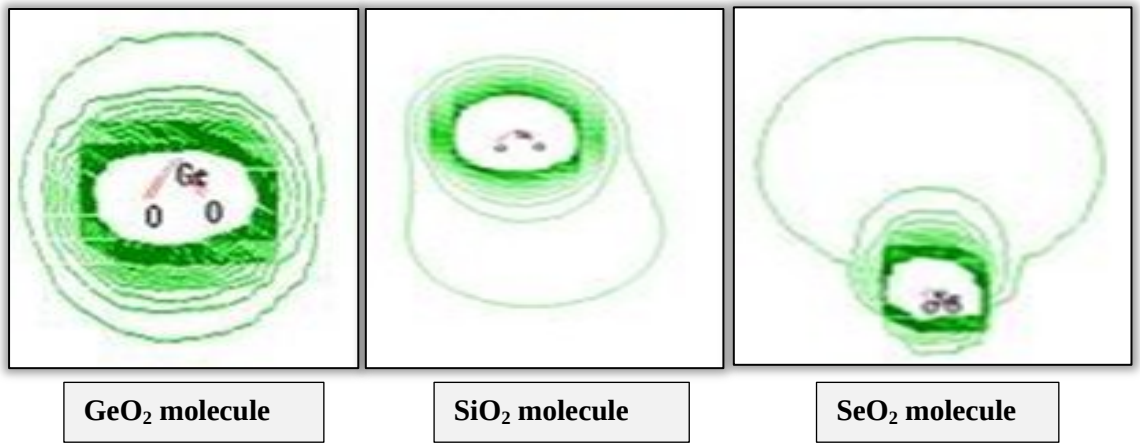
Fig.8 : Molecules of GeO2, SiO2, and SeO2 total charge density



GeO_2 molecule **SiO_2 molecule** **SeO_2 molecule**

Fig.9Distribution Geometry The electrostatic potential of molecules

of GeO2, SiO2, and SeO2

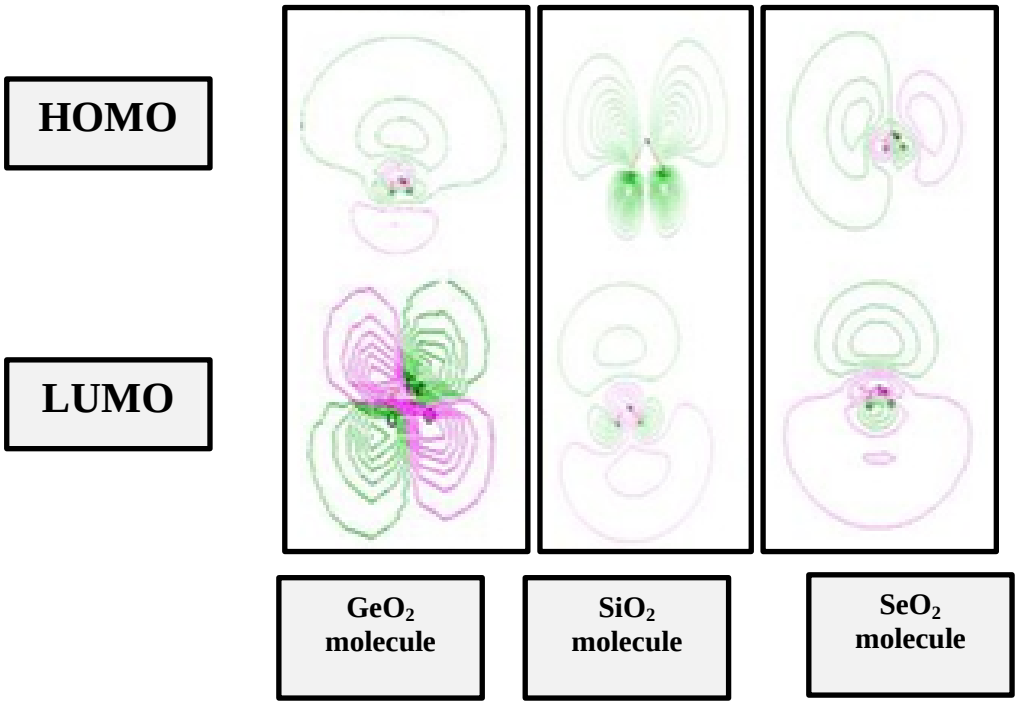


Fig.10: HOMO and LUMO molecular orbitals of GeO2, SiO2, and SeO2 molecules

1. Conclusions

When the distance between the atoms is more than the equilibrium distance, the total energy of all the molecules under study increases. The equilibrium distance of GeO2.The lowest total energy is found in SeO2 molecules. The molecules' thermal characteristics made it abundantly evident that their behavior matched the temperature range of (100-2000)K.The relationship between temperature and enthalpy and heat of formation is linear. In contrast to heat of capacity, entropy varies somewhat at low temperatures and considerably at high ones. The high space energy value of all molecules indicates that the oxide has an effect on them since they are insulators. This is due to oxygen's high electronegativity, which has a big impact on all molecules. Because of their strong electronegativity, the electrical characteristics data indicated that the electron lines congregated near the two oxide atoms.

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