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Transition State interaction between Tin-Dioxide and Water using the Density Functional Theory (DFT)

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Abstract

Tin dioxide $Sn_{10}O_{16}$ clusters reaction with water H_2O is examined utilizing the transition state method and Density Functional Theory (DFT) with (B3LYP) level and two basis set SDD for heavy atoms such as (Sn) and 6-311G** for light atoms, such as (O, H). Gaussian 09W program is used to calculate electronic properties like (HOMO, LUMO) levels, energy gap, density of state. Spectroscopic properties, such as IR and Raman in addition, the thermodynamic features, such as Gibbs free energy, enthalpy, and entropy. In order to study reaction and activation, Gaussian View 05 is used for geometrical structure optimization. It was found that an increase in conductivity results from a decrease in the energy gap of tin dioxide in water. The Gibbs free energy of the interaction of tin dioxide with water is positive which indicates that the reaction is endergonic, and the process of reaction could be photocatalysis with a photon energy of 3.7 eV.

Keywords: Tin- dioxide, humidity sensor, Transition state method and density functional theory (DFT).

تفاعل الحالة الانتقالية بين ثنائي اوكسيد القصدير والماء باستخدام نظرية دالية الكثافة

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الخلاصة

تم دراسة تفاعل مجموعات ثاني أكسيد القصدير $Sn_{10}O_{16}$ مع الماء H_2O باستخدام طريقة الحالة الانتقالية ونظرية دالية الكثافة (DFT) بمستوى (B3LYP) ومجموعتي أساس SDD للذرات الثقيلة مثل (Sn)و 6-311G**للذرات الخفيفة مثل (O, H).تم استخدام برنامج Gaussian 09W لحساب الخصائص الإلكترونية مثل مستويات (HOMO, LUMO)وفجوة الطاقة وكثافة الحالة. تم التحقيق في الخصائص الطيفية مثل الأشعة تحت الحمراء ورامان بالإضافة إلى السمات الديناميكية الحرارية مثل طاقة جيبس الحرة والانثالبي والإنتروبي للتفاعل والتنشيط. تم استخدام طريقة Gaussian View 05 لتحسين البنية الهندسية. وقد وجد أن انخفاض قيمة فجوة الطاقة لثاني أكسيد القصدير في وجود الماء يؤدي إلى زيادة في الموصلية. إن طاقة جيبس الحرة لتفاعل ثاني أكسيد القصدير مع الماء موجبة مما يدل على أن التفاعل هو

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تفاعل ماص للحرارة وأن عملية التفاعل ممكن ان تتم بتحفيز ضوئي باستخدام طاقة فوتون 3.7 الكترون فولت.

1. Introduction

Tin dioxide (SnO_2) is a stable metal oxide with a crystal structure. It is an n-type with wide-bandgap of approx. (3.4–3.6) eV. According to SnO_2 intriguing characteristics, this metal oxide may interfere with the chemical and physical perception of oxygen and water vapor [1-9]. SnO_2 is the best choice for applications in photocatalysis, photodetection, solar cells, catalysis, lithium-ion batteries, and humidity sensors due to its long-term stability, low pollution level, and extremely high thermal resistance. On the one hand, it exhibits very stable chemical behavior and is environmentally friendly. On the other hand, the material is susceptible to change in electrical properties after deposition. Besides, the addition of precious metals in catalyst compositions allows SnO_2 to display the highest electrical conductivity [10-14].

Water vapor in the atmosphere has increased due to the rising greenhouse effect, affecting several industries. Humidity sensors are essential for monitoring moisture levels, ensuring optimal conditions in climate studies, healthcare, agriculture, aerospace, and industry [15-17]. The use of metal oxides or metal ions improved the sensing performance of SnO_2-based sensors. This treatment ensures the structural integrity while introducing heterogeneous interfaces that lead to optimal water adsorption and desorption, thus improving efficiency [18-21].

Theoretical aspects of the sensing mechanisms are less investigated than experimental procedures. Most of these calculations used density functional theory [22-25]. The novelty of this computational theoretical research lies in studying the electronic and spectroscopic properties, as well as the reaction between a tin dioxide cluster and water, using the transition state method and density functional theory, with the aim of developing a humidity sensor.

