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Computational Investigation of B_6 Particle for H_2S Capturing

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ABSTRACT

Hydrogen sulfide (H_2S) hazardous gas capturing by a model of boron-6 (B_6) cyclic particle was investigated in this work using computational methodology. To this aim, density functional theory (DFT) calculations were performed to obtain optimized geometries of individual H_2S and B_6 counterparts in addition to their complex systems. Two sides of H_2S including H and S sides were located towards the B_6 surface to explore gas capturing through H@B_6 and S@B_6 interacting complex formations. Interestingly, serious differences were observed for the complexes with more stability for S@B_6 complex formation in comparison with H@B_6. Indeed, that of S@B_6 was almost a chemisorption in contrast with that of physisorption of H@B_6 complex. Further analyses based on the obtained molecular descriptors described various features of complex models in details. This work was done actually for proposing small B_6 cyclic particle for H_2S capturing regarding the importance of environmental issues for humankind health care.

KEYWORDS Boron-6, Particle, Hydrogen sulfide, DFT, Gas capturing.

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INTRODUCTION

Gas pollutants are such hazardous materials in the modern industrial cities mostly produced from fuels of machines and factories threatening the health level of humankind.[1] These gases are very much harmful because of their easily inhaling inside the body through every time regular breathing processes.[2] Therefore, designing novel materials for gas capturing purposes are important regarding sensing and removal of hazardous gas materials for maintain humankind health care.[3-5] For achieving this purpose, several materials including nanostructures have been developed for gas capturing.[6-9] In addition to initial carbon nanotube (CNT), various types of nanostructures have been developed to this time for specified applications even gas capturing.[10-12] In this case, molecular scale studies employing computational methodology could help for providing novel insights regarding the development of such capturing materials.[13-17] Hence, this computational work was performed to investigate hydrogen sulfide (H_2S) gas capturing by a model of boron-6 (B_6) cyclic particle (Fig. 1). H_2S is one of the most hazardous gases produced by several machines and factories in modern cities with harmful effects for environmental issues of health care.[18] This small molecule should be captured in the environment avoiding its inhaling in breathing processes.[19] Earlier works introduced candidate materials for H_2S capturing, but the results have not been yet qualified the conditions of such gas capturing processes. Therefore, further works are still required to recognize such capturing features regarding the innovation of novel adsorbing materials or details of adsorption processes.

In this work, density functional theory (DFT) calculations were performed to investigate H_2S gas capturing by B_6 cyclic particle at the molecular scale. The structures were optimized and two models of $H@B_6$ and $S@B_6$ interacting complex systems were characterized regarding the starting geometrical position of H_2S molecule from H side or S side towards the B_6 surface. The interacting complexes were analyzed to achieve information to describe the processes of H_2S capturing by the B_6 particle. All results were summarized in Table 1 and Fig. 1 for providing further discussion in the direction of main problem solving of this work for H_2S capturing by B_6 particle.

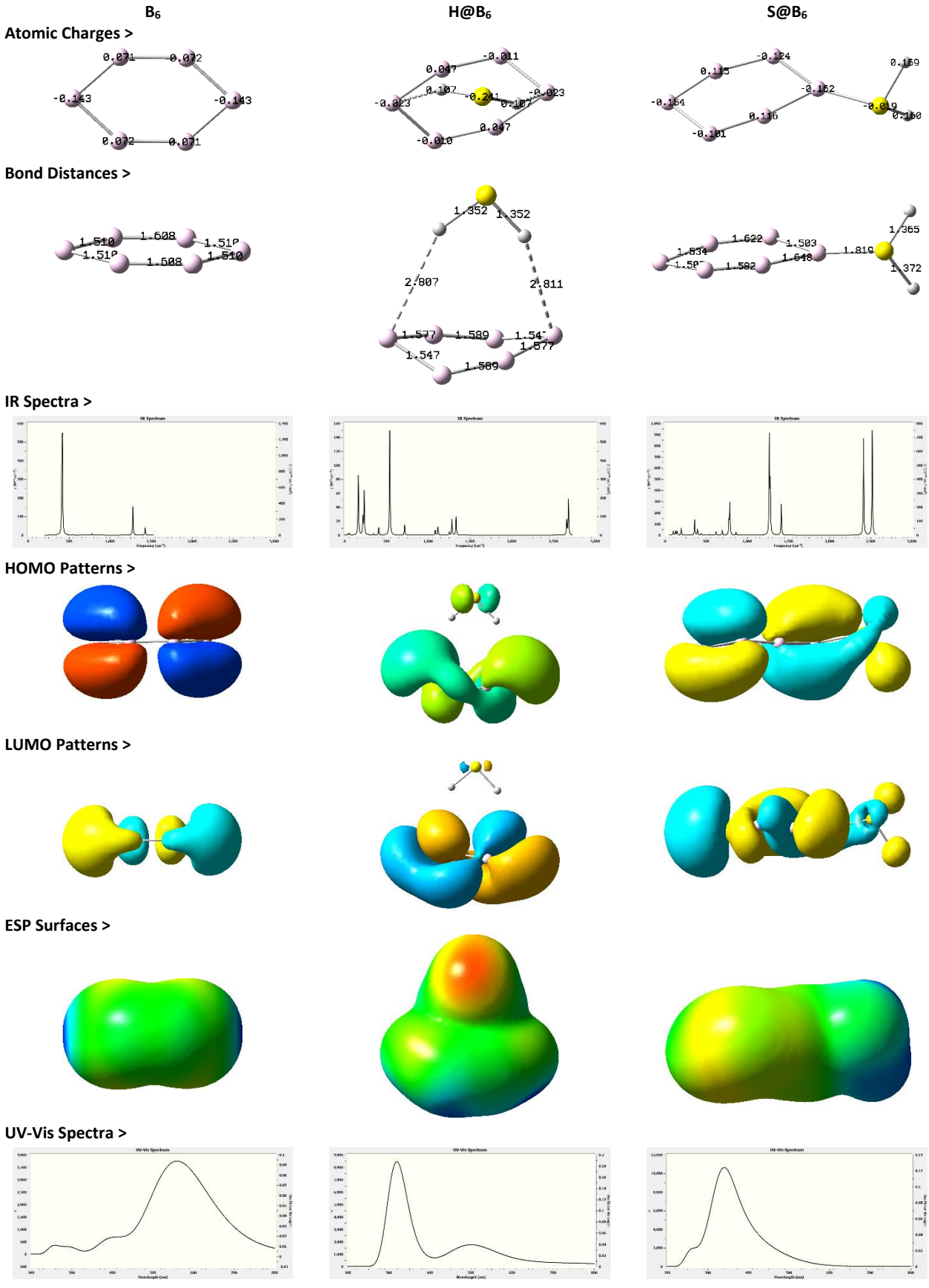

Fig. 1: Molecular features for the optimized model systems.

MATERIALS & METHODS

DFT calculations were performed to optimize geometries of individual H_2S and B_6 molecules first. Interacting complex formations of $H@B_6$ and $S@B_6$ systems were obtained by performing further optimization processes next. The H side and S side of H_2S were initially located towards the B_6 surface for complex formation of each of $H@B_6$ and $S@B_6$ systems (Fig. 1). In addition to obtaining the optimized geometries, other molecular features including total energies (E), adsorption energies (E_{Ads}) of energy differences of total energies for complex and components, atomic charges, bond distances, infrared (IR) spectra, quantitative levels and qualitative representations of the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO), electrostatic potential (ESP) surfaces, and ultraviolet-visible (UV-Vis) spectra, energy gaps (EG) of the HOMO and LUMO differences and Fermi energy (FE) of the HOMO and LUMO averages, dipole moments (DM), and volume (V), all summarized in Table 1 and Fig. 1. All calculations were performed using the B3LYP exchange-correlation functional and the 6-31G* standard basis set as implemented in the Gaussian program.[20] Additionally, IOp(3/124=3) was included in the calculations of bimolecular systems regarding dispersion correction purposes. As a consequence, required information were provided for further discussion of the results to approach the main goal of this work for H_2S capturing by the B_6 cyclic particle surface. As mentioned before, computer-based works could provide *in silico* environment for investigating chemical systems at the lowest possible molecular and atomic scales.[21-25]

Table 1: Molecular descriptors for the optimized model systems.

Descriptor	B_6	$H@B_6$	$S@B_6$
E eV	-4047.631	-14916.679	-14918.412
E_{Ads} eV	n/a	-0.972	-2.705
HOMO eV	-5.258	-6.341	-4.892
LUMO eV	-4.651	-4.567	-2.776
EG eV	0.607	1.774	2.116
FE eV	-4.954	-5.454	-3.834
DM Debye	0	3.592	6.118
V cm^3/mol	54.127	117.121	89.798

E(H_2S) = -10868.076 eV

RESULTS & DISCUSSION

The main problem of this work was to investigate B_6 model for capturing H_2S hazardous gas for sensing and removal of this gad regarding environmental health issues. To this aim, DFT calculations were performed to explore the chemical systems at the lowest molecular and atomic scales. Required information (Table 1 and Fig. 1) were provided for discussing the results to approach solution for the problem of this fork. To carefully examine the capturing process, two sides of H_2S including S side and H side were individually located towards the B_6 surface resulting two interacting complexes of $H@B_6$ and $S@B_6$ systems. In this case, visual representations indicated that the complex formation of $H@B_6$ could be considered as physisorption whereas that of $S@B_6$ could be considered as chemisorption. Indeed, bond distances of interactions between two molecular components were significantly shorter for $S@B_6$ in comparison with $H@B_6$. Furthermore, corresponding values of E and E_{Ads} indicated more stability for $S@B_6$ rather than that of $H@B_6$. Variations of atomic charges also indicated that the particle was detected effects of gas adsorption at the atomic scale, in which the molecular shape was also somehow deformed in this case. As an interesting point, the type of adsorption of H_2S at the B_6 surface was dominantly dependent on initial configuration of gas molecule at the surface yielding different structural system. This achievement could be proposed by the advantage of performing computer-based works to provide insightful information for solving the problems of chemical systems.

Variations of molecular orbital features were recognized by obtaining quantitative and qualitative values, in which HOMO and LUMO distribution patterns could show the effects of H_2S capturing on the electronic properties of B_6 particle. Moreover, representations of ESP surfaces could reveal the changes of electric charges distributions at the investigated surface systems with fluctuations of electric charges for the interacting complexes of $H@B_6$ and $S@B_6$ systems. Worthy to note that the complex formations of bimolecular systems could be very well confirmed by ESP surface representations, in which sharing the electric charges between the molecular components could reveal the formation of interacting complexes. Moreover, values of EG and FE could approve such effects regarding variations

of electronic properties for molecular orbital distribution. Values of DM and V also indicated that such complex formations could yield different properties regarding the capturing processes of two interacting complex formations. Indeed, such obtained molecular descriptors were useful tools for describing various features of the chemical systems in singular and bimolecular states to show the effects of interacting media on the original properties of the molecules and atoms. In this work, the results were obtained for achieving such purpose by evaluating qualitative and quantitative features of DFT calculations. The results indicated that only investigating adoption process was not enough for obtaining knowledge for the interacting processes but details of such adsorption processes were very much important. In this regard, formation of $S@B_6$ system was more favorable than that of $H@B_6$ system regarding several obtained molecular and atomic scales features. Although experiments are crucial for finalizing the achievements of chemical systems, but such computer-based works could provide insightful information about details of such chemical systems.

CONCLUSION

This DFT work was performed to investigate H_2S capturing by B_6 particle for sensing and removal of hazardous gases regarding the environmental health issues. The molecules were optimized to obtain $H@B_6$ and $S@B_6$ interacting complexes by initial locating of H side and S side of H_2S towards the B_6 surface. The results indicated that $S@B_6$ complex formation could be obtained more favorable than $H@B_6$ complex formation. Indeed, $S@B_6$ complex was obtained by chemisorption whereas $H@B_6$ complex was obtained by physisorption. The achievement indicated the importance of adsorption details clarification for exploring gas capturing processes of molecular systems. Variations of other molecular and atomic features in singular and bimolecular systems indicated significant impacts of such molecular adsorption on electronic properties of original systems. Molecular orbital features including quantitative levels and qualitative representations all confirmed the formation of such complexes of $H_2S@B_6$ interacting systems with significant detected impacts of structural and electronic features. As a consequence, B_6 particle could be proposed as a small surface for H_2S gas capturing.

DISCLOSURE STATEMENT

The author(s) did not report any potential conflict of interest.

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