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The effect of biointerface of chemicals and inhibitors in the cerebral cortex of brain on language cognition

Fatemeh Mollaamin [1, *]

[1] Department of French Language and Literature, Science and Research Branch, Islamic Azad University, Tehran, Iran

*corresponding author e-mail address: ***smollaamin@gmail.com***

ABSTRACT

Brain neurotransmitters are essentials in language mechanism to conduct language progress using chemical neurotransmitters in the brain like dopamine that leads human talking path by theoretical levels. At first, the most organized of dopamine-N or -O linked to BNNT has been discussed by the best minimized situation to localize the structure by the delivery method in the brain to excite the part of learning language through a simulated model due to the theoretical properties of Lagrangian kinetic energy G(r), Hamiltonian kinetic energy , Potential Energy density , Laplacian of electron density, Localized orbital locator (LOL) , Local information entropy , average local ionization energy , ESP from nuclear charge and ESP from electrons. Second, it has been simulated the disability modeling function of dopamine as a neurochemical transporter in the brain for learning the language after adsorption on Boron Nitride (BN) and Titanium dioxide (TiO2 Anatase) surfaces through the theoretical methods using thermodynamic data which can produce a structural criteria by comparison between dopamine-Boron Nitride and dopamine-TiO_2 clusters. Then, this work attempts to discover the inhibitors of language development due to blocking of dopamine (DA) by cocaine (CA) when brain cannot control the functions of learning and reward. So, it has been investigated the decrease of DA effectiveness in the brain using modeling the structures of DA, CA, DA-CA , TiO_2 nano-surface, and DA-CA-TiO_2 nano-cluster due to discovering the presence of cocaine (CA) as a stopper of DA release in the brain.

Keywords: *Language cognition; neurochemical transmitters; dopamine; BNNT complex; brain; TiO_2.*

1. INTRODUCTION

Passing the chemical messages in the brain lets routines activities like thinking, learning, movements, speaking, listening and other works through the communication of the brain with itself which transfers the chemical data from one neuron to another.

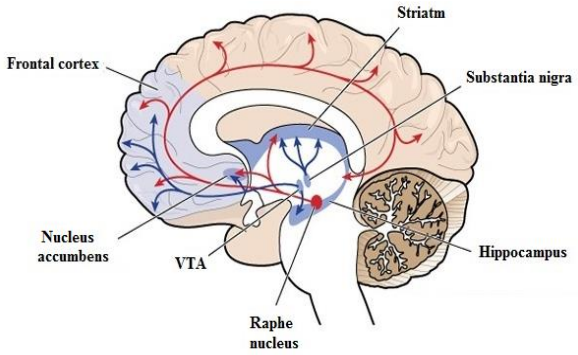
Communicating among the human has been investigated by discovering the neurochemicals in the human's brain to perceive chemical changes produced by people activities and experiences.

MR spectroscopic (magnetic resonance) has introduced an account how the children and adults brain develop. Neurochemicals through MR spectroscopy have allowed researchers to study disease processes and mutagenic evolution of subjects in vivo. They have approved that there is a complex association between structural brain development and changes in levels of metabolites, which are organic compounds used or produced by metabolism [1].

Neurological experiments have illustrated a central part of function by dopamine in a proper motor commands, learning and higher-order cognitive process with language institute [2].

It has been also found that the human has the most improved susceptibility for producing different languages [3]. The neuroscience learning through condition changes of the brain has been discovered by scientists [4].

It has been approved that learning a foreign language changes the structure and function of the brain to be more adaptable and releasing neurochemicals can help powerful learning. There are some characteristics of the dopaminergic system consisting of brain systems, domain general language functions and related genes. These characteristics can construct the basis for improving informed hypotheses about the genetic fundamental of grammar cognition and memory and the cerebral cortex responsible for higher-order functions such as language and information processing. So, this total part is known as the brain's reward or pleasure center (scheme 1) [5].



Scheme 1. The pathway of chemical neurotransmitters in the brain.

The procedure of dopaminergic deals with brain structures, procedural memory level but encoded dopamine DA gene receptors and deliverers in nonlinguistic elements are connected to various brain answers and learning rules [6].

Learning is satisfying and excited for all people, so the amount of dopamine increases in the brain to take our information. On the other hand, some learners cannot keep the new knowledge and lose them through the lack of dopamine. The amount of dopamine increases by encouraging students and generates excitement to learn and remember the categorized data in their brain.

BNNTs of boron and nitrogen atoms in graphite like structure with electrostatic interactions have an important role in gaining the elastic properties of BNNTs [7]. The theoretical properties show a variety of parameters of electron structures which are calculated by the method of wave function analysis [8].
It has been done a theoretical debate of adsorption of dopamine by nanoparticles in the brain to study the disability of language learning, because dopamine is one of the most significant neurochemicals for learning new things such as a second language.

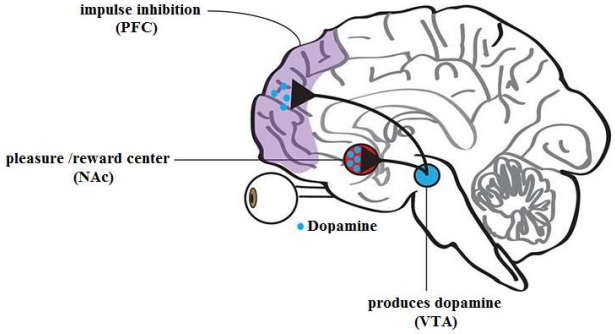
The differences among nanoparticles are related to chemical and physical properties and sometimes are harmful to nature, especially medicine. They can traverse the protective membrane barrier surrounding cells due to their small size and chemical properties [9].

