

Methamphetamine causes the exhilaration in the brain by dumping dopamine

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ABSTRACT

Neurochemical transmitters in the brain lead speaking mechanism and its path by physical and chemical interactions in the various environments. Fundamental neurotransmitter, Dopamine (DA), is infectious by Methamphetamine (Meth) through the language status; so this work strives to demonstrate the lack of language progress after blocking of DA by Meth while brain is not capable to manage the operation of learning. Meth is an important loss of DA transmitters which creates a reduced memory through the slower motor operation. Then, in this work, it has been discussed the damage of DA effectiveness in the brain by simulating the compounds of Meth, DA, Meth-DA, TiO₂ nanosurface, and Meth-DA-TiO₂ nanocluster due to discovering the effect of Methamphetamine (Meth) as a stopper of DA release in brain. Theoretical calculations have been run on these compounds to achieving the chemical and physical effects. So, it has been shown that after blocking of dopamine by Meth, brain cannot indicate its function for dispersing the neurochemical transmitters which cause the role of learning a foreign language.

Keywords: neurochemical transmitters; methamphetamine (meth); dopamine (DA); language; brain; TiO₂.

1. INTRODUCTION

Methamphetamine (C10H15N) is a common abuser as a significant loss of DA transporters which produces a decreased memory through the slower motor function.

The scientists think that the loss of DA transports which predisposes methamphetamine abusers to neurodegenerative cause some disorders like Parkinsonism. It has been evaluated the perspective of protracted abstinence on the loss of DA transmitter in methamphetamine by DA transmitter radio ligand and positron emission. Brain DA transmitters in some methamphetamine abusers experimented on six months and then reexamined during 12–17 months which indicated important increases with protracted abstinence. The DA transmitter increasing with abstinence is able to show that methamphetamine-induced DA transmitter loss reflects temporary adaptive [1, 2].

Conversation among the human has been researched by unraveling the neurochemical transmitters in the brain to understand the chemical changes caused by activities. Magnetic resonance has been applied to show a value of how the brain improves. Neurochemical transmitters through magnetic resonance spectroscopy have led scientists to research the disease mechanism. They have illustrated that there is a significant association between structural brain improvement and fluctuations in steps of metabolites which are organic structures applied or produced with metabolism [3].

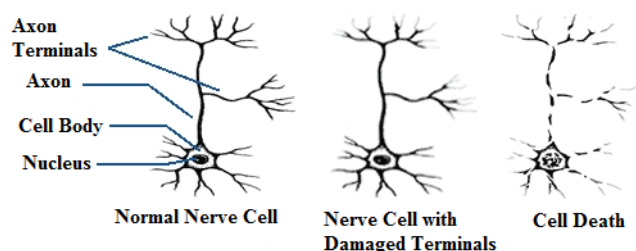
Neurological experiences have debated a central part of the role by DA in a suitable motor commands, learning and higher-order cognitive process with language system [4, 5].

It has been also perceived that the human has the most developed capabilities for forming different languages. The neuroscience learning through condition fluctuations of brain has been investigated by researchers [6, 7].

It has been discovered that learning a new language alters the foundation and the role of the brain to be more flexible and flowing neurochemical transmitters can help powerful learning.

There are some properties of the dopaminergic system including the brain systems, domain general language roles and related genes. These properties can form the basis for developing updated hypotheses of the genetic fundamental in grammar cognition, memory and the cerebral cortex of responsible for higher-order roles such as language and information steps [8].

The scheme 1 shows that methamphetamine harms the nerve terminals of DA-producing brain cells by activating a natural mechanism of apoptosis that causes the death of additional nerve cells in other brain regions [9, 10].

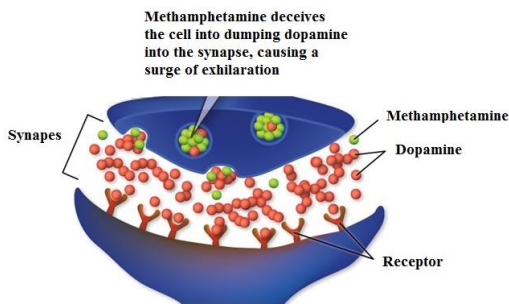


Scheme 1. Neurotoxic effects of Methamphetamine in the brain.

The method of dopaminergic accompanies with brain structures, procedural memory step, however encoded DA gene receptors and deliverers in nonlinguistic parameters are related to different brain replies and learning instructions [11, 12].

Meth releases DA fast as the high values in the brain which tightly reinforces drug-taking behavior, making the user want to repeat the experience. Meth like other excitants such as amphetamines and cocaine can conclude a lot of similar results such as deteriorating the physical activity, the decreasing of appetite, decreasing, fast and irregular heartbeat through rising body temperature and the blood pressure.

