

What is the effect of body's chemical messengers in the brain?

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ABSTRACT

Neurochemical transmitters in the brain are fundamental to normal brain function and this investigation aims to introduce a study on the center of neuroscientific through an account of language development which conducts human speech mechanism using theoretical methods. In the process of this work, new understanding has been gained from the neurochemistry of several important neurotransmitters of dopamine (DA), epinephrine (EN), norepinephrine (NE), histamine (HA) and serotonin (ST) in brain by Monte Carlo simulation (MC) which uses the increased temperature to the potential energy of the neurochemicals in the brain considering the geometry optimization of the compounds as an additional conformational level. Moreover, the results of optimized DA, EN, NE, HA, ST neurochemical transmitters by running the physicochemical parameters as a practical model using Gaussian 09 program package can approve the twisting of language-brain due to these structures using density electron deliverers.

The most stable of these compounds through the active sites of nitrogen and oxygen atoms has illustrated the best optimized position for localizing the structure through delivery technique in the brain to activate the center of learning a language as a simulated model. So, the best results with the calculated amounts conduct us to analyze the perspective of language learning process and enhancing this ability.

Keywords: DA, EN, NE, HA, ST, neurochemical transmitters, brain, normal mode, MC method.

1. INTRODUCTION

Communicating among humans has been studied by unraveling neurochemicals in the brain for exhibiting chemical changes produced by people's activities and experiences.

Neurotransmitters by MR spectroscopy have let scientists' research disease processes and mutagenic evolution of subjects in vivo. They have shown that there is a complex relationship between structural brain development and changing the levels of metabolites which are used organic structures or produced by metabolism [1-3].

The body's chemical transmitters are responsible for simplifying the communications among nerve cells in the nervous system. While dopamine (DA) is most commonly associated with the brain's movement, pleasure and reward, serotonin (ST) and norepinephrine (NE) strongly influence mental behavior patterns.

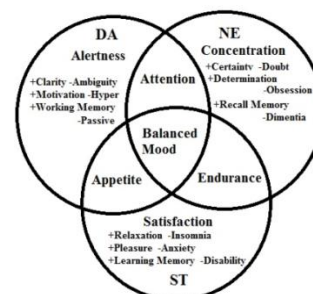
We can find dopamine in two different parts of the brain; substantia nigra, the responsible for both rewards and movement and the ventral tegmental area (VTA) of the brain which has the main role in pleasure and reward signaling.

A reward response is needed for humans through dopamine for some behaviors that motivate us to continue them. Flowing dopamine in the brain which causes us to feel pleasure from these things is our body's mechanism to ensure that we follow doing things that we need to do in order to keep the body running optimally and feel healthy.

Norepinephrine and Serotonin affect mental behavior patterns, while dopamine is involved in the movement. These three substances are therefore fundamental to normal brain function.

Dopamine is usually associated or confused with serotonin which has some similarities with DA that they are both chemical messengers for the brain and both have positive associations in

regards to mood, but their principal functions are completely different (Scheme 1). DA shows positive feelings based on a certain action and ST plays a role as a mood stabilizer. However, a deficiency in either ST or DA can negatively influence mood and happiness.



Scheme 1. Principal functions of three chemical neurotransmitters (DA, NE, and ST) in the brain.

Movement, speaking, listening, thinking, learning, and other activities are possible by transferring the chemical messengers in the brain which allow routine functions due to communicating of brain with itself through sending out the chemical information from one neuron to another. It has been shown that there are some ways for the verdict of cognitive criteria which cross different subjects' borders and model a specific viewpoint of language mechanism. The effort to discover the linguistic perspectives with neurological subjects has just commenced increasing the understanding of cerebral zone for language due to the applying of imaging methods and chemical alteration [3]. Some Neurological works have explained a central part of function by DA in proper motor commands, learning and higher-order cognitive process with language laboratory that leads

us to know about the ability of humans for generating different languages [4, 5].