Although the recent studies have shown that nanoparticles such as boron-nitride and Titanium dioxide nanotubes can treat cancer in the brain and other parts of the body such as lung, liver, prostate, head and neck, kidney and pancreas, can also damage the cell brain [10].

BNNTs show electrical properties such as superconductors, semiconductors and insulators, so scientific efforts focused on the electrostatic properties of these materials [11, 12].
Some experimental studies have been done on these compounds by Raman spectroscopy and phonon dispersion. The electronic structure and the reverse of the diameter (1/d) dependence of the frequency of the radial breathing mode (RBM) were employed [13].

Some investigations have been launched to the study of TiO_2 Nano-clusters because of their multiple applications in chemistry [14].

In this study, it has been illustrated dopamine as one of the effective brain neurochemical transmitters in language processing, adsorption of dopamine by Boron Nitride and Titanium dioxide surfaces through the brain and a comparison with them which can cause the disability of language learning has been indicated. Finally, it has been investigated the inhibitive role of cocaine which increases the amount of dopamine in the nucleus accumbens and causes a shortcut to the brain's pleasure center.
After blocking of DA (dopamine) by CA (cocaine), brain cannot monitor the special functions by the flow of information from other areas of the brain with the happiness and satisfaction of the brain through reinforcement and enjoyment to encourage us to do activities based on neurobiological theories and information flowing to the brain will stop due to learning and conducting the human knowledge (Scheme 2).



Scheme 2. The increase of dopamine in the cerebral cortex of brain.

2. EXPERIMENTAL SECTION

Theoretical method of simulation model

Multiwfn software is suitable for the visual study of real space functions like ELF (electron localization function) and ESP (electrostatic potential). Also, there is some wave function analysis software limited to the principal analysis methods. The electron density surface of dopamine jointed to Boron Nitride nanotube (BNNT) has been calculated as [15,16]:

$$\rho(r) = \eta_i \left|\varphi_i(r)\right|^2 = \sum_i \eta_i \left|\sum_l C_{l,i}\,\chi_i(r)\right|^2 \qquad (1)$$

η_i is occupation number of orbital *i*, χ is the basis function, φ is orbital wave function , and
C is Bader which explains the zones by large electron localization including enormous Fermi-hole parameter with a six-dimension function. Probability of spin conditional pair as the spherically averaged has a direct correlation with Fermi hole and the electron localization function [17]:

$$\mathrm{ELF(r)} = \frac{1}{1+[D(r)/D_{0(r)}]^2}, \quad \mathrm{D(r)} = \frac{1}{2}\sum_i \eta_i \left|\nabla\varphi_i\right|^2 - \frac{1}{8}\left[\frac{\left|\nabla\rho_\alpha\right|^2}{\rho_\alpha(r)} + \frac{\left|\nabla\rho_\beta\right|^2}{\beta(r)}\right] \qquad (2)$$

$$D_{0(r)} = \frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}} \qquad (3)$$

Kinetic energy illustrates ELF for post HF wave function and Kohn Sham DFT wave function. Thomas-Fermi kinetic energy density, $D_0(\mathbf{r})$ and $D(\mathbf{r})$, indicates the excess kinetic energy density of Pauli repulsion. In fact, a correction value of 10-5 to $D(\mathbf{r})$ is shown by Multiwfn program and kinetic energy term changes by Kirzhnits type second order gradient expansion:

$$\frac{1}{2}\sum_i \eta_i \left|\nabla\varphi_i\right|^2 \approx D_0(r) + \frac{1}{72}\frac{\left|\nabla\rho\right|^2}{\rho(r)+\frac{1}{6}\nabla^2\rho(r)} \qquad (4)$$

ELF is totally free of the wave-function and can be used to discuss electron density from X-ray diffraction results. Besides, LOL, localized orbital locator, is used for placing high localization areas. LOL has an expression and specified significant chemical zones; it is also comparable to ELF. The obtained values of LOL denote more clear and certain amounts than ELF [18].
In this study, the computational methods have been done using Gaussian 09 on the 8, 0- zigzag dopamine BNNT complexes [19]. The calculated parameters have been done by density functional theory and the Kohn-Sham equation in a plane-wave set with the

projector increased wave pseudo-potentials [20]. Simulation indicates the methods which aim to produce a representative sampling of a system at a finite temperature that calculate most of the properties from partition function [21].

The adsorption of bioorganic structures such as dopamine on nanoparticles of Boron Nitride and Titanium dioxide clusters were calculated in this work, and the most stable ones are shown in Figs.1 and 2.

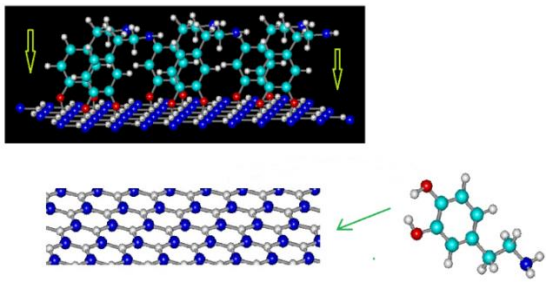


Figure 1. The adsorption of neurochemical, dopamine, on the Boron Nitride nanostructure.

