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RESEARCH ARTICLE

DETECTION OF GLYCINE AND SEROTONIN NEUROTRANSMITTERS BY HEXAGONAL BORON NITRIDE 2-D NANOSHEET

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Abstract

Neurotransmitters, called as chemical messengers, play a significant role in human body by transmitting message or signal between neurons or neurons to muscles, and their disorder badly affects the human body. In this study we have analyzed the sensing capability ofhexagonal boron nitridenanosheet (BNNS), which is of great interest because of their remarkable physical and chemical properties, to detect several neurotransmitters like glycineand serotonin. Structuraland electronic properties of the materials have been calculated using density functional theory analysis by Gaussian09 package. A significant change has been observed inhexagonal boron nitridesheet when neurotransmitters come in contact with this. This study will be helpful for the detection of the chemical messengers in human body.

Introduction:-

Nanomaterials, in the range of 1-100 nm, are of great interest because of their unique optical, electrical, magnetic, thermal, mechanical, and other emerging properties. Because of having notable characteristics, nanomaterials have a wide range of applications including in the chemical industry, power generation industry, waste management, cosmetic industry, water purification, and sensor etc[1]. Researchers are working on different nanomaterials also different shaped nanomaterials such as nanoparticles, nanosheets, nanotubes, and nanocones as the properties of nanomaterials vary over shape. Our interest in this study is on nanosheet since it has a large surface area; the large surface area facilitates in adsorption process. Boron nitride nano sheet(BNNS) consists of boron and nitrogen atoms, attached by covalent bond, exhibiting a honeycomb-like network analogous to graphene sheet and has some fascinating properties like broad energy band gap, high thermal conductivity, high mechanical strength, high thermal stability[2–4].These appealing properties have attracted researchers to sense or detect neurotransmitters using hexagonal BNNS besides carbon-based nanomaterials.

Neurotransmitters are the essential chemical messengers in the human nervous system and more than 100 different types of neurotransmitters are acquainted to date.The human body cannot work properly without its proper functioning, and almost all the neurotransmitters have an inevitable effect on mental and physical health; severe diseases like Parkinson, Alzheimer and mental disorder can create due to any abnormality in neurotransmission[5].Therefore, monitoring or detectingneurotransmitters is needed for medical treatment and analysis.

H. Tavassoli Larijani et al worked on the interaction of glycine with three different monolayers, namely graphene, h-BN and h-SiC; they used ORCA quantum chemistry software with generalized gradient approximation (GGA)

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approximation and Perdew-Burke-Ernzerhof (PBE) functional and reported the physisorption of glycine with h-BN sheet[6].P. Chaudhuri et al also have shown adsorption of glycine on BN nanotube using density functional theory (DFT) analysis through Quantum Espresso software based on GGA approximation and PBE functional[7].R. Zhiani has reported on the adsorption of various types of amino acids on graphene and BN nanosheet where he used the Gaussian 09 software using B3LYP/6-31G(d) and B3LYP-D3/6-31G(d) functional[8].

In this study,density functional theory (DFT)analysis was performed to see the adsorption capability of boron nitride nanosheet(BNNS) towards the two neurotransmitters-glycine and serotonin.Structural, electronic, and opticalproperties of the adsorbed structures were observed to see the interaction between BNNS and neurotransmitters.

Computational details

All the calculations were accomplished on using Gaussian 09 simulation package based on a hybrid functional-HSEH1PBE and 6-31G(d) basis set.The adsorption energy was calculated using the formula, $E_{Ads} = E_{(BNNS+Neurotransmitter)} - (E_{BNNS} + E_{Neurotransmitter})$.

Results And Discussion:-

Optimized structures

Optimization refers to the process of minimization of total energy of a structure by changing its geometry, specifically its nuclear coordinates and lattice vectors. The optimized structures of BNNS, Glycine, Serotonin, adsorbed structure of BNNS with Glycine and Serotonin are shown in Figure 1.

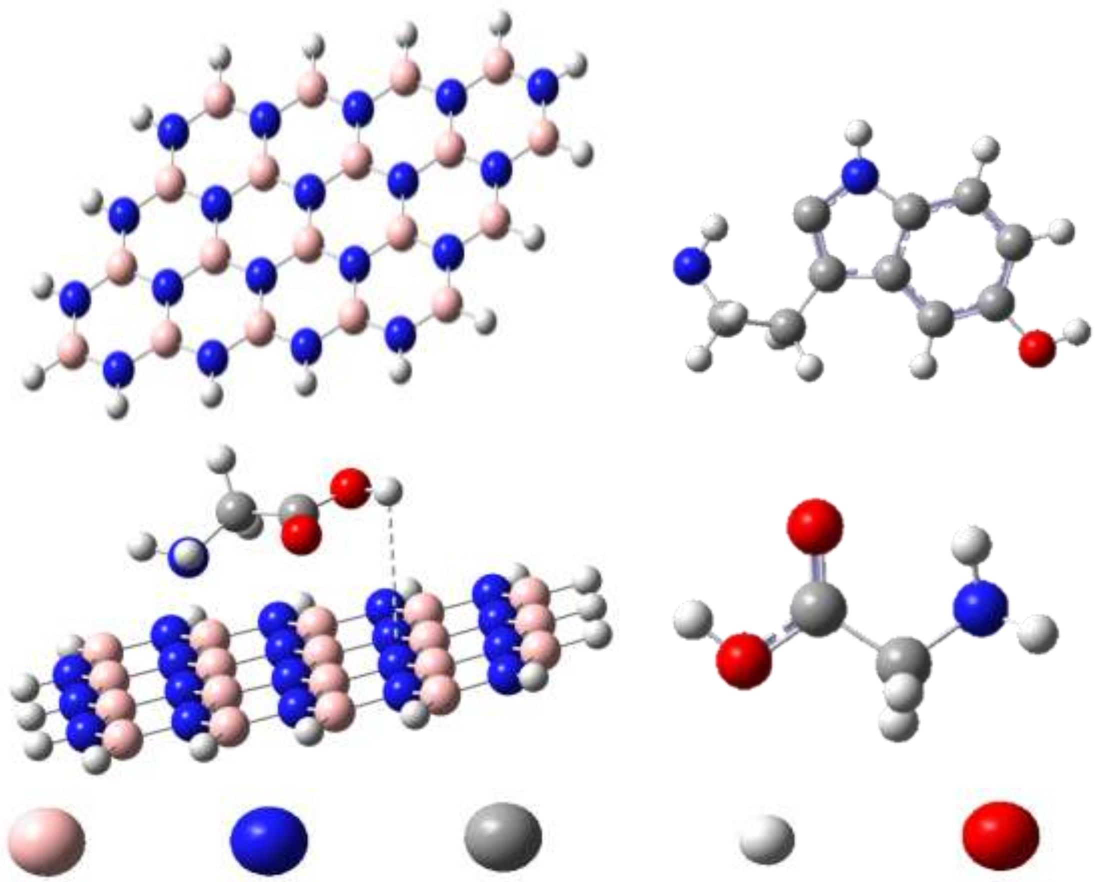


Figure 1:- Optimized structures of (a) BNNS (b) Glycine (c) Serotonin (d) BNNS with Glycine (e) BNNS with Serotonin.

A slight deformation of the BNNS adsorbent is observed when both glycine and serotonin come near the adsorbent. The bond lengths between different atomic species in the structures are shown in Table 1; there are little changes in bond length of the adsorbent, which confirms the interaction between BNNS and the neurotransmitters-glycine and serotonin.

Bonds	Bond lengths in Å				
	BNNS	Glycine	Serotonin	BNNS with neurotransmitters	
				Glycine	Serotonin
B-N	1.44			1.44	1.44
N-H	1.02	1.016	1.01	1.01	1.01
B-H	1.2			1.2	1.19
O-C		1.27	1.365	1.27	1.37
O-H		0.97	0.966	0.97	0.96
C-H		1.1	1.09	1.1	1.01
C-N		1.445	1.4	1.45	1.4
C-C		1.507	1.43	1.5	1.51

Table 1:- Bond lengths in the structures.

Adsorption energy

Adsorption is the process of adhering of atoms, ions or molecules to a surface, and this process can happen by weak van der walls forces or covalent bonding. The adsorption energy refers to the difference in energy between the adsorbed system and the individuals which indicates how strongly adsorbate molecules are adsorbed to adsorbent. The adsorption energies and corresponding adsorption heights of the adsorbed structures are tabulated in Table 2.

Molecules adsorbed on BNNS	Adsorption energies in eV	Adsorption lengths in Å
BNNS + Glycine	-0.18	2.99
BNNS + Serotonin	-0.18	2.89

Table 2:- Adsorption energies and adsorption heights.

From the table it is observed that both the adsorption energies are negative which means the process is exothermic, and the adsorption length is notable that indicates there is no contact of the neurotransmitters with the BNNS which is also seen from the optimized structures; thus, physisorption occurs here for both the neurotransmitters.

Mulliken charge analysis

Mulliken charges represents the partial atomic charges in a molecule, and this partial charges for the structures are shown in Table 3.

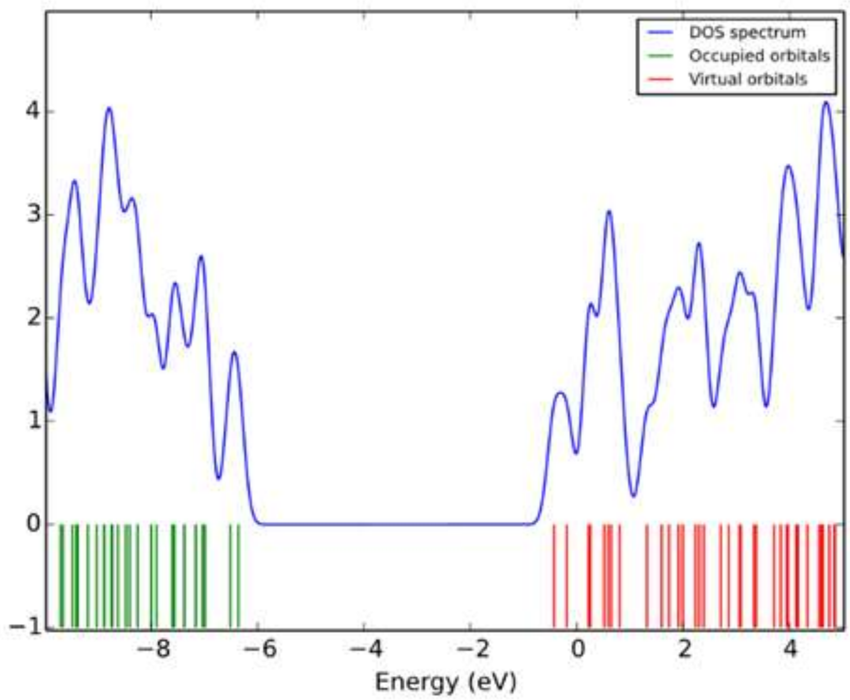
Atoms	Average Mulliken charges in units of e						
	BNNS	Glycine	Serotonin	BNNS with neurotransmitters			
				BNNS with Glycine		BNNS with Serotonin	
				BNNS	Glycine	BNNS	Serotonin
B	0.46			0.41		0.44	
N	-0.51	-0.756	-0.735	-0.56	-0.767	-0.55	-0.72
H	0.14	0.296	0.238	0.28	0.30	0.29	0.24
C		0.16	-0.048		0.167		-0.03
O		-0.52	-0.665		-0.52		-0.68

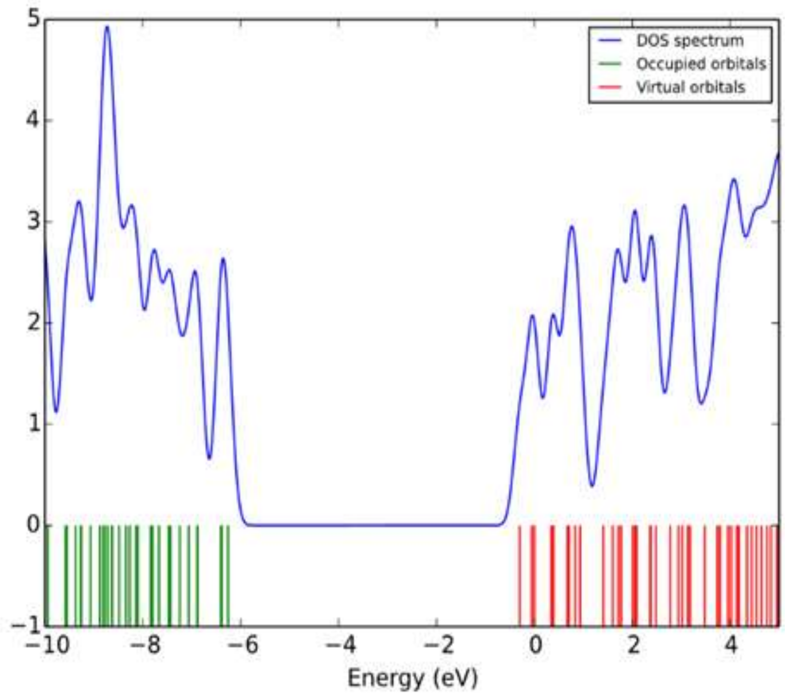
Table 3:- Average Mulliken charges of the adsorbent and adsorbates.