Serotonin (ST) is a monoamine neurochemical transmitter which has a common image as a participant to understand the comfort, health and being happy with several complicated and multiple biological activities including learning, modulating cognition, memory, reward, and various physiological steps [6]. ST is not managed clinically as a drug itself as it is not specific enough, but drugs that selectively target special ST receptor subtypes are used therapeutically for antidepressant impacts [7, 8]. In the brain, noradrenaline (NE) is generated in nuclei that are small yet exert strong impacts on other brain parts. NE, outside the brain, is used as a neurochemical transmitter by sympathetic ganglia which is near the spinal cord or in the abdomen, releasing into directly the bloodstream by the adrenal glands [9, 10]. The neurochemical science education and grammar learning have been focused by researchers through media changes of the brain which can be renewed by altering its function for reacting to cognition, environmental reflections or behavioral experience [11, 12].

Learning a foreign language alters the foundation and the role of brain to be more flexible and flows out neurochemical

2. EXPERIMENTAL SECTION

Normal mode calculation is the study of harmonic potential wells by analytic means which include simultaneous motion of all atoms during the vibration leading to a natural description of molecular vibrations. Therefore, they are good candidates for representation of the molecular Hamiltonian. Since a transformation between different sets of coordinates is possible, the anharmonic terms can be calculated in one representation and then transformed into another one [18].

The theoretical calculations were done at different steps of theory to investigate the more accurate equilibrium geometrical parameters and IR spectral data for each of the determined structure. It is supposed that the polarization functions into the basis set used in the calculation always lead us to the considerable improvements on the obtained results in theory [19-22].

The Simulation exhibits the methods which produce a popular sample of a system at a specific temperature using calculating most of the properties through the partition function [23].

Monte Carlo, MC, force fields used in simulating physical and mathematical systems are computational algorithm classes based on repeated occasional samples to computing their consequences. MC method is a statistical sampling technique which discovers a number of scientific questions. Computation of random or pseudo-random numbers causes the accuracy of calculation particularly for unfeasible or impossible to estimate

3. RESULTS SECTION

In this project, the chemical neurotransmitters of DA, EN, NE, HA, ST have been calculated using theoretical methods to evaluate the effects of these compounds in the brain. The values have indicated that EN has the lowest optimized energy and the most stabilized compound compared to some other neurochemical transmitters; DA, NE, HA and ST (Table 1).

compounds which help scientific learning. So, the most important interdisciplinary subjects of anthropology cognitive science, neurobiology, and chemical interdisciplinary science are generated by language mechanism and brain [13].

Besides, epinephrine (EN) is normally generated by both certain neurons and the adrenal glands and which has a significant role in the fight-or-flight response by boosting blood flow to muscles, the output of the heart, blood sugar degree and pupil dilation reply [14, 15].

Histamine (HA) is another neurochemical transmitter which is released from histaminergic neurons projecting out of the mammalian hypothalamus. The cell bodies of these neurons are situated in a part of the posterior hypothalamus known as the tuberomammillary nucleus. The histamine neurons equilibrate the brain's histamine system which acts throughout the brain including axonal projections to the cortex and medial forebrain bundle [16, 17].

In this work, it has been illustrated some neurochemical transmitters in the brain including dopamine, epinephrine, norepinephrine, histamine and serotonin for discovering immense chemical properties such an experienced sample.

exact data with a deterministic algorithm [24]. It doesn't always need random numbers to apply deterministic, pseudo-random sequences, making it easy to test and re-run simulations [25].

In MC methods, a sequence of points in phase space is produced from an initial geometry by adding a random "kick" to the coordinates of a randomly chosen atom or molecule. The new configuration is approved if the energy decreases and with a probability of $e^{-\Delta E/kT}$ if the energy increases. Based on metropolis procedure, the configurations in the ensemble obey a Boltzmann distribution, and the possibility of approving higher energy configurations allows MC methods to increase and escape from a local minimum [25].

MC simulations are widely applied in biology, chemistry, physics, and engineering for determining the structural and thermodynamic properties of complex systems at the atomic level. MC simulations need only the ability to evaluate the energy of the system which may be advantageous if calculating the first derivative is difficult or time-consuming. Moreover, since only a single particle is moved in each step, only the energy changes associated with this move should be calculated, not the total energy for the whole system. A disadvantage of MC methods is the lack of the time dimension and atomic velocities, and they are therefore not appropriate for studying time-dependent phenomena or properties depending on momentum [25].

As it has been shown, a vibrational calculation with its own eigenvector for finding thermodynamic values of neurochemical transmitters including Total Energy, Binding Energy, Isolated Atomic Energy, Electronic Energy, Core-Core Interaction, Heat of Formation, and Gradient have been studied (Table 1 and Figