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RESEARCH ARTICLE

Studying the Physisorption and Reaction Between In_9SnO_{15} Pyramid Nanocluster With Water Molecule via Transition State Theory

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ABSTRACT

This study investigates two binary semiconductors, $Sn_{10}O_{15}$ and $In_{10}O_{15}$, to form a ternary In_9SnO_{15}, a potential indium tin oxide (ITO) pyramid nanocluster for a humidity sensor, using density functional theory and transition-state theory. B3LYP hybrid functional was applied with the 6-311G** basis set for light elements (H, O) and (SDD) basis set for heavy elements (In, Sn). Steady-state geometrical structures were obtained using a complementary program, Gaussian View 05, and the corresponding electronic properties. HOMO and LUMO were calculated via the Gaussian 09W software program to obtain the energy gap of $Sn_{10}O_{15}$, $In_{10}O_{15}$, and In_9SnO_{15} pyramid nanoclusters, which were analyzed before and after adsorption (physisorption) with a single water molecule. Thermodynamic parameters such as enthalpy, entropy, and Gibbs free energy were calculated to evaluate the energetic feasibility of water interaction. The vibrational changes that followed the physisorption of water were analyzed by simulating the IR and Raman spectra. The simulations reveal that exposure to water leads to changes in the energy gap and electronic structure, and thus, it implies that the conductivity of indium tin oxide (ITO) would be reduced, which is a promising indicator for humidity sensing. The calculated Gibbs free energy as a function of the interaction coordinates between In_9SnO_{15} and H_2O to give In_9SnO_{16} and release H_2 with the required energy was 3.13 eV; the positive value of Gibbs free energy means an endergonic reaction, suggesting a thermodynamically stimulated pathway under standard conditions, also known as the photocatalysis process.

Keywords: DFT, Electronic and spectroscopic study, Humidity sensing, Indium tin oxide, Transition state theory

Introduction

Indium tin oxide (ITO) is a solid mixture of indium oxide (In_2O_3) and tin oxide (SnO_2). It exhibits interesting optoelectronic characteristics, such as high electrical conductivity and high visibility in the visible region. These properties have led to extensive applications in transparent electrodes, gas-detection devices, and photocatalytic systems.[1–3] To enhance the functioning of humidity sensors and photocatalytic devices, we must have a complete understanding of the interaction of ITO nanostructures with environmental molecules, particularly water. Water molecules have been demonstrated to play a major role in modifying the electronic structure and surface reactivity of oxide semiconductors.[4,5]

These interactions can alter charge-transport behavior, influence the effects of surface defects on charge transport, and align energy bands at the nanoscale. This is significant for catalytic and sensing behavior.[6,7] Density Functional Theory (DFT) is an applicable method for investigating these

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phenomena at the molecular level. The B3LYP hybrid functional, which is characterized by the combination of Hartree-Fock exact exchange with density functional approximation, has been effectively applied to investigate transition metal oxides and their reactions with adsorbates.[8,9]

Density Functional Theory (DFT) allows the calculation of both thermodynamic and spectroscopic quantities, such as Gibbs free energy, enthalpy, entropy, and infrared (IR) and Raman frequencies. This provides significant information regarding the behavior of ITO clusters in water.[10] Recent studies have highlighted the critical role of hierarchical nanostructures in metal-oxide semiconductor gas sensors. Investigations on pristine and Ni-doped In_2O_3 interacting with NO_2 have demonstrated that the pyramidal architecture increases the density of active sites and reduces the adsorption barriers, thereby improving the sensitivity and minimizing the response time.[11] Similarly, studies on pristine and Rh-doped SnO_2 clusters interacting with acetone, analyzed using transition-state theory (TST) and the modified Evans–Polanyi principle, revealed that doping directly affects the activation energies and reaction kinetics, enabling accurate theoretical predictions of the sensor response and response time, which are in good agreement with experimental observations.[12]

Furthermore, research on porous ZnO/SnO_2 composites has shown that controlled porous growth and oxygen ratios enhance the specific surface area and charge transport, thereby increasing water molecule adsorption and improving both sensitivity and response/recovery rates. Altogether, these results highlight the fact that the combination of hierarchical architecture, transition-metal doping, and customized porosity is a successful approach to optimize sensor functionality and explain the gas-surface interactions at the nanoscale.[13] This study used DFT calculations with the B3LYP functional and appropriate basis sets to model the interactions between ITO clusters and water molecules. In addition to examining the thermodynamic behavior and activation energy of water dissociation, special attention was paid to changes in the electronic properties, modulation of the energy gap, and vibrational spectra. These results support the idea that ITO nanostructures could be useful in photocatalytic and humidity-sensing applications.

Methodology

Density functional theory (DFT) was employed to investigate the electronic structure, thermodynamic behaviour, and vibrational properties of indium tin oxide (ITO) nanoclusters that interact with water molecules. All calculations were carried out using the Gaussian 09W software package[14] (relevant: Gaussian 09 is indeed the software used for DFT calculations), and molecular visualizations were performed with Gaussian View 05.

Computational method and functional

The B3LYP hybrid functional was chosen due to its validated performance in modeling metal oxide systems and its strong agreement with experimental data[15,16] (see all cited works for use or validation of B3LYP in metal oxide or semiconductor systems). This functional, which combines Becke's three-parameter exchange with the Lee-Yang-Parr correlation function, includes a portion of the exact Hartree-Fock exchange energy[17] (relevant). B3LYP has demonstrated reliability in describing transition-metal oxides and semiconductor clusters. Fig. 1 shows the geometrical optimization of (a) $Sn_{10}O_{15}$, (b) $In_{10}O_{15}$, (c) In_9SnO_{15}, and (d) $In_9SnO_{15} + H_2O$.