In BNNS, the Mulliken charge value of Nitrogen (N) is negative while it is positive for Boron (B) atom, and this is due to the electronegativity difference between N and B atoms. Nitrogen is more electronegative than Boron atom, and that's why N pulls the covalently bonded electrons more towards it; therefore, N becomes partially negative and B becomes partially positive. In both glycine and serotonin, the more electronegative atoms become partially negative while others become partially positive. It is observed that after adsorption of neurotransmitters the Mulliken charge values of the atoms change which means the deformation of electron density in the structures, and this confirms interaction or adsorption of glycine and serotonin on BNNS.

Electronic properties

The available electronic energy states of the structures are shown by the Density of States (DOS) spectra in Figure 2.


DOS spectrum
Occupied orbitals
Virtual orbitals
Energy (eV)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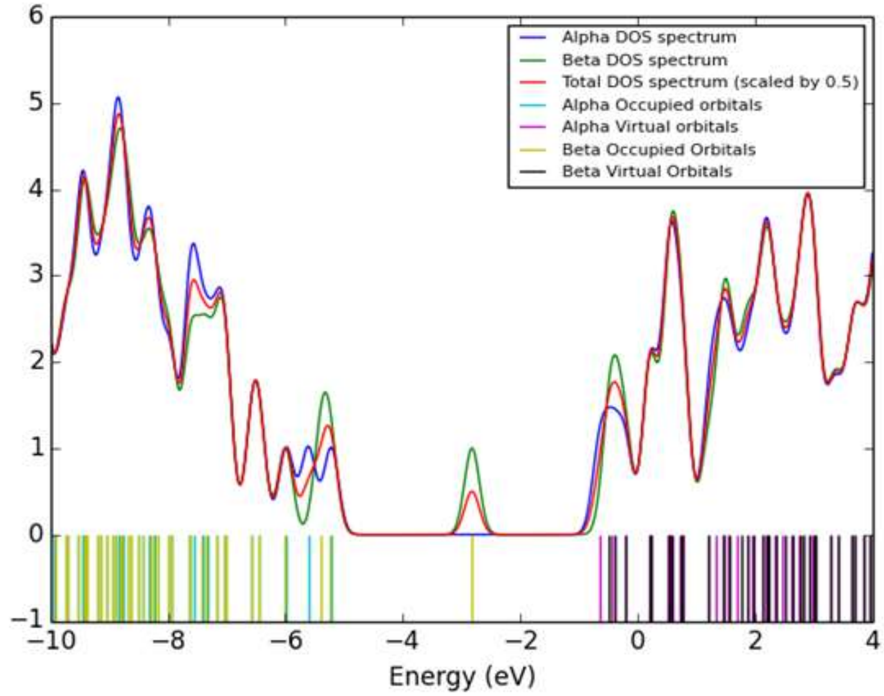

Figure 2:- DOS spectra of (a) BNNS (b)BNNS with Glycine (c) BNNS with Serotonin.

From the DOS spectra, it is observed that the available electronic energy states or density of electronic states change in BNNS when neurotransmitters come in contact with glycine and serotonin; the change in DOS confirms the adsorption or interaction of the neurotransmitters with adsorbent BNNS. In the Figure 2, the rightmost vertical line on the energy axis represents the HOMO (Highest occupied molecular orbital), and the leftmost represents the LUMO (Lowest unoccupied molecular orbital); these HOMO and LUMO of the different structures are shown in Figure 3.

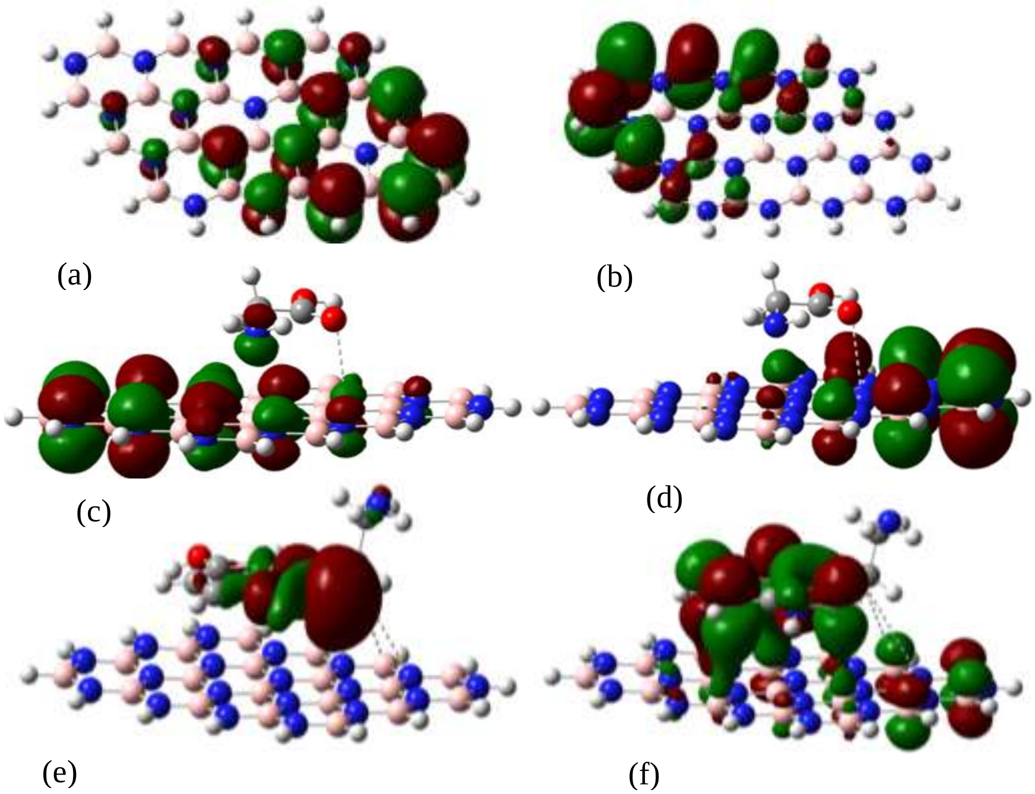

Figure 3:- HOMO of (a)BNNS (c) BNNS with Glycine (e) BNNS with Serotonin and LUMO of (b)BNNS (d) BNNS with Glycine (f) BNNS with Serotonin.

The energy gap between the HOMO and LUMO are called the HOMO-LUMO gap which are tabulated in Table 4 for the different structures.

Structures	HOMO-LUMO gaps in eV
BNNS	5.93
BNNS with Glycine	5.96
BNNS with Serotonin	2.93

Table 4:- HOMO-LUMO gaps of the structures.

The band gap obtained for BNNS is compatible with that obtained by other researchers[9-10]. It is seen that the energy band gap of pristine BNNS changes when both glycine and serotonin are brought near to BNNS. This means that both glycine and serotonin interact with BNNS and adsorbed on BNNS. This change of band gap is desirable for sensing purpose.

Optical Properties

The absorbance or electronic transition properties of the structures in different wavelengths can be visualized from Figure 4. The peaks in the spectra represent electronic transition by absorbing that corresponding wavelength's light which is near to the band gap of the structures. It is seen that the optical absorption peaks after adsorption shifted towards high wavelength region or low energy region; this is because of the reduction of band gap energy after adsorption.

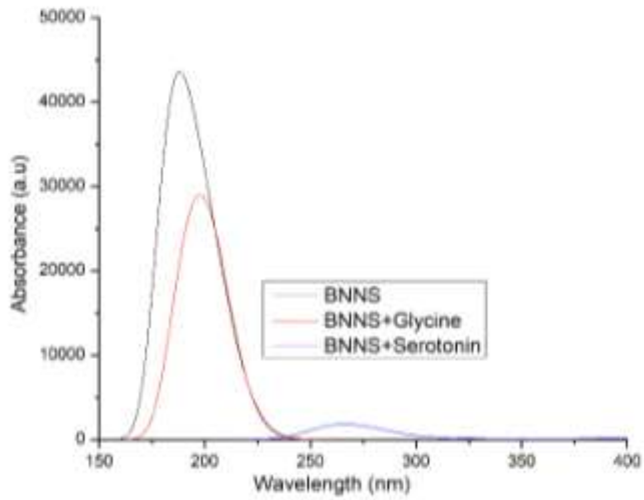

Figure 4:- Optical absorbance spectra of the structures.

Conclusion:-

The geometric structure of the adsorbent BNNS has undergone slight deformation due to interaction of the glycine and serotonin neurotransmitters. The adsorption energy was negative indicating the process of adsorption as exothermic. The band gap of the adsorbent changed due to the adsorption of both glycine and serotonin while there was a huge change in band gap in case of serotonin adsorption. Therefore, the glycine and serotonin neurotransmitters can be sensedordetected by using BNNS as adsorbent.

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