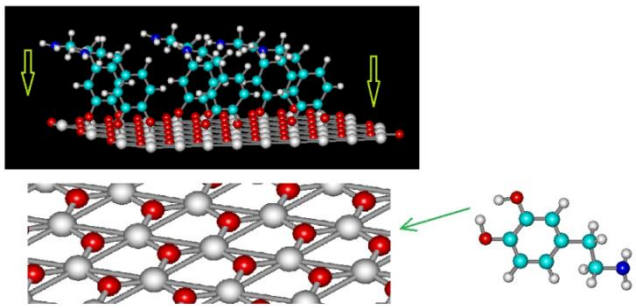


Figure 2. The adsorption of neurochemical, dopamine, on the TiO_2 surface.

Dopamine is released by a neuron into the synapse in the natural communication process, where it can be linked to dopamine receptors on neighboring neurons. Then, it is recycled back into the transmitting neuron by a specific protein of dopamine transporter. In the presence of cocaine, dopamine transporter is attached by cocaine which blocks the normal recycling process, appearing in a structure of dopamine in the synapse, and contributes to motivation and pleasurable effects of cocaine (Fig.3).

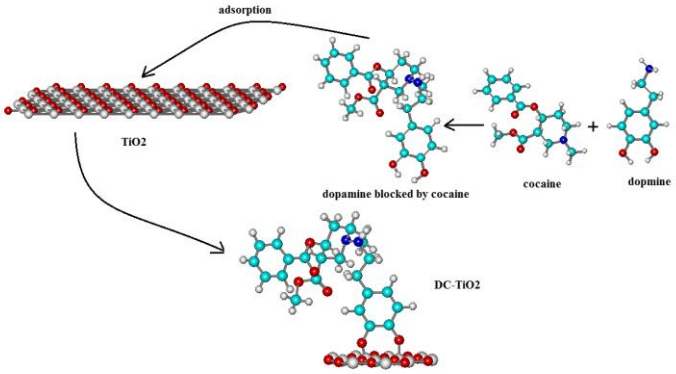


Figure 3. The path of cocaine functions through the blocked dopamine in the brain.

Dopamine-cocaine (DA-CA) dissociates by its OH bonds and adsorbs on TiO_2 nano-surface as the bidentate mode that DA-CA places perpendicular to the surface of TiO_2 (Fig.3).

During brain is fulfilled unexpectedly, dopamine releases largely, making the Limbic pleasure center to take note for remembering how to copy the positive experience.

In contrast, negative thoughts reduce dopamine as a signal to avoid repeating them which is a key learning mechanism dealing with memory-formation and motivation because researchers believe that brain proves a new temporary neural network to process a new development.

3. RESULTS SECTION

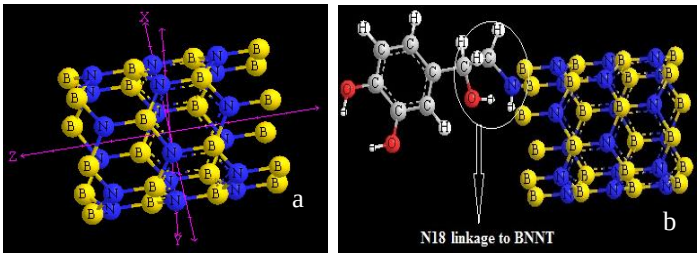
Dopamine is not only a neurochemical transmitter released by the brain in humans and other animals, but also has some noteworthy roles such as "cognition", "memory", "behavior" and "learning" which has been researched in the previous works [22-29]. So, in this work, the surface geometry coordination (x,y,z) of dopamine jointed to zigzag BNNT complex as a dopamine-nanotube neurotransmitter (N and O active sites) has been optimized (Fig.4 a-c).

Also, Some properties such as density of all electrons , Lagrangian kinetic energy G(r), Hamiltonian kinetic energy , Potential Energy density , Laplacian of electron density; Localized orbital locator (LOL), Local information entropy , average local ionization energy , ESP from nuclear charge , ESP from electrons and Total ESP have been calculated for dopamine structure (table1.a and Figs.5a,b) , dopamine with N jointed to BNNT (table1.b) and O jointed to BNNT (table1.c) as neurochemical transmitters using the Multifunctional Wave function Analyzer (Table1 and Figs.6 a-c)[13].

Table 1. b, and c show two sites of N and O atoms from dopamine molecule which linked to BNNT (Fig.5a-c).

Theoretical properties of Lagrangian kinetic energy G(r), potential energy density V(r) and Laplacian of electron density (LED) for dopamine-BNNT complex \ have been plotted due to N and O linkages, respectively (Figs.6a-c).

Obviously, more stable of dopamine with N or O linked to BNNT has been investigated the best coordination for citing the structure using the delivery technique in the brain to promote the center of learning the language as a model (Tables1 b, c , Figs. 6a-c).



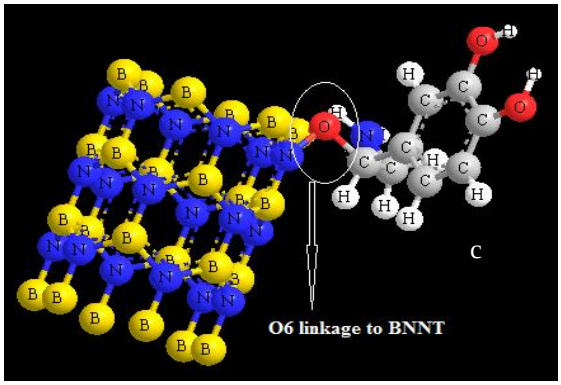


Figure 4. (a) Boron Nitride Nanotube with Inertial Axes, dopamine-BNNT deliverer of different citations of **(b)** N18 and **(c)** O6 linkage as the optimized models for junction of dopamine to zigzag BNNT complex as dopamine-nanotube neurotransmitter (N and O active sites).

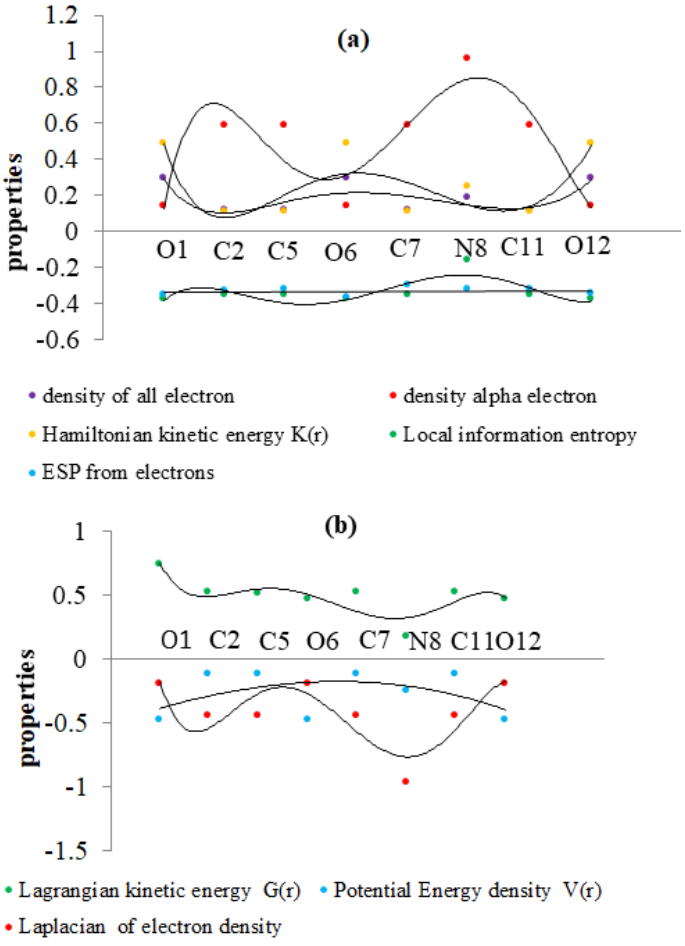


Figure 5. Theoretical properties of **(a)** density of all electron, density alpha electron, Hamiltonian kinetic energy , Local information entropy ,ESP from electrons and **(b)** Lagrangian kinetic energy , Potential density ,Laplacian of electron density for dopamine as a neurotransmitter in the brain.