Moreover, meth can produce significant alterations in the brain's DA system brain complicated with emotional and cognitive difficulties which are involved with the loss of impaired verbal learning (scheme 2) [13].



Scheme 2. The mechanism of dopamine (DA) level increasing in the cerebral cortex of brain.

Although some changes in the brain might reverse after being off the drug during some years, other changes might not regain even after a long time of abstinence [14]. Recently, it has been studied that using the meth has an increased risk of developing Parkinson's disease to ruin the nerves and their movement [15].

Some people cannot save the new knowledge and lose them through the lack of dopamine (DA). The number of DA increases by encouraging students and generates excitement to learn and remember the categorized data in their brain. Learning is satisfying and excited for all people, so the number of DA increases in the brain to take our information. It has been studied a theoretical discussion of adsorption of DA by nanoparticles in the brain to investigate the damage of language learning because DA is one of the most important neurochemical transmitters for learning the new skills such as a new language. Chemical and physical properties are different in nanostructures and sometimes toxic to nature. They are able to traverse the protective membrane barrier

2. MATERIALS AND METHODS

In this work, the appropriate software is Multiwfn which is used for the visual study of real space functions like ELF (electron localization function) and ESP (electrostatic potential). It has been shown some wave function inspection software restrain to the main analysis approaches. The electron density surface of DA and Meth jointed to TiO₂ nano-surface has been calculated as (Fig.1) [30, 31]:

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

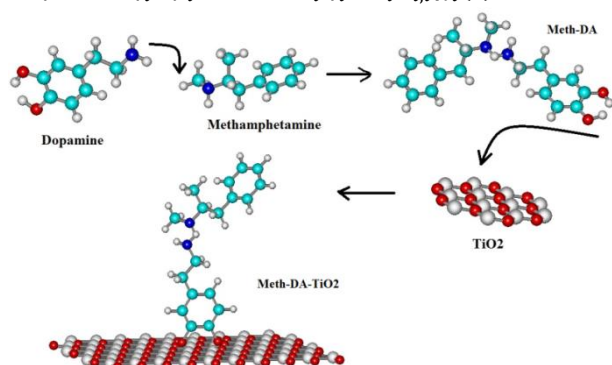


Figure 1. Schematic of the adsorption mechanism including Dopamine, Methamphetamine, Meth-DA complex and Meth-DA-TiO₂.

η_i is occupation number of orbital i ; χ the basis function; φ orbital wave function, and C Bader which illustrates the areas by ground electron localization consisting of large Fermi-hole

surrounding cells through their small size and chemical properties [16].

Nanoparticles such as Titanium dioxide nanotubes and boron-nitride can treat the cancer in the brain and other parts of body, however, can ruin the cell brain [17-20].

Electrical properties such as superconductors, semiconductors and insulators are shown in BNNTs, and researchers concentrated on the electrostatics parameters of these compounds [21-25].

Some investigations have been run on these structures by phonon dispersion and Raman spectroscopy. The electronic compound and the reverse of the diameter ($1/d$) dependence of the frequency of the radial breathing mode (RBM) were applied [26-28].

Some studies have been done to achieve TiO₂ Nano-clusters because of their multiple functions in science [29].

In this investigation, it has been approved dopamine as one of the effective brain neurochemical transmitters in language processing and the inhibitive role of Methamphetamine which increases the amount of DA in the nucleus accumbens and causes a shortcut to the brain's pleasure center.

After blocking of DA (dopamine) by Meth (Methamphetamine), brain cannot control the special roles by the release of information from other parts of the brain with the content and joy of the brain through constraint and enjoyment to persuade us to do activities based on neurobiological theories and information releasing to the brain will stop through learning and conducting the human knowledge (Scheme 2).

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:

$$ELF(r) = \frac{1}{1+[D(r)/D_0(r)]^2}, D(r) = \frac{1}{2} \sum_i \eta_i |\nabla \varphi_i|^2 - \frac{1}{8} \left[\frac{|\nabla \rho_\alpha|^2}{\rho_\alpha(r)} + \frac{|\nabla \rho_\beta|^2}{\rho_\beta(r)} \right] \quad (2)$$

$$D_0(r) = \frac{3}{10} (6\pi^2)^{\frac{2}{3}} [\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}] \quad (3)$$

Kinetic energy indicates ELF for post HF wave function and Kohn Sham DFT wave function. Thomas-Fermi kinetic energy density, $D_0(r)$ and $D(r)$, debates the extra kinetic energy density of Pauli repulsion. A correction amount of 10^{-5} to $D(r)$ is shown by Multiwfn program and kinetic energy term changes by Kirzhnits type second order gradient expansion: $\frac{1}{2} \sum_i \eta_i |\nabla \varphi_i|^2 \approx D_0(r) +$

$$\frac{1}{72} \frac{|\nabla \rho|^2}{\rho(r) + \frac{1}{6} \nabla^2 \rho(r)} \quad (4)$$

ELF is totally free of the wave-function and can be applied to debate electron density from X-ray diffraction conclusions. Moreover, LOL, localized orbital locator, is used for localizing high localization zones. LOL has a definition and special important chemical parts. The gained amounts of LOL indicate more specified and certain values than ELF [32]. The measured 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 by Gaussian 09. The simulation illustrates the ways which aim to produce a representative templet of a system at a certain temperature that evaluates most of the parameters from partition function [33].

The adsorption of bioorganic structures such as DA and Meth on nano-surface of Titanium dioxide clusters (TiO₂) were calculated in this paper and the most stable ones have been denoted in Fig 2.

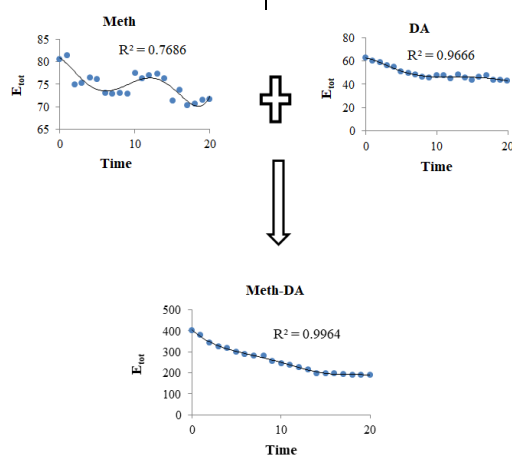


Figure 2. Total energy simulation of Methamphetamine (Meth), Dopamine (DA) and composition of Meth-DA.

3. RESULTS

Dopamine which is flown with a neuron into the synapse in the natural communication process, it can be connected to dopamine receptors on beside neurons [34-36]. After that, it returns back into the transferring neuron by a specific protein of dopamine transporter. Then, dopamine transporter is attached by Methamphetamine which blocks the normal recycling process, revealing in a structure of dopamine in the synapse, and capable of encouragement and happiness impacts of Methamphetamine [37-40]. The linkage of bioorganic molecule of Methamphetamine (Meth) to dopamine (DA) has been calculated in this investigation, and the most stable ones based on total energy gained by Monte Carlo simulation was shown in Figs.3a and b.

Besides, it has been discovered infrared radiation technique (IR) on the indicated system, to understand how dopamine cannot do its duties in the brain because of linkage to Methamphetamine via N atom (Fig. 4). Meth-DA is dissociated by its OH bonds and adsorbs on TiO₂ nano-structure as the bidentate mode that Meth-DA is situated vertically to the surface of TiO₂ (Fig. 1). When the brain is ecstatic unexpectedly, dopamine flows largely, making the limbic pleasure center to take note for remembering how to imitate the positive experience. Inversely, negative thoughts decrease dopamine as a sign to prevent repeating them which is a key learning mechanism handling with memory-formation and motivation because scientists think that brain shows a new temporary neural network to process a new development.

In this paper, the surface geometry coordination (x,y,z) of Meth to TiO₂ complex as DA-nanotube neurotransmitter (N and O active sites) has been optimized (Table 1) .

Table 1. Optimized coordination of Methamphetamine.

atom	Z	x	y	z
C1	6	-20.64384	-10.93902	-0.15565
C2	6	4.61130	-25.60943	0.04475
C3	6	10.58342	1.15043	2.95793
C4	6	-26.82626	43.81532	10.53806
C5	6	18.79042	17.60000	0.03436
C6	6	23.47443	-7.62148	-0.25539
C7	6	-36.29389	-11.58941	0.87460
C8	6	0.74968	20.61332	-25.73755
N16	7	22.18505	-3.17247	5.54567
C17	6	28.69402	-2.20313	3.11247
C18	6	13.41139	2.11300	9.18622
H12	1	-1.76460	10.56904	0.01548
H13	1	-10.46280	3.76729	0.00275
H14	1	-8.09116	-7.16665	0.10656
H15	1	-16.87001	-11.89947	24.17418
H9	1	6.38572	8.09529	7.93302
H10	1	6.72778	7.74389	-7.99152
H11	1	9.38570	7.34867	-0.02553

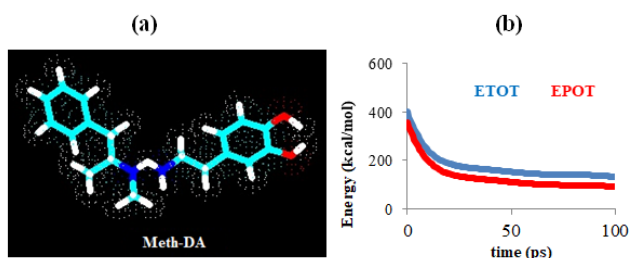


Figure 3. (a) The structure of Methamphetamine (Meth) - dopamine (DA) complex. (b) Total energy of Meth-DA calculated by Monte Carlo simulation.

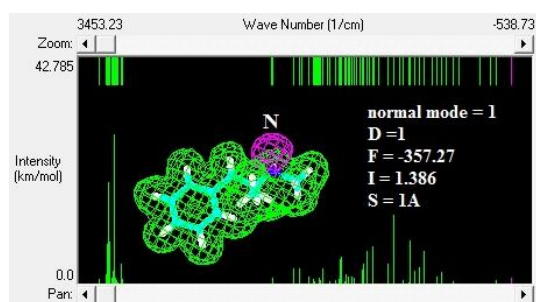


Figure 4. IR spectra of neurochemical transmitters of dopamine linked to Methamphetamine.

atom	Z	x	y	z
H19	1	-14.30150	-6.80198	18.85082
H20	1	-3.21265	-1.55413	-8.57263
H21	1	-2.39684	-8.44335	-5.48993
H22	1	-0.44978	-0.56238	-7.56715
H23	1	-2.38436	-6.19045	-25.82553
H24	1	4.38417	-2.34551	-0.73673
H25	1	-2.76131	-5.41991	-6.47054
H26	1	-2.92405	-11.29748	5.45128

The adsorption energy, E_{ads} , was calculated for DA, Meth-DA and Meth-DA-TiO₂ as the energy difference between the energy of the adsorption complex based on electron density of these structures with different relation coefficients (Table 2 and Fig. 5).

Table 2. Thermodynamic parameters for DA, Meth-DA and Meth-DA-TiO₂ structures.

Energy-Gradient	DA	Meth-DA	Meth-DA-TiO ₂
Total Energy	-43042.94731	-78892.07024	684002.4684
Binding Energy	-2226.33791	-4569.303741	863503.089
Isolated Atomic Energy	-40816.6094	-74322.7665	-179500.6206
Electronic Energy	-217763.8073	-583542.8822	-1327566.884
Core-Core Interaction	174720.86	504650.812	2011569.352
Heat of Formation	-53.9779099	154.384259	870184.881

4. CONCLUSIONS

The conjunction of Methamphetamine to dopamine on the surface of TiO₂ was modeled in different positions through transferring the electron. Our theoretical calculations have approved that such extrapolation schemes estimate the dopamine-TiO₂ by active site of structure (N and O linkage) which is the most active point of the target molecule.

It has been debated the interface of DA, Meth-DA and Meth-DA-TiO₂ on an atomic level by means of theoretical methods to discover the features connecting geometrical and electronic structures which reduce the role of dopamine in the brain due

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Energy-Gradient	DA	Meth-DA	Meth-DA-TiO ₂
Gradient	19.0289186	41.728372	5422.431647

This method lets giving an illustration of the adsorption energy of the electronic states for DA which was blocked by Meth on the surface (Fig. 5).

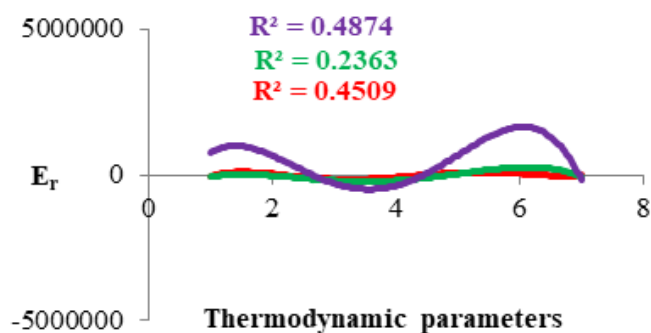


Figure 5. The curve of relative energy via Thermodynamic parameters for DA, Meth-DA and Meth-DA-TiO₂.

Moreover, the core-core interaction and the electronic energy were plotted to show the distribution points of DA ($R^2 = 0.4509$), Meth-DA ($R^2 = 0.2363$) and Meth-DA-TiO₂ ($R^2 = 0.4874$) (Fig.5).

motivating and learning. Thus, it has been indicated how dopamine can be less active with adsorbing on Methamphetamine on the surface of TiO₂. It will be illustrated that the electronic structure of the surface of Meth-DA-TiO₂ systems is essential to prove the basic features of their activity and disability. Finally, it has been proved that after blocking of dopamine by Methamphetamine inhibitor, the brain cannot play its role for releasing neurotransmitters which have the function of learning a foreign language aspect of the didactic process.

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