Basis sets

To treat the different elements present in the cluster, two types of basis sets were employed. The 6-311G** basis set, a 6-311G (d, p) variant, was used for light atoms such as hydrogen and oxygen, providing triple-zeta-quality and accurate valence electron descriptions. For heavy atoms such as indium and tin, the Stuttgart/Dresden (SDD) effective core potentials were used to reduce computational cost while preserving accuracy.[18–20]

Geometry optimization

The first structures of $In_{10}O_{15}$, $Sn_{10}O_{15}$, as well as In_9SnO_{15}, along with their reactions with H_2O nanoclusters, were built and optimized in the gas phase with no symmetry restrictions. Geometry optimizations were carried out with strict convergence criteria: the forces were kept at less than 1×10^{-5} a.u. and the energy changes at less than 1×10^{-6} a.u.

Spectroscopic simulations

Infrared (IR) and Raman vibrational spectra were simulated using the same level of theory (B3LYP/6-311G**/SDD). These spectra were used to evaluate the vibrational behavior of the ITO clusters before and after interaction with a single water molecule, helping to interpret the spectroscopic response of the sensor to humidity.

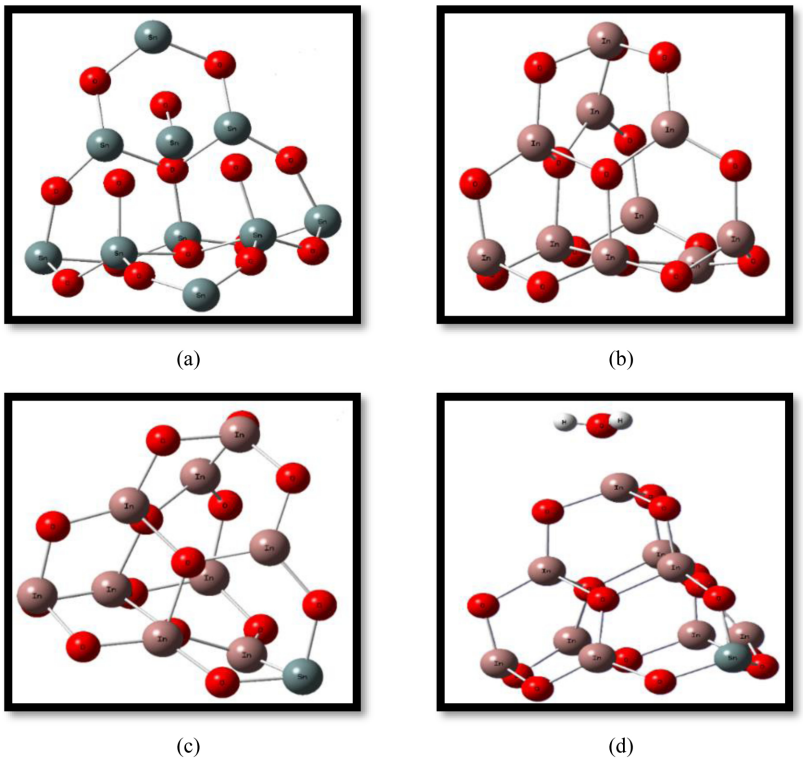


Fig. 1. Geometrical optimization of (a) $Sn_{10}O_{15}$, (b) $In_{10}O_{15}$, (c) In_9SnO_{15}, and (d) In_9SnO_{15}+H_2O.

Transition state analysis

Transition-state (TS) theory was used to explore the reaction pathway for the interaction between a water molecule and the In_9SnO_{15} cluster. A TS search was performed using the synchronous transit-guided quasi-Newton (STQN) algorithm (Berny algorithm), which was provided by Gaussian. The existence of a single imaginary frequency and intrinsic reaction coordinate (IRC) calculations were used to establish the identified transition state and provide a proper relationship between the product and reactant states.

Thermodynamic calculations

The thermodynamic properties, including enthalpy (ΔH), entropy (ΔS), and Gibbs free energy (ΔG), were obtained through frequency calculations conducted at 1 atm and 298.15 K. The resulting values illustrate the spontaneity and energetic feasibility of water adsorption and its interaction with ITO surfaces.

Results and discussion

Electronic properties

The electronic structures of the investigated nanoclusters were measured by analyzing the energy levels of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The energy gap (Eg) was determined based on Eq. (1). This gap is a critical parameter for evaluating the electronic conductivity and reactivity of semiconducting materials.

$$Eg = | \text{LUMO} - \text{HOMO} | \quad (1)$$

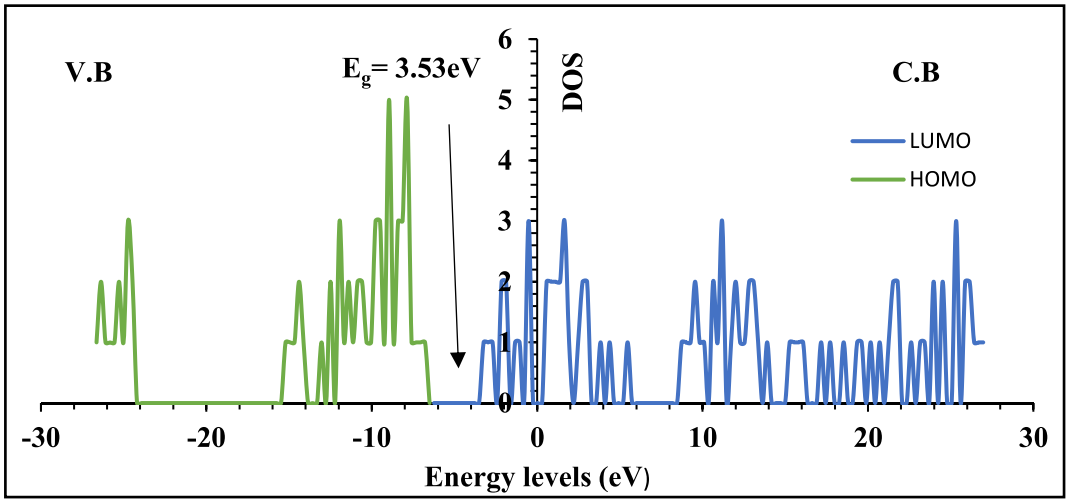
Density of state

Gaussian 09 W software was used to estimate the electronic characteristics of $Sn_{10}O_{15}$, $In_{10}O_{15}$, In_9SnO_{15}, H_2O, and ($In_9SnO_{15}+H_2O$), yielding energy gaps of 3.53, 2.99, 3.36, 8.69, and 3.37 eV, respectively (Fig. 2). These numbers were juxtaposed with the theoretical and experimental findings of the energy gap for SnO_2 and In_2O_3, ranging from 3.4 to 3.6 eV.[21,22] The density functional theory calculation results are presented in Table 1.

The calculated HOMO-LUMO energy gap of In_9SnO_{15} with water showed only a few changes, slightly increasing (~0.01 eV) upon H_2O adsorption, implying that the modulation of electronic conductivity was minimal in the isolated cluster model.

Spectroscopic analysis (IR and Raman)

Figs. 3 and 4 illustrate the simulated infrared (IR) and Raman spectra of the In_9SnO_{15} nanocluster



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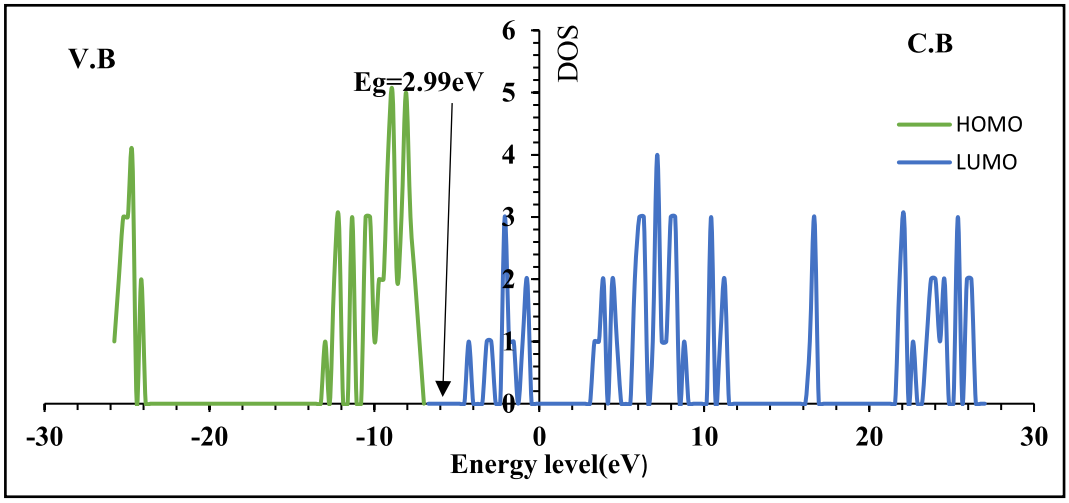

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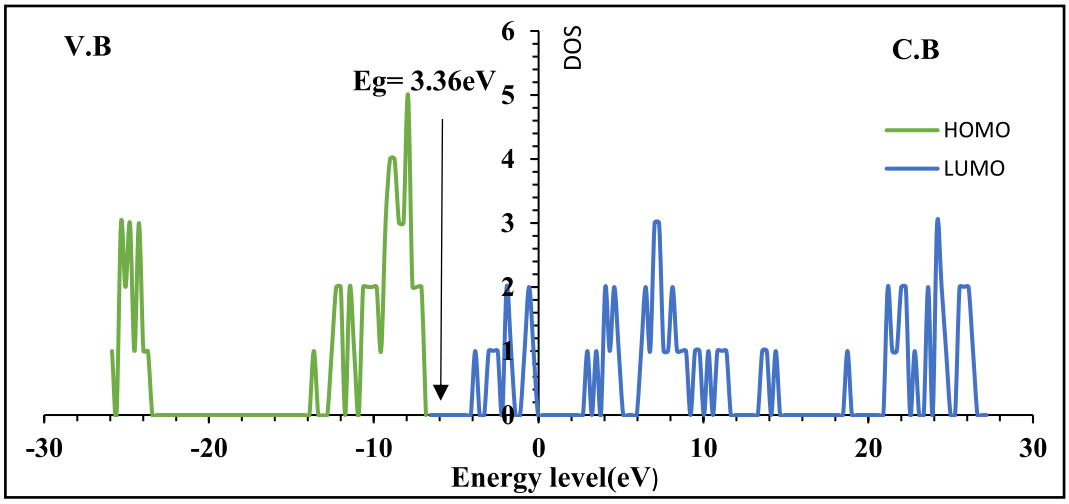
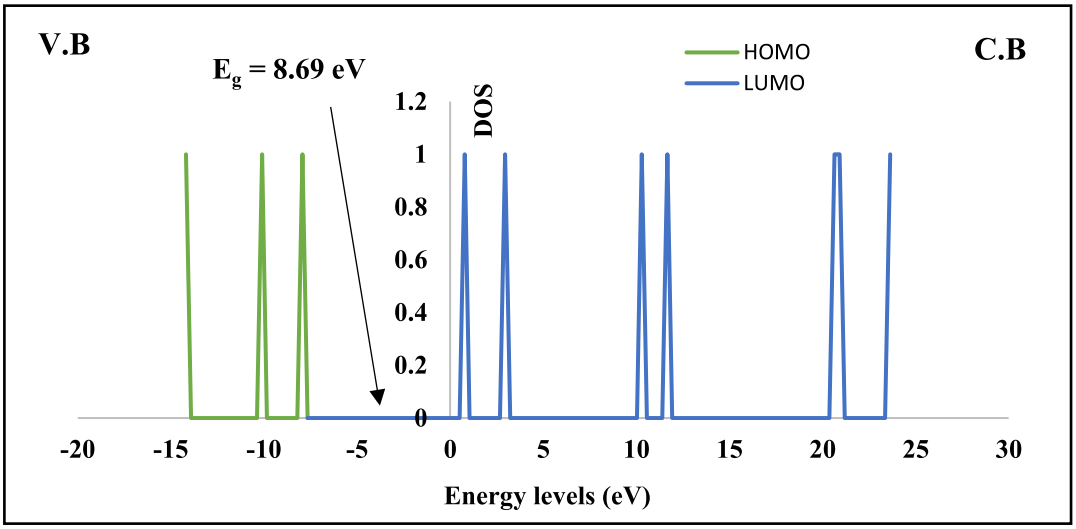


Fig. 2. Continued.



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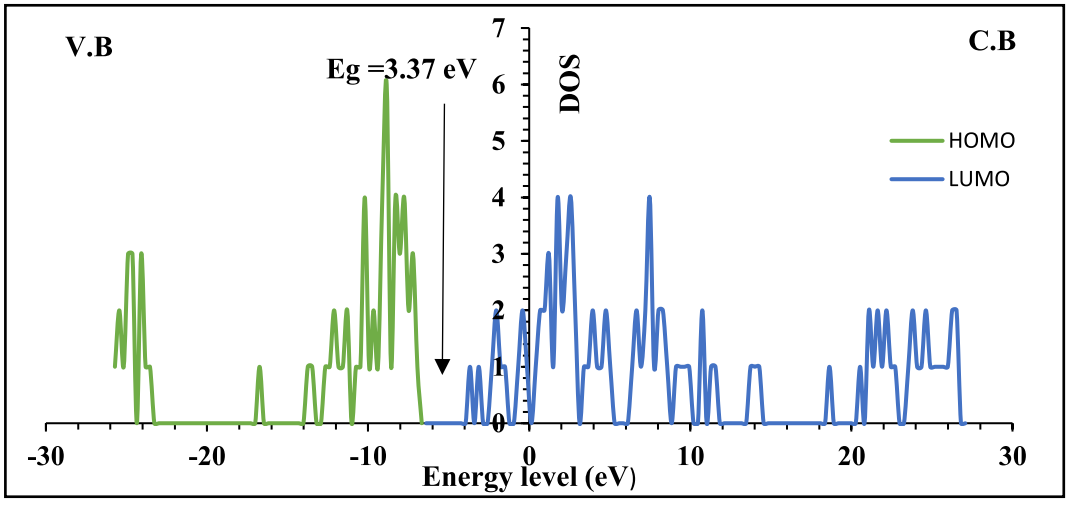


(e)

Fig. 2. Density of state of (a) $Sn_{10}O_{15}$, (b) $In_{10}O_{15}$, (c) In_9SnO_{15}, (d) H_2O, (e) In_9SnO_{15} with H_2O.

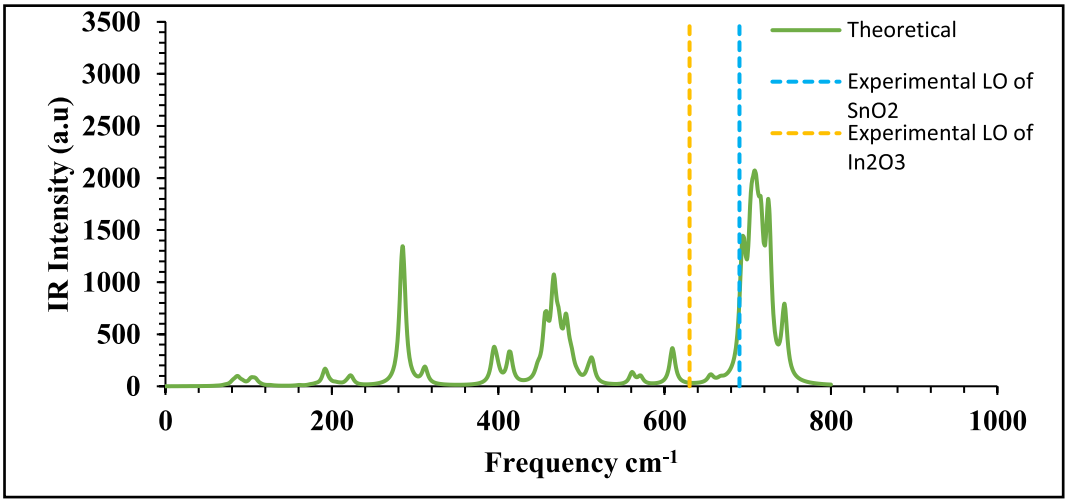
Table 1. DFT-calculated energy levels of (HOMO), (LUMO), and (Eg) for the investigated systems.

Material Structure	HOMO (eV)	LUMO (eV)	Eg(eV)
1. $Sn_{10}O_{15}$	–6.776	–3.238	3.53
2. $In_{10}O_{15}$	–7.268	–4.275	2.99
3. In_9SnO_{15}	–7.20	–3.84	3.36
4. H_2O	–7.92	0.77	8.69
5. $In_9SnO_{15} + H_2O$	–7.213	–3.842	3.37

before and after its interaction with a water molecule. These spectra provide insights into the vibrational behavior of the cluster and the effects of water adsorption at the molecular level.[23]

IR spectroscopy

Fig. 3 shows the IR spectrum, which reveals major absorption peaks at approximately 711 cm^{-1} and 690 cm^{-1}, corresponding to O-H bending, and at 1606 cm^{-1} and 3253 cm^{-1}, corresponding to O-H stretching of the water molecules. The bands in the 700 cm^{-1} region are attributed to the In–O and Sn–O stretching vibrations, consistent with the typical lattice vibrations observed in metal oxide clusters.[24,25] The high-frequency band at 3253 cm^{-1} corresponds to the O–H stretching mode of the adsorbed water molecule, indicating the successful binding of H_2O to the cluster surface. These assignments align with previously reported experimental longitudinal optical (LO) phonon modes: SnO_2: ~690 cm^{-1}, In_2O_3: ~630 cm^{-1}, and H_2O: ~1430 cm^{-1} (bending) and ~3600 cm^{-1} (stretching).[26–28] Although the simulated O–H stretching mode appears at a slightly lower frequency (~3253 cm^{-1}) than the experimental value (3600 cm^{-1}), this deviation is typical of



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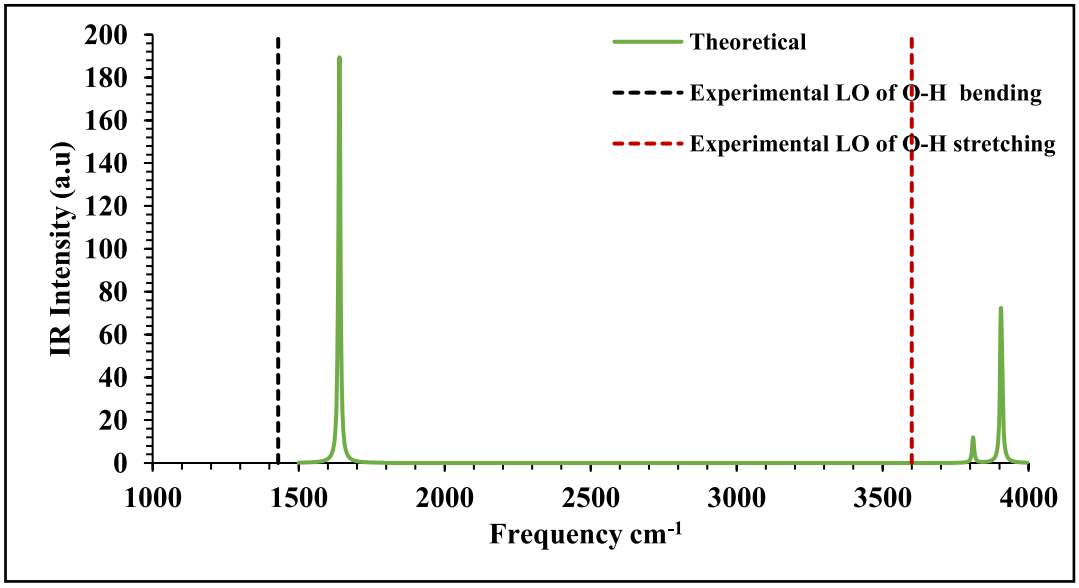

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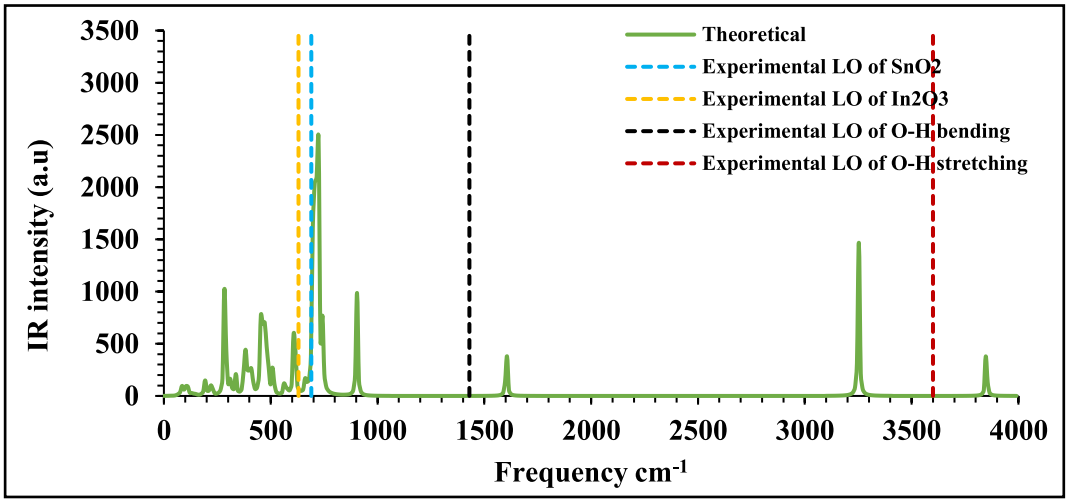
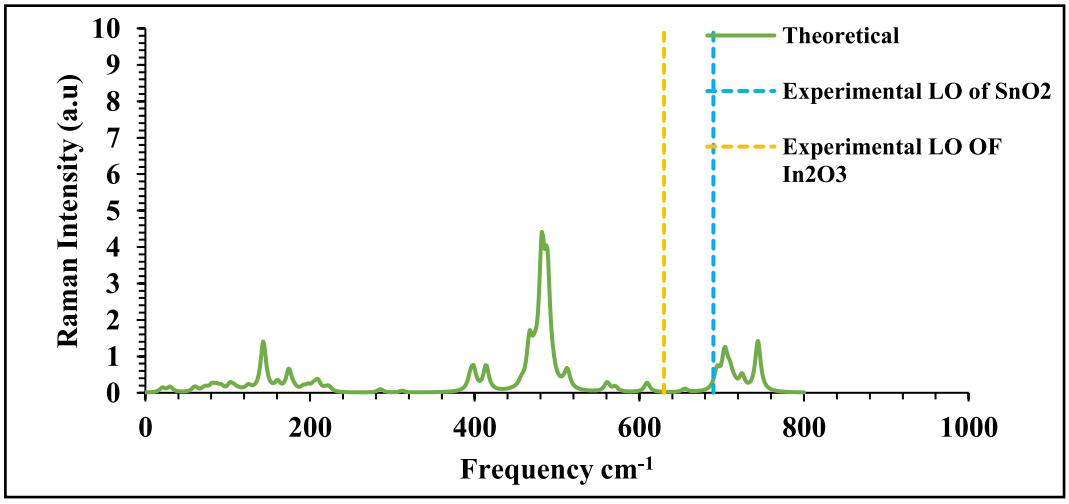
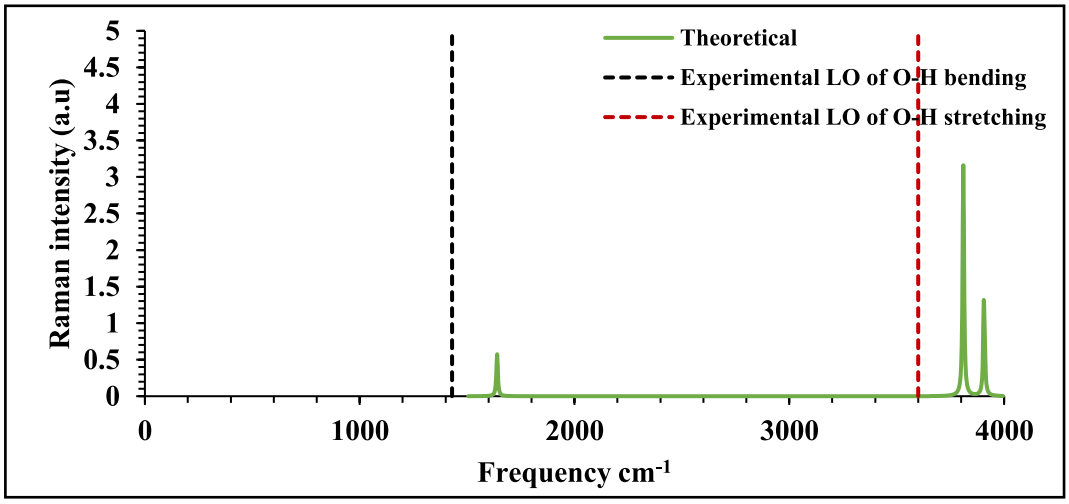


(c)

Fig. 3. IR spectrum as a function of the frequency of (a)In_9SnO_{15}, (b) H_2O, and (c) $In_9Sn\ O_{15}$ +H_2O, compared with the experimental longitudinal mode of frequency of In_2O_3, SnO_2, and H_2O.



(a)



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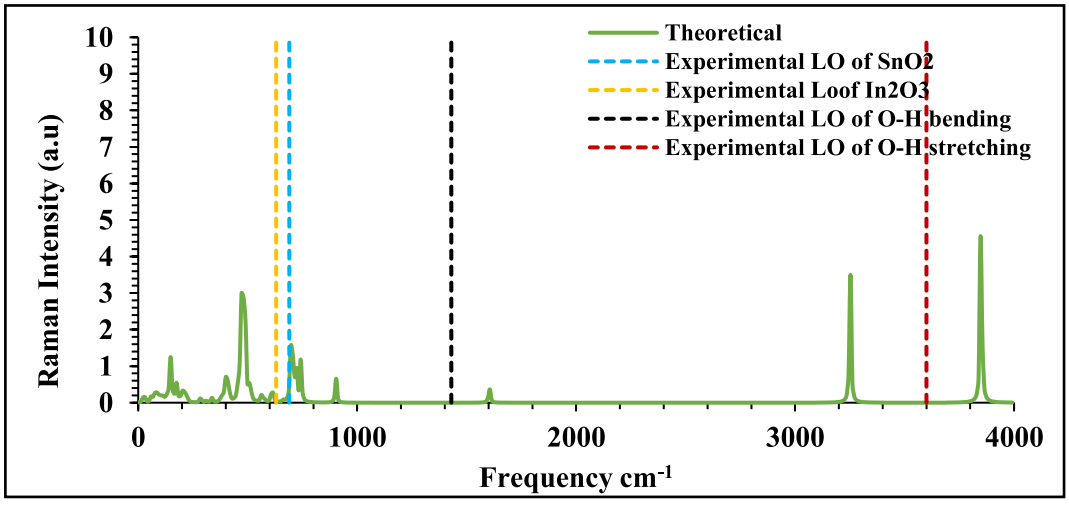

(c)

Fig. 4. Raman spectrum as a function of the frequency of (a) In_9SnO_{15}, (b) H_2O, and (c) In_9SnO_{15} with H_2O compare with the experimental longitudinal mode frequency of In_2O_3, SnO_2, and H_2O.

DFT-calculated spectra, which often underestimate vibrational frequencies due to the neglect of anharmonic effects.[29,30]

Raman spectroscopy

Fig. 4 shows the Raman spectrum with relatively low-intensity peaks in the same regions as those in the IR spectrum. Raman signals near 690–711 cm^{-1} represent symmetric metal–oxygen vibrations, while a broad, weak peak around 3250 cm^{-1} indicates minimal polarizability change in the O–H bond of the water molecule, which is expected since Raman activity depends on bond polarizability rather than dipole moment. The low Raman intensities are consistent with the highly ionic nature of the metal-oxygen (M–O) bonds in the cluster, which tend to be more IR-active than they are Raman-active. Nonetheless, the changes in the peak position and intensity upon water adsorption suggest slight structural distortions and electron redistribution around the adsorption site.[31,32]

The appearance of O–H-related vibrational modes in both spectra confirms the physical interaction between the water molecule and the ITO nanocluster. Spectral variations, particularly in the O-H stretching region, can form reliable signals for humidity measurements in practical sensor applications. This highlights the usefulness of infrared and Raman spectroscopy as diagnostic tools for the real-time determination of water adsorption on metal-oxide surfaces. However, the current simulations involved only one H_2O molecule; further extension of the research to cover several molecules and different surface coverages would provide a spectral response that better represents ambient humidity conditions. The density functional theory-calculated IR and Raman spectra intensities as a function of frequency for the investigated materials are listed in Table 2.[33]

Transition state modeling and thermodynamic pathway

In order to obtain a better understanding of the potential reaction mechanisms of the In_9SnO_{15} nanocluster with a water molecule, the thermodynamic and kinetic factors of a potential reaction pathway involving the dissociation of water were considered.

Table 2. DFT-calculated IR and Raman spectra intensities as a function of frequency for the investigated materials.

Material Structure	Frequency (cm^{-1})	IR Intensity (a.u)	Raman Intensity (a.u)
1. In_9SnO_{15}	710	2029.36	1.097
2. H_2O	1640	189.443	0.574
3. $In_9SnO_{15} + H_2O$	724	2464.47	1.182

This analysis was performed to determine whether hydrogen evolution at the surface of the cluster was possible and thus could be used to understand its behavior in humidity sensing or photocatalysis. The Berny optimization algorithm in Gaussian 09 W was used to identify the transition state (TS). An intrinsic reaction coordinate (IRC) calculation was performed to ensure that the transition-state assignment was accurate. This calculation confirmed the first step of the reaction, from the reactant complex to the product, thereby confirming the proposed reaction pathway. The reaction occurs in the following consecutive elementary steps, as shown by the equations in Eqs. (2) to (4), with the dissociation of water explained by Eq. (5).

$$In_9SnO_{15} + H_2O \rightarrow [In_9SnO_{15}\ldots H_2O]^{A} \rightarrow [In_9SnO_{15}\ldots H_2O]^{\dagger\dagger} \rightarrow In_9SnO_{16} + H_2 \quad (2)$$

$$[In_9SnO_{15}\ldots..H_2O]^{A} \rightarrow In_9SnO_{16} + H_2 \qquad \Delta G = 3.13\,(eV) \quad (3)$$

$$[In_9SnO_{15}\ldots H_2O]^{A} \rightarrow [In_9SnO_{15}\ldots H_2O]^{\dagger\dagger} \qquad \Delta G = 0.04\,(eV) \quad (4)$$

$$H_2O \rightarrow H_2 + {}^1\!/_2O_2 \qquad \Delta G = 2.84\,(eV) \quad (5)$$

The relationship between the Gibbs free energy change (ΔG), enthalpy (ΔH), and entropy contribution (TΔS) is explained in Eq. (6). These values were calculated for each step under standard conditions (T = 298.15 K, P = 1 atm) using vibrational thermodynamic functions derived from frequency analysis.

$$\Delta G = \Delta H - T\Delta S \quad (6)$$

Where:

ΔH: is the enthalpy of activation,

ΔS: is the entropy change associated with the activation process,

T: is the temperature (typically 298.15 K under standard conditions).

Fig. 5 schematically illustrates the computed Gibbs free energy profile along the reaction coordinate. The energy of the transition state exceeds that of the reactant and product states, with the final product (In_9SnO_{16} + H_2) being at a higher energy than the reactants. This suggests that, under standard conditions, the proposed transformation is not spontaneous and requires catalytic or photonic assistance.

Although the computational model successfully captured a possible pathway for H_2 evolution on the In_9SnO_{15} cluster, the large positive ΔG suggests that this process is unlikely to occur spontaneously under typical humidity-sensing conditions. This supports

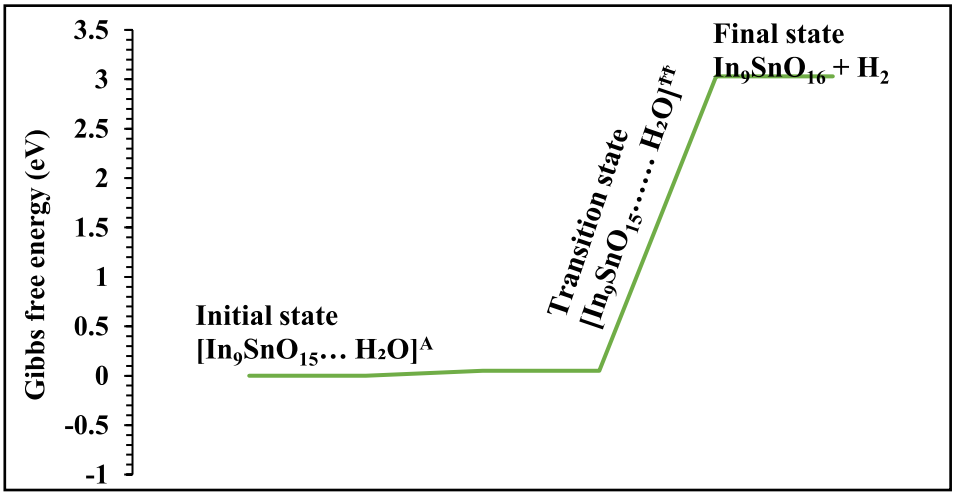

Fig. 5. Gibbs free energy change during the oxidation process of In_9SnO_{15} in the presence of H_2O.

Table 3. Gibbs' energy, enthalpy, and entropy of reaction under standard conditions (T = 298.15 K, P = 1 atm).

Reactions	ΔG (eV)	ΔH (eV)	TΔS (eV)
1. $[In_9SnO_{15}..... H_2O]^A \rightarrow In_9SnO_{16} + H_2$	3.13	3.32	0.19
2. $[In_9SnO_{15}..... H_2O]^A \rightarrow [In_9SnO_{15}..... H_2O]^{\dagger\dagger}$	0.04	0.05	0.01
3. $H_2O \rightarrow H_2 + {}^1/_2\, O_2$	2.84	2.94	0.10

the view that the dominant sensing mechanism is more likely to involve physical adsorption, hydrogen bonding, or charge transfer phenomena rather than chemical water dissociation. The transition state reaction, characterized by a positive Gibbs free energy, is presented in Table 3.

The activation barrier for the reaction step from the adsorbed complex to the transition state was relatively low (ΔG = 0.04 eV), suggesting that the reaction could proceed under mild excitation. However, the total Gibbs free energy of the overall reaction (ΔG= + 3.13 eV) was significantly positive, indicating an endergonic reaction, that is, a thermodynamically non-spontaneous process under ambient conditions. This finding implies that an external energy input, such as light or heat, is required to drive the reaction. It has been found that the energy required to split one mole of water into hydrogen and oxygen is approximately 237 kJ, or about 2.46 eV per molecule.[32] This is the theoretical minimum electrical energy input for water electrolysis, which is in good agreement with our calculations (2.84 eV).

Conclusions

Density functional theory (DFT) and transition-state theory were used to investigate the interaction mechanisms between a defective In_9SnO_{15} cluster and a water molecule, with the aim of evaluating its potential role in humidity-sensing applications. Thermodynamic analysis revealed that the oxidation reaction pathway involving the In_9SnO_{15} cluster and H_2O exhibited a Gibbs free energy change (ΔG) of + 3.13 eV, indicating that it was non-spontaneous and endergonic under standard conditions. The transition state was located and confirmed by vibrational analysis, with an associated energy barrier (ΔG) of 0.04 eV. These results suggest that water dissociation on the In_9SnO_{15} cluster requires external energy input, such as thermal or photonic excitation, which supports the possibility of photocatalytic behavior but challenges the feasibility of spontaneous water splitting under ambient humidity. Moreover, IR and Raman analyses revealed vibrational mode shifts upon water interaction, highlighting specific structural perturbations within the cluster. However, the calculated HOMO-LUMO gap showed only a few changes, with a slight increase (~0.01 eV) upon H_2O adsorption, implying that the modulation of electronic conductivity was minimal in the isolated cluster model. Therefore, the observed changes may not directly translate into a significant humidity sensor response unless surface-level adsorption mechanisms (rather than bulk reaction pathways) dominate the sensing behaviour of the sensor. Overall, while the present computational model provides valuable insights into the energetic and spectroscopic aspects of ITO–water interactions at the molecular

level, it remains a simplified representation of real sensor environments.

Acknowledgment

The authors would like to express their sincere thanks to the College of Science at Al-Nahrain University for providing an academic environment and resources necessary to complete this study.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the figures and tables in the manuscript are ours. Besides, the figures and images, which are not ours, have been given permission for re-publication attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at Al-Nahrain University.

Authors' contributions statement

A. H.M and M. T. H designed the study.N. A. F. performed the experiments.N. A. F performed simulations.

N. A. F. and M. T. H expressed and purified all proteins.N. A. F and A. H. M analyzed the dataA.H. M wrote the paper with input from all authors.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request

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دراسة الامتزاز الفيزيائي والتفاعل بين In_9SnO_{15} العنقودي النانوي الهرمي مع جزيء الماء باستخدام نظريه الحالة الانتقالية

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الخلاصة

تتناول هذه الدراسة تحليل خصائص مركبين شبه موصلين هما $Sn_{10}O_{15}$ و $In_{10}O_{15}$ بالاضافة الى مركب ثلاثي In_9SnO_{15} على شكل عنقود نانوي هرمي من أكسيد القصدير والإنديوم (ITO)، لاستخدامه كمستشعر للرطوبة، تم استخدام نظرية دالية الكثافة الى جانب نظرية الحالة الانتقالية (Transition State Theory). في هذا التحليل اعتمدت الدراسة على الدالة التهجينية B3LYP (Becke's three-parameter Lee-Yang-Parr) باستخدام مجموعة الأساس 6- 311G**للعناصر الخفيفة (H, O)، ومجموعة الأساس Stuttgart/Dresden (SDD) للعناصر الثقيلة (In, Sn).تم تحليل الخصائص البنيوية والالكترونية المستقرة باستخدام البرنامج المساعد Gaussian View 05، كما جرى حساب الخصائص الإلكترونية مثل HOMO (أعلى مدار جزيئي مشغول) وLUMO (أدنى مدار جزيئي غير مشغول) عبر برنامج Gaussian 09W باستخدام منهجيات ميكانيكا الكم، وذلك لتحديد فجوة الطاقة في $Sn_{10}O_{15}$ و$In_{10}O_{15}$ و In_9SnO_{15} على شكل عناقيد نانوية هرمية، قبل وبعد التفاعل مع جزيء ماء واحد.تم كذلك حساب المعلمات الثرموديناميكية، مثل الإنثالبي، والإنتروبيا، وطاقة غيبس الحرة، بهدف تقييم الجدوى الطاقية لتفاعل الماء. كما جرى محاكاة أطياف الاهتزاز IR وRaman لرصد التغيرات الاهتزازية المصاحبة لامتصاص الماء (تفاعل الامتزاز الفيزيائي).أظهرت النتائج أن التفاعل مع الماء يؤدي إلى تغيّر في فجوة الطاقة والبنية الإلكترونية، مما يشير إلى انخفاض في التوصيلية الكهربائية لـ ITO، وهو ما يعد مؤشراً جيداً لكفاءة استشعار الرطوبة. كما استُخدمت تقنية نظرية الحالة الانتقالية لحساب طاقة غيبس الحرة بوصفها دالة لمعامل التفاعل بين In_9SnO_{15} وH_2O لإنتاج In_9SnO_{16} وانطلاق H_2 بطاقة مطلوبة مقدارها 3.03 إلكترون فولت. وتشير القيمة الموجبة لطاقة غيبس الحرة إلى أن التفاعل ماص للطاقة (Endergonic Reaction)، مما يدل على إمكانية حدوثه عبر مسار محفَّز حرارياً تحت الظروف القياسية، ويُعرف هذا أيضاً بعملية التحفيز الضوئي (Photocatalysis Process).

الكلمات المفتاحية: دراسة الكترونية- طيفية، اكسيد الانديوم والقصدير، مستشعر الرطوبة، نظرية داليه الكثافة ، نظرية الحالة الانتقالية.