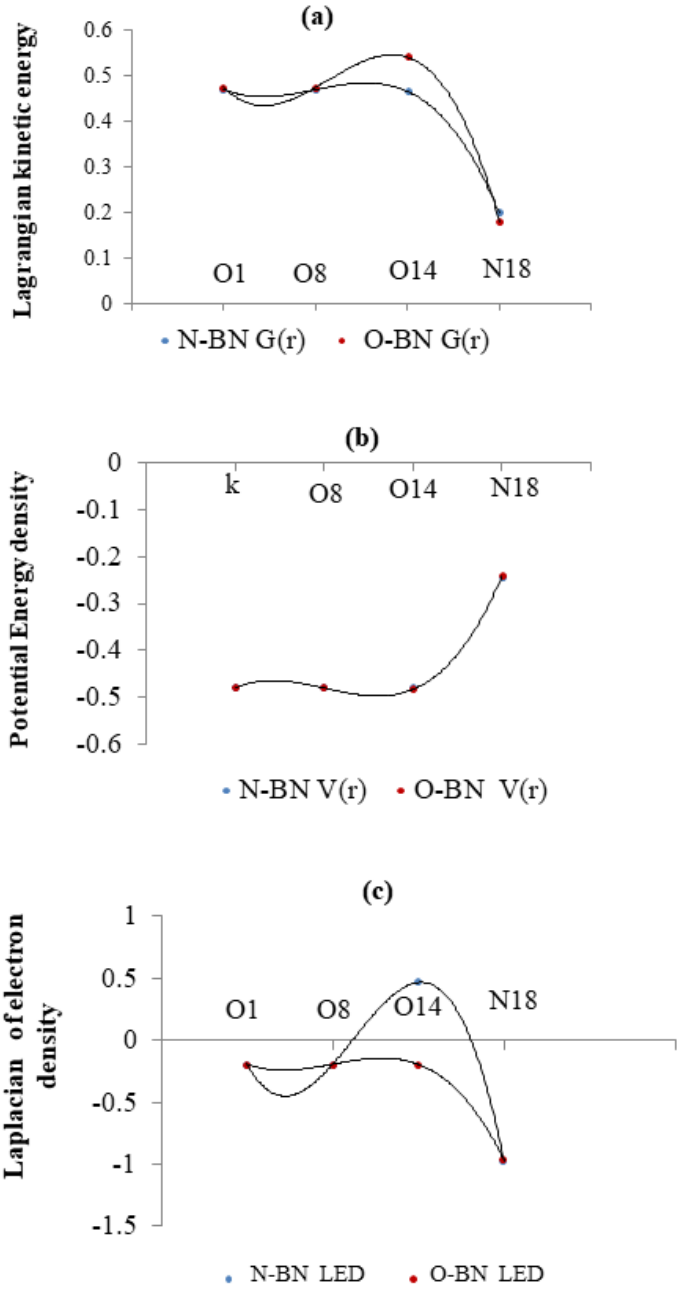


Figure 6. (a) Lagrangian kinetic energy G(r), **(b)** potential energy density V(r) and **(c)** Laplacian of electron density via active atoms of Nitrogen and Oxygen formed the complex of N-BN and O-BN.

Geometrical optimization was done on two surfaces of TiO_2 Anatase and BN for unraveling a description of the electronic structures through vibrational calculations.

This approach allows giving an estimate of the relative energy of the electronic states for TiO_2, BN and the clusters of adsorption with bioorganic structure, dopamine.

An analysis of the electron spin density was carried out to get a picture of the charge transfer occurring upon dopamine adsorption on TiO_2 anatase and BN surfaces (Figs.7a,b).

Table 1. Calculated properties on **a)** dopamine **b)** 8, 0 zigzag dopamine BNNT deliverer due to N linkage **c)** 8, 0 zigzag dopamine BNNT deliverer due to O linkage in the brain.

aatoms	Density of all electron	Density Alpha electron	Lagrangian kinetic energy	Hamiltonian kinetic energy	Potential Energy density V(r)	Laplacian of electron density	Localized orbital locator (LOL)	Local information entropy	Average local ionization energy	ESP from electrons	Total ESP
(a)											
O1	0.29	0.14	0.74	0.48	-0.48	-0.19	0.9987	-0.38	0.18	-0.35	0.96
C2	0.12	0.59	0.52	0.11	-0.11	-0.43	0.9993	-0.35	0.99	-0.33	0.97
C5	0.12	0.59	0.51	0.11	-0.11	-0.44	0.9993	-0.35	0.99	-0.32	0.97
O6	0.29	0.14	0.46	0.48	-0.48	-0.19	0.9987	-0.38	0.18	-0.36	0.96
C7	0.12	0.59	0.52	0.11	-0.11	-0.43	0.9993	-0.35	0.99	-0.30	0.97
N8	0.19	0.95	0.17	0.24	-0.24	-0.96	0.9990	-0.16	0.14	-0.32	0.97
C11	0.12	0.59	0.52	0.11	-0.11	-0.43	0.9993	-0.35	0.99	-0.32	0.97
O12	0.29	0.14	0.47	0.48	-0.48	-0.19	0.9987	-0.38	0.18	-0.35	0.96
(b)											
O1	0.29	0.14	0.47	0.48	-0.48	-0.19	0.9987	0.12	0.18	-0.48	0.95
O8	0.29	0.14	0.47	0.48	-0.48	-0.19	0.9987	0.12	0.18	-0.48	0.95
O14	0.29	0.14	0.46	0.48	-0.48	0.46	0.9987	0.12	0.18	-0.54	0.94
N18	0.19	0.96	0.20	0.24	-0.24	-0.97	0.9989	0.32	0.14	-0.61	0.94
(c)											
O1	0.29	0.14	0.47	0.48	-0.48	-0.19	0.9987	0.12	0.18	-0.50	0.95
O8	0.29	0.14	0.47	0.48	-0.48	-0.19	0.9987	0.12	0.18	-0.48	0.95
O14	0.29	0.14	0.54	0.48	-0.48	-0.19	0.9985	0.12	0.18	-0.67	0.93
N18	0.19	0.95	0.18	0.24	-0.24	-0.96	0.9990	0.32	0.14	-0.54	0.94

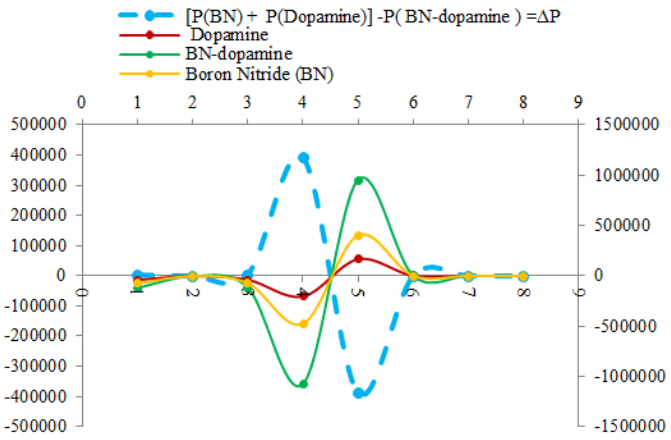


Figure 7a. Simulated thermodynamic parameters of dopamine-BN surface.