2. Methodology

The theoretical results, when compared with practical results, were well matched by the electron density-based technique known as density functional theory. Using the B3LYP level of Density Functional Theory (DFT) (Becke three-parameter, Lee-Yang-Parr), the structure and various properties of the sensing materials were analyzed. For lighter atoms like oxygen and hydrogen, the 6-311G** basis set was applied, while the Stuttgart/Dresden (SDD) basis set was used for heavier atoms like tin. The Gaussian 09W molecular software was employed during the calculations, along with Gaussian View 05, which served as a supplementary tool to examine the geometric structure [26-43]. Figure 1 shows the geometrical optimization of (a) $Sn_{10}O_{16}$ cluster, (b) H_2O molecule, (c) reaction between $Sn_{10}O_{16}$ cluster, and H_2O molecule, where a scaling factor of 0.967 was applied to the computed vibrational frequencies.

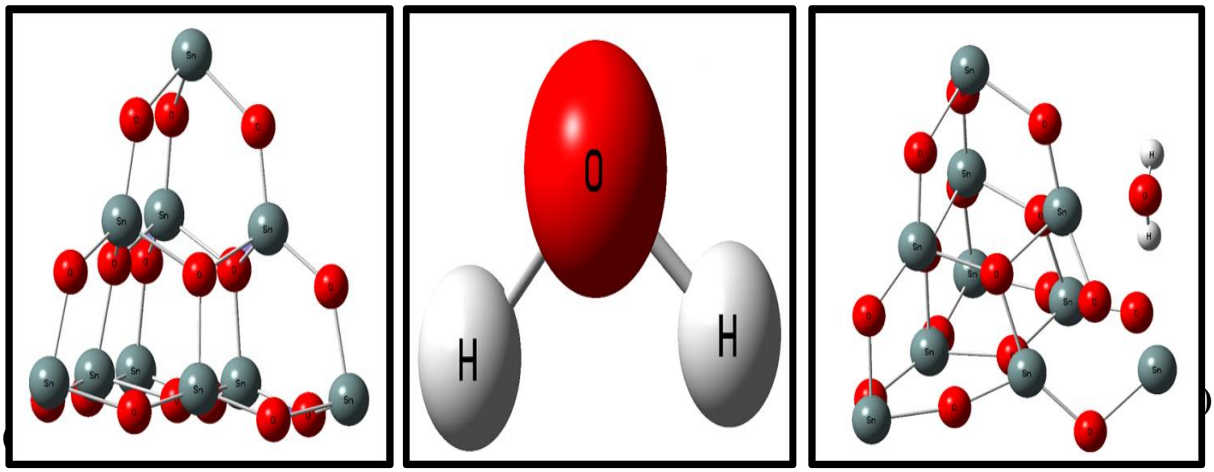


Figure 1: Geometrical optimization of (a) $Sn_{10}O_{16}$ cluster (b) H_2O molecule (c) reaction between $Sn_{10}O_{16}$ cluster with H_2O molecule using Gaussian view 05 program.

The following equations clarify the interaction amongst $Sn_{10}O_{16}$ cluster and H_2O:

$$Sn_{10}O_{16} + H_2O[Sn_{10}O_{16}... H_2O]^A \rightarrow [Sn_{10}O_{16}... H_2O]^{\dagger\dagger} \rightarrow Sn_{10}O_{17} + H_2 \quad (1)$$

$$[Sn_{10}O_{16}.....H_2O]^A \rightarrow Sn_{10}O_{17} + H_2 \qquad \Delta G = 3.7 \text{ (eV)} \quad (2)$$

$$[Sn_{10}O_{16}.... H_2O]^A \rightarrow [Sn_{10}O_{16}.... H_2O]^{\dagger\dagger} \qquad \Delta G = 4.54 \text{ (eV)} \quad (3)$$

$$H_2O \rightarrow H_2 + \tfrac{1}{2} O_2 \qquad \Delta G = 2.83 \text{ (eV)} \quad (4)$$

Eq.1 summarises all the reaction. In the provided equations, ΔG represents the difference in Gibbs free energy related to the reaction. Eqs.2 and 3 represent the adsorption mechanisms and transition state. It can be seen that the cluster $Sn_{10}O_{16}$ is unstable and converts to $Sn_{10}O_{17}$ when it is exposed to oxygen from water. It is noted that ΔG activation is the Gibbs free energy with a positive value, and the system needs a photon with energy equal to (3.70 eV), this process is called photocatalysis. Eq.4 represents the probability of water analysis.

3. Results and Discussion

3.1 Electronic properties

Electronic characteristics, such as density of state as a function of energy levels, HOMO levels, LUMO levels, and energy gap were studied. The following equation was used to compute the energy gap. The difference in energy between the last level of HOMO and the first level of LUMO is described by Eq. 5 [44,45]:

$$Eg = |LUMO - HOMO| \quad (5)$$

Fig. 2 shows the density of state of (a) $Sn_{10}O_{16}$, (b) H_2O, and (c) $Sn_{10}O_{16}$ reaction with H_2O as a function of the energy levels. The energy gap between HOMO and LUMO was calculated, which was (3.8, 8.9, and 3.75) eV, respectively. It was found that the tin dioxide energy gap decreased in the presence of water due to the addition of levels within the tin dioxide energy gap, which decreased the resistivity and increased the conductivity.

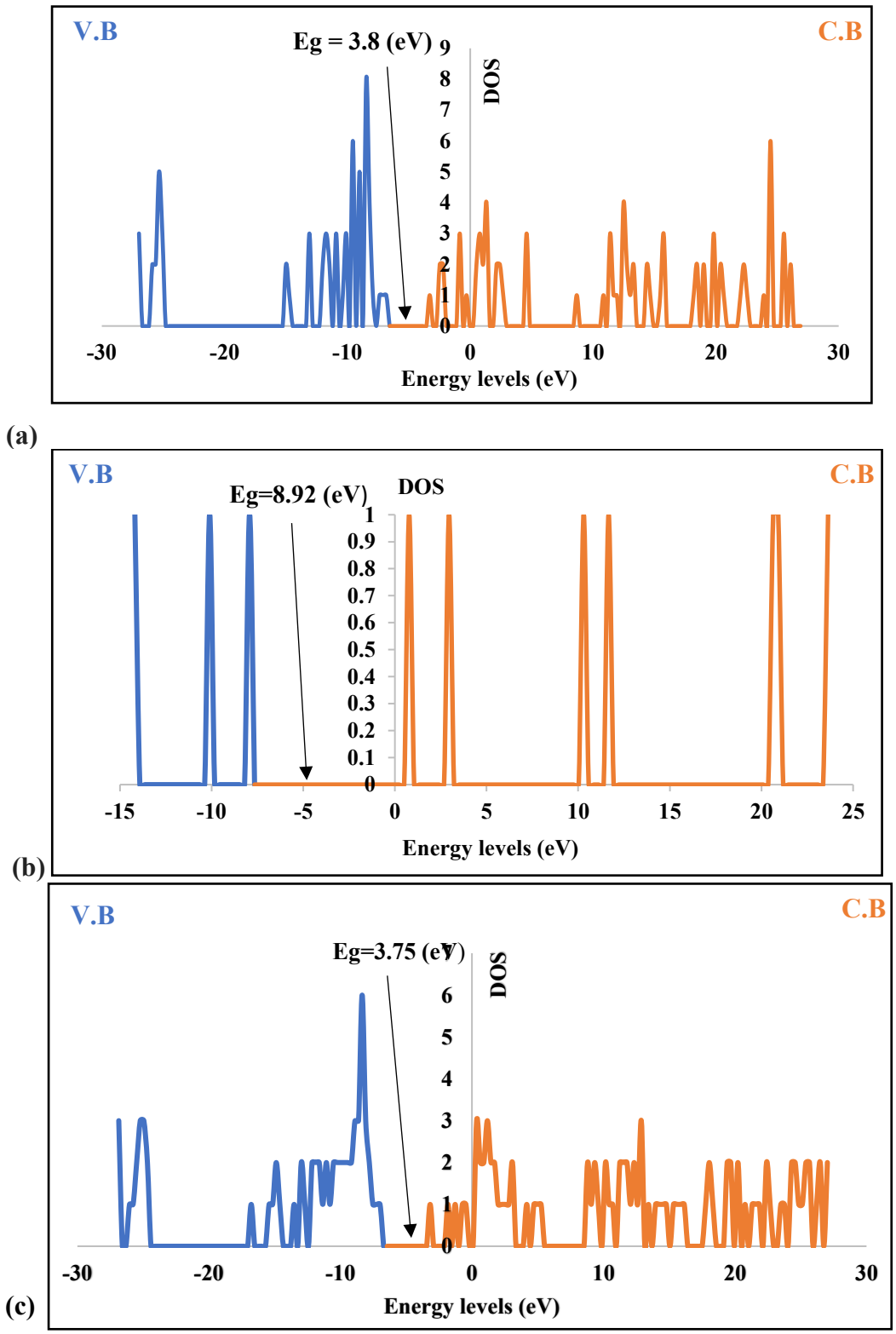


Figure 2: Density of states for (a) $Sn_{10}O_{16}$ (b) H_2O and (c) reaction $Sn_{10}O_{16}$ with H_2O

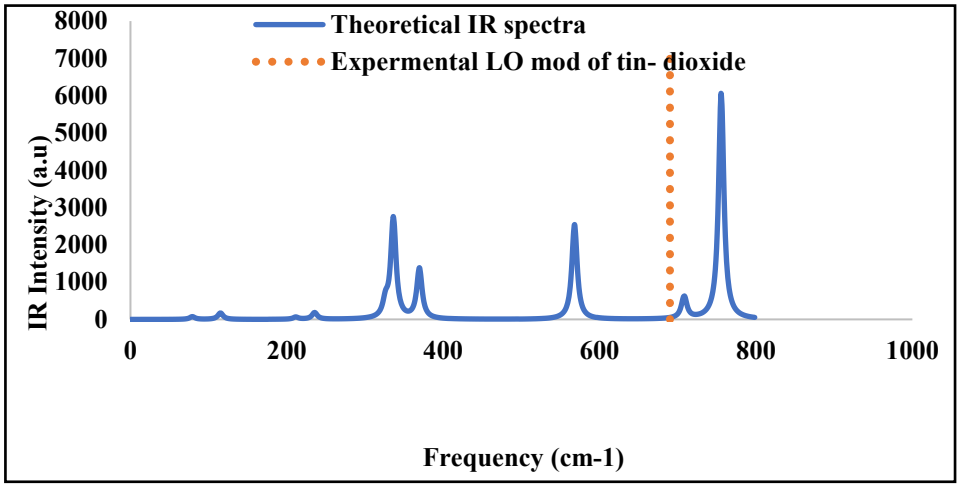
3.2 Spectroscopic properties

Figures 3, 4, and 5 display the IR and Raman spectra of tin dioxide, water and their reactions. The findings were compared with the Longitudinal Optical (LO) mode experimental value of tin dioxide, which is 690 cm^{-1} [46]. Whereas O-H bending and O-H stretching occurred at

about 1400 cm^{-1}, 3600 cm^{-1} and 3649 cm^{-1}, respectively [47,48].

High-intensity peaks in the IR spectrum were observed at frequencies of 744 cm^{-1}, 1640 cm^{-1}, 2944 cm^{-1}, and 3840 cm^{-1} due to the interaction between tin dioxide and water, which is in good agreement with the experimental results.

(a)



(b)

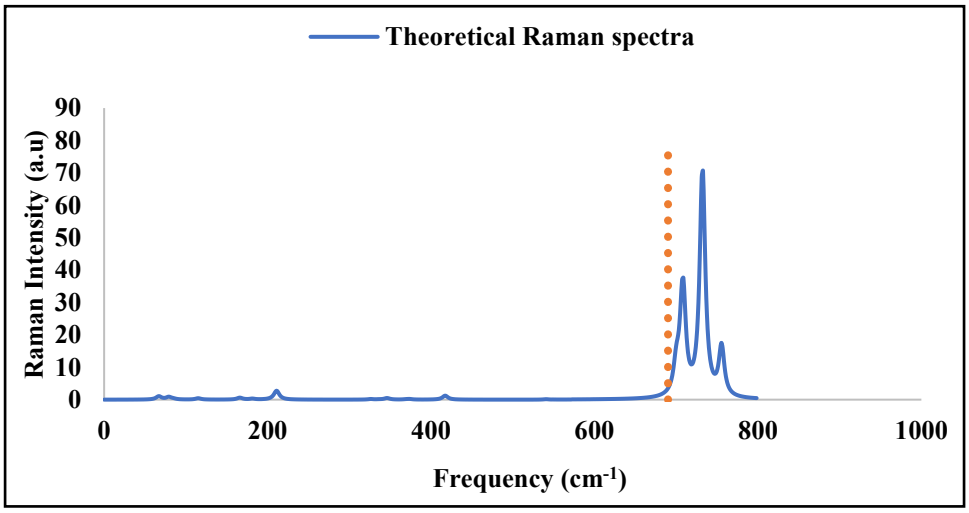
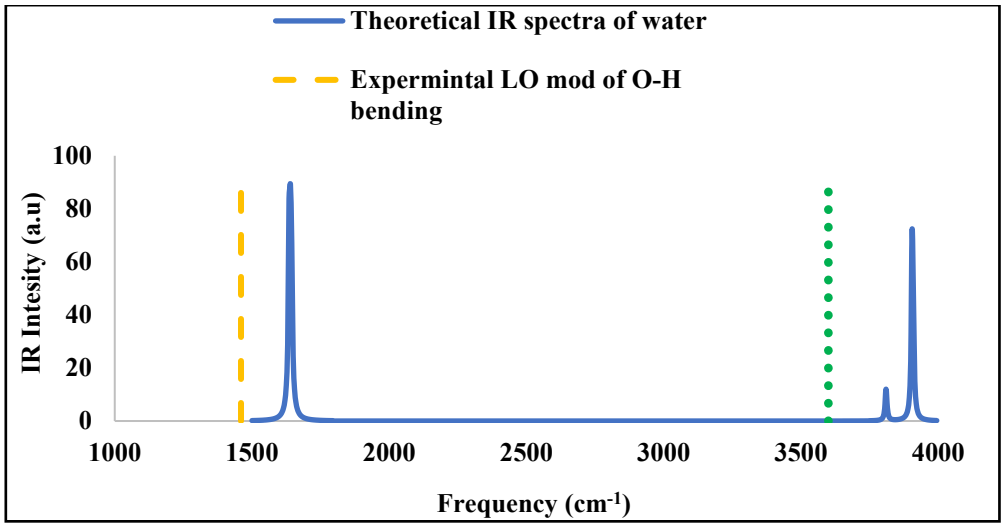
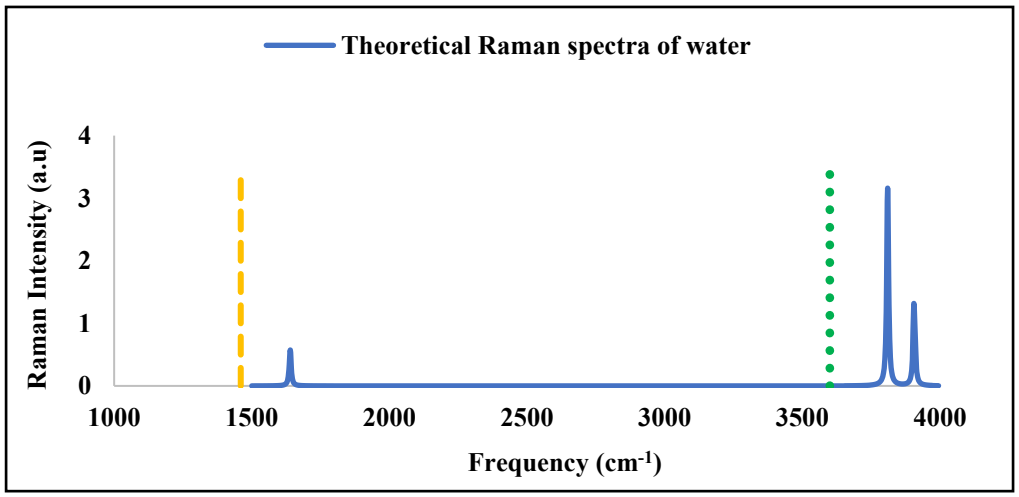


Figure 3: (a) IR intensity (b) Raman intensity for tin dioxide ($Sn_{10}O_{16}$) as a function of frequency compared with the experiment longitudinal optical (LO) mode.



(a)



(b)

Figure 4: (a) IR intensity (b) Raman intensity for H_2O as a function of frequency compared with the experiment longitudinal optical (LO) mode.

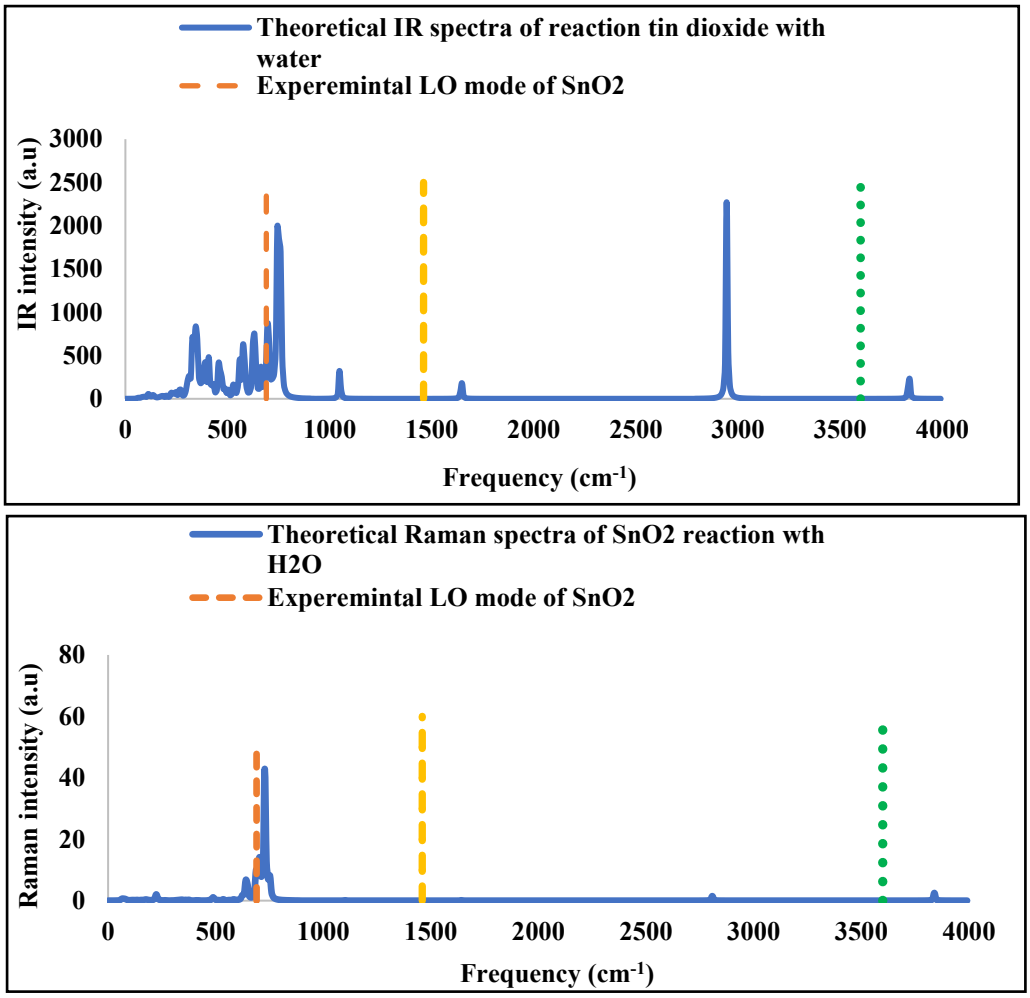


Figure 5: (a) IR intensity (b) Raman intensity for interaction between ($Sn_{10}O_{16}$+H_2O) as a function of frequency compared to the experiment longitudinal optical (LO) mode.

3.3 Thermal properties

Transition state

Transition state theory, one of the most important models in the field of reaction kinetics, has been limitedly utilized in gas sensor studies. This theory involves the existence of a transition state, specified by the Gibbs free energy, which has been employed throughout many reactions of different mechanisms [49-51]. In this paper, the total Gibbs free energy of activation is the maximum energy barrier along the reaction path. Furthermore, as shown in Fig. 6, the energy level of the product is higher than that of the reactants at the activation state, and the value of Gibbs free energy is positive, indicating that the reaction is endergonic.

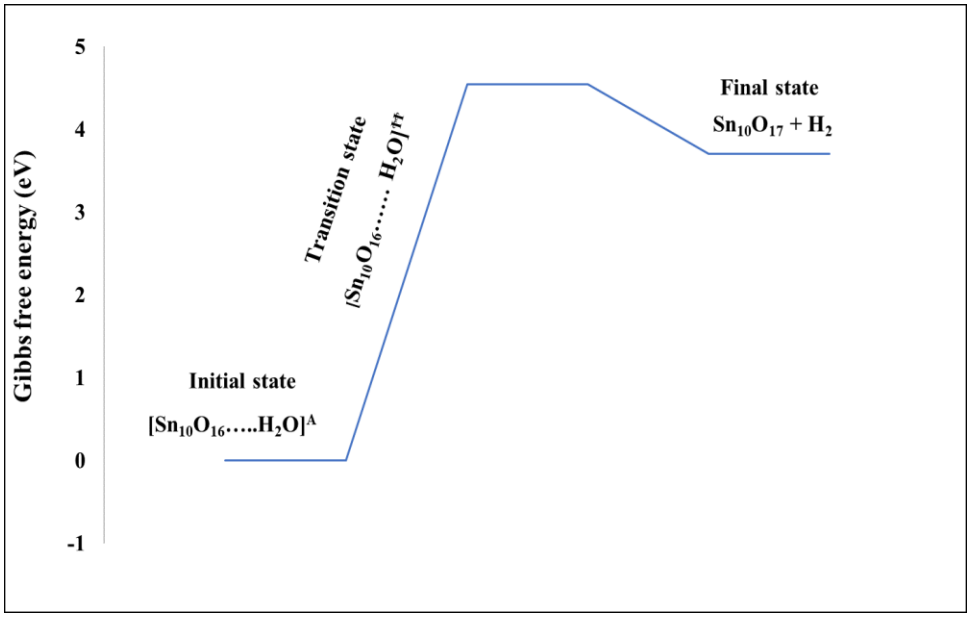


Figure 6: $Sn_{10}O_{16}$ clusters reacting with water and the transition state of the reaction pathway.

The following Eq. 6 explains the change in Gibbs free energy ΔG, enthalpy ΔH, and entropy ΔS [52].

$$\Delta G=\Delta H-\Delta ST \quad (6)$$

Table (1) indicates that the majority of reactions lead to a greater number of product molecules than the reacting ones. The augmentation of the molecular count is responsible for an increase in entropy, which in turn is one of the reasons a positive entropy change is brought up in the system.

Table 1: The Gibbs free energy of reactions along with activation, as well as their entropy, and enthalpy components examined in the standard conditions (temperature of 298.15 K and pressure of 1 atm)

n	Reaction	ΔG (eV)	ΔH (eV)	TΔS (eV)
1	$[Sn_{10}O_{16}…..H_2O]^A \rightarrow Sn_{10}O_{17} + H_2$	3.70	4.12	0.42
2	$[Sn_{10}O_{16}…..H_2O]^A \rightarrow [Sn_{10}O_{16}…..H_2O]^{††}$	4.54	4.49	-0.05
3	$H_2O \rightarrow H_2 + ½\ O_2$	2.83	2.94	0.10

4. Conclusions

Density functional theory and transition state calculations were performed on the reaction of tin dioxide nanoclusters with water molecules, and the theoretical values were compared with experimental results. In the presence of water, the value of the tin dioxide energy gap decreased due to the addition of levels within the tin dioxide energy gap which decreased resistivity and increased conductivity.

The results of the IR and Raman spectra are another indication to explain the interaction between tin dioxide and water. With the help of the transition state theory, the change of Gibbs free energy of $Sn_{10}O_{16}$ and water as a function of the reaction coordinates gave a positive value, indicating that the reaction is endergonic and that it requires heat or a photon; it is called a photocatalytic process.

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