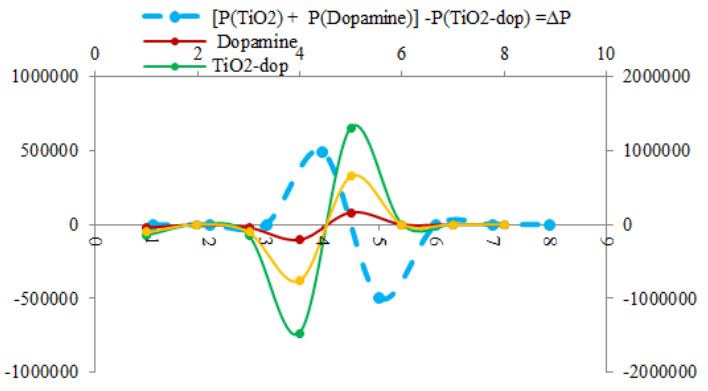


Figure 7b. Simulated thermodynamic parameters of dopamine-TiO_2 surface.

The adsorption energy, E_{ads}, was calculated as the energy difference between the energy of the adsorption complex and the sum of dopamine, the bare slab. In this work, if the adsorption stabilizes the system, then E_{ads} <0. Thus, the more negative E_{ads}, the more stable structure (Tables 2 and 3 and Fig.7) based on following eqs.5,6;

$[P_{(BN)} + P_{(dopamine)}] - P_{(dopamine-BN)} = \Delta P$ (5)

(5)

$[P_{(TiO2)} + P_{(dopamine)}] - P_{(dopamine-TiO2)} = \Delta P$ (6)

Where P is the thermodynamic parameter such as Total Energy, Binding Energy, Isolated Atomic Energy, Electronic Energy, Core-Core Interaction, Heat of Formation, Gradient (kcal/moll/Nag) and Dipole (Debye).

Table 2. Thermodynamic properties of adsorption of dopamine on the Boron Nitride surface.

Thermodynamic property (kcal/mol)	Dopamine	BN-dopamine	Boron Nitride (BN)	$[P_{(BN)} + P_{(Dopamine)}] - P($ BN-dopamine $) = \Delta P$
Total Energy	-42250.07	-121679.05	-76451.55	2977.43
Binding Energy	-2036.41	-4132.52	-2806.25	-710.14
Isolated Atomic Energy	-40213.65	-117546.53	-73645.30	3687.57
Electronic Energy	-206713.81	-1076705.32	-478541.61	391449.89
Core-Core Interaction	164463.75	955026.27	402090.06	-388472.46
Heat of Formation	31.74	920.034	178.15	-710.14
Gradient (kcal/mol/Ang)	67.47	198.05	100.99	-29.58
Dipole (Debyes)	184.88	4.71	1.051	181.22

Table 3. Thermodynamic properties of adsorption of dopamine on the TiO_2 surface.

Thermodynamic property (kcal/mol)	Dopamine	TiO_2-dopamine	TiO_2	$[P_{(TiO2)} + P_{(Dopamine)}] - P_{(TiO2\text{-}dop)} = \Delta P$
Total Energy	-42250.07	-146156.54	-106948.53	-3042.05
Binding Energy	-2036.41	-162.08	-170.43	-2044.76
Isolated Atomic Energy	-40213.65	-145994.46	-105780.81	0
Electronic Energy	-206713.81	-1457995.69	-758628.85	492653.02
Core-Core Interaction	164463.75	1311839.15	651680.32	-495695.08
Heat of Formation	31.74	3968.38	894.58	-3042.05
Gradient (kcal/mol/Ang)	67.47	764.59	359.16	-337.96
Dipole (Debyes)	184.88	10.48	7.61	182.01

After simulating the model, relative energy (ΔE_r) of DA, CA, DA-CA, TiO_2 nano-surface, and DA-CA-TiO_2 nano-cluster based on electron density of these structures has been debated.

This method lets giving an illustration of the adsorption energy of the electronic states for DA which was blocked by cocaine on the surface (Table 4).

An analysis of the electron density was carried out to gain the charge transfer upon dopamine blocked by cocaine adsorption on TiO2 nano-surface (Fig.3).

The relative energy ($\mathbf{\Delta E_r}$) is attained as the energy difference between the energy of the adsorption of DA-CA-TiO_2 nano-cluster , $E_{(DA\text{-}CA\text{-}TiO2)}$, and the sum of DA , CA, DA-CA, TiO_2 nano-surface, $E_{DA}+E_{CA}+E_{DA\text{-}CA}+E_{TiO2}$ (eq.7) .

$$\Delta E_r = [E_{DA}+E_{CA}+E_{DA\text{-}CA}+E_{TiO2}] - [E_{(DA\text{-}CA\text{-}TiO2)}] \quad (7)$$

Moreover, the core–core interaction and the electronic energy were plotted to show the distribution points of DA, CA, DA-CA, TiO_2 nano-surface, and DA-CA-TiO_2 nano-cluster with R^2 = 0.8029 for core-core interaction and R^2 = 0.7833 for electronic energy (Fig.8) .Fig.8 has estimated the most important value of change and stability for DA-CA-TiO_2 nano-surface .

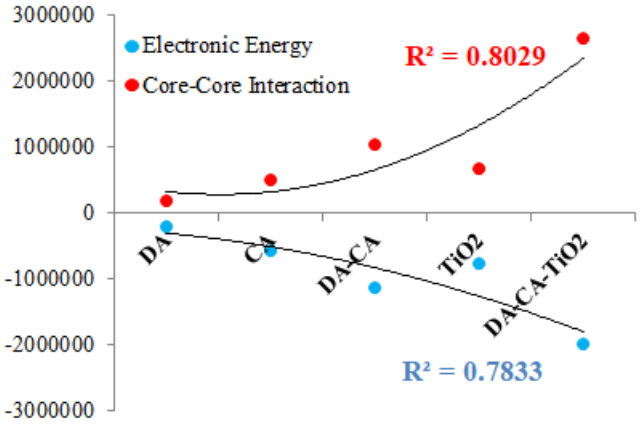


Figure 8. The core–core interaction and the electronic energy were drawn to show the distribution points of DA, CA, DA-CA, TiO_2 nano-surface, and DA-CA-TiO_2 nano-cluster.

The relative energy of dopamine, cocaine, DA-CA, TiO_2 nano-surface, and DA-CA-TiO_2 nano-surface have been simulated to achieve the structural model and parameters based on the results of the most minimized adsorption energy for DA-CA-TiO_2 nano-surface in compared to dopamine, cocaine, DA-CA and TiO2 nano-surface (Table 4, Fig.8).

Table 4. Optimized properties of dopamine, cocaine, TiO_2 surface, DA-CA and DA-CA-TiO_2 nano-surface.

properties	dopamine	cocaine	DC	TiO2	DC-TiO2	$\Delta E=(E_D+E_C+E_{DC}+E_{TiO2}) - (E_{(DC\text{-}TiO2)})$
Total Energy	-43042.95	-78498.97	-120106.10	-106834.98	630926.06	-979409.95
Binding Energy	-2226.34	-3969.99	-5062.89	-1054.17	851148.02	-863461.42
Isolated Atomic Energy	-40816.61	-74528.98	-115044.11	-105780.81	-220221.96	-115948.54
Electronic Energy	-217763.81	-575615.22	-1151163.88	-762710.91	-1994461.59	-712792.23
Core-Core Interaction	174720.86	497116.25	1031056.89	655875.93	2625387.65	-266617.72
Heat of Formation	-53.97791	-65.47	961.89	1008.13	859130.91	-857280.33
Gradient	19.03	31.24	125.98	371.44	6260.96	-5713.26

4.CONCLUSIONS

Linkage of dopamine on the edge of (8, 0) zigzag BNNT is modeled in different positions through transferring the electron. The jointed atoms of nitrogen and oxygen by large electron localization and magnitudes of Fermi-hole integration have been approved through considering the spherical average of the spin for the Fermi hole. Our calculations have demonstrated that such extrapolation schemes significantly overestimate the dopamine- BNNT by the active site of a molecule (N and O linkage) which are the most active points of the indicated structure.

Then, it has been illustrated the interface dopamine-BN and dopamine-TiO_2 nano-surfaces on an atomic level by means of theoretical methods to unravel the features connecting geometrical and electronic structures which inactivate the role of dopamine in the brain due motivating and learning. Thus, it has been indicated how dopamine can be less active with adsorbing on the surface of BN and TiO_2 Anatase Nanoclusters. It will be discussed that the electronic structure of the surface of dopamine-BN and dopamine-TiO_2 systems is crucial to prove the basic features of their activity and disability.

Finally, it has been indicated that after blocking of dopamine by cocaine inhibitor, the brain cannot play its role for releasing neurotransmitters which have the responsibility of learning a new language and enjoying in daily life.

5. REFERENCES

[1] Baslow M.H., Guilfoyle D.N., Using proton magnetic resonance imaging and spectroscopy to understand brain "activation", *Brain and Language*, 102, 153-164, **2007**.

[2] Ueno A., Akabane Y., Kato T., Hoshino H., Kataoka S., Ishiyama Y., Capacitive sensing of electrocardiographic potential through cloth from the dorsal surface of the body in a supine position: a preliminary study, *IEEE Trans Biomed Eng*, 54, 4, 759-66,**2007.**

[3] Jürgens U., Neural pathways underlying vocal control, *Neurosci Biobehav Rev*, 26, 2, 235-58,**2002.**

[4] Merzenich M.M., Nelson R.J., Stryker M.P., Cynader M.S., Schoppmann A., Zook J.M., Somatosensory cortical map changes following digit amputation in adult monkeys, *Journal of Comparative Neurology* **,** 224, 4, 591-605, **1984.**

[5] Opitz B.,Friederici A.D., Interactions of the hippocampal system and the prefrontal cortex in learning language-like rules, *NeuroImage*, 19, 4, 1730-1737, **2003.**

[6] Shohamy D., Adcock R.A., Dopamine and adaptive memory, *Trends in Cognitive Sciences*, 14, 10, 464-472, **2010.**

[7] Chopra N.G., Luyken R.J., Cherrey K., Crespi VH., Cohen M.L., Louie S.G., Zettl A., Boron nitride nanotubes, *Science*, 269, 5226, 966-967, **1995.**

[8] Jensen F., *Introduction to Computational Chemistry; Wiley: Chichester* ,second edition, 293-314, **2007.**

[9] Wang J., Liu Y., Jiao F., Lao F., Li W., Gu Y., Li Y., Ge C., Zhou G., Li B., Zhao Y., Chai Z., Chen C., Time-dependent translocation and potential impairment on central nervous system by intranasally instilled TiO(2) nanoparticles, *Toxicology* , 254, 1-2, 82-90, **2008.**

[10] Zheng M., Ke C., Bae I.T., Park C., Smith M.W., Jordan K., Radial elasticity of multi-walled boron nitride nanotubes, *Nanotechnology*, 23, 9, 095703, **2012.**

[11] Mollaamin F., Features of Parametric Point Nuclear Magnetic Resonance of Metals Implantation on Boron Nitride Nanotube by Density Functional Theory/Electron Paramagnetic Resonance, *J. Comput. Theor. Nanosci*, 11, 11, 2393-2398, **2014.**

[12] Monajjem M., Non-covalent attraction of $B_2N^{(-,0)}$ and repulsion of $B_2N^{(+)}$ in the B_nN_n ring: a quantum rotatory due to an external field, *Theor Chem Acc*, 134, 77, 1-22, **2015.**

[13] Ouyang M., Huang J.L., Lieber C.M., Fundamental Electronic Properties and Applications of Single-Walled Carbon Nanotubes, *Acc Chem Res*, 35, 12, 1018-1025, **2002.**

[14] Urdaneta I., Keller A., Atabek O., Palma J.L., Finkelstein-Shapiro D., Tarakeshwar P., Mujica V., Calatayud M., Dopamine adsorption on TiO_2 anatase surfaces, *J PHYS CHEM C*, 118, 35, 20688-20693, **2014.**

[15] Weinhold F., Landis C.R., Natural bond orbitals and extensions of localized bonding concepts, *Chemistry education research and practice*, 2, 91-104, **2001.**

[16] Kohout M., Bonding indicators from electron pair density functionals, *Faraday Discuss,* 135 , 43-54 ,**2007.**

[17] Bader R.F.W., *Atoms in Molecule: A quantum Theory (Oxford Univ. press, Oxford)*, **1994**.

[18] Lu T., Chen F., Multiwfn: a multifunctional wave function analyzer, *J Comput Chem*, 33, 5, 580-592, **2012.**

[19] Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Mennucci B., Petersson G.A., Nakatsuji H., Caricato M., Li X., Hratchian H.P., Izmaylov A.F., Bloino J., Zheng G., Sonnenberg J.L., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Montgomery Jr., J.A., Peralta J.E., Ogliaro F., Bearpark M., Heyd J.J., Brothers E., Kudin K.N., Staroverov V.N., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J.C., Iyengar S.S., Tomasi J., Cossi M., Rega N., Millam J.M., Klene M., Knox J.E., Cross J.B., Bakken V., Adamo C., Jaramillo J., Gomperts R., Stratmann R.E., Yazyev O., Austin A.J., Cammi R., Pomelli C., Ochterski J.W., Martin R.L., Morokuma K., Zakrzewski V.G., Voth G.A., Salvador P., Dannenberg J.J., Dapprich S., Daniels A.D., Farkas O., Foresman J.B., Ortiz J.V., Cioslowski J., Fox D.J. , *Gaussian 09*, Gaussian Inc., Wallingford CT, **2009.**

[20] Perdew J.P., Burke K., and Ernzerhof M., Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett*, 78, 3865**, 1996.**

[21] van Gunsteren W.F., Berendsen H.J. C., Computer Simulation of Molecular Dynamics: Methodology, Applications, and Perspectives in Chemistry, *Angewandte Chemie International Edition in English*, 29, 9, 992-1023, **1990**.

[22] Grandy DK., Miller GM., Li JX .,TAARgeting Addiction"-The Alamo Bears Witness to Another Revolution: An Overview of the Plenary Symposium of the 2015 Behavior, Biology and Chemistry Conference". *Drug Alcohol Depend*, 159, 9-16,**2016.**

[23] Ayano G., Dopamine: Receptors, Functions, Synthesis, Pathways, Locations and Mental Disorders: Review of Literatures ,*Journal of Mental Disorders and Treatment*,2,2,1-4,**2016.**

[24] Hare DJ., Double KL., Iron and dopamine: a toxic couple, *Brain*, 139, 4, 1026-35,**2016.**

[25] Pavăl D., A Dopamine Hypothesis of Autism Spectrum Disorder, *Dev Neurosci* ,39:355-360 ,**2017.**

[26] Orefici G., Cardona F., Cox CJ., et al: Pediatric autoimmune neuropsychiatric disorders associated with streptococcal infections (PANDAS); in Ferretti JJ, Stevens DL, Fischetti VA (eds): *Streptococcus pyogenes*: Basic Biology to Clinical Manifestations. Oklahoma City, University of Oklahoma Health Sciences Center, **2016.**

[27] Fischer AG., and Ullsperger M., An Update on the Role of Serotonin and its Interplay with Dopamine for Reward, *Front Hum Neurosci***,** 11, 484, 2017.

[28] Sebastian Kruss, Daniel P. Salem, Lela Vuković, Barbara Lima, Emma Vander Ende, Edward S. Boyden, and Michael S. Strano, High-resolution imaging of cellular dopamine efflux using a fluorescent nanosensor array ,*PNAS* ,114 ,8, 1789-1794 ,**2017.**

[29] Polo E., Kruss S., Nanosensors for neurotransmitters. *Anal Bioanal Chem* ,408, 11,2727–2741 ,**2016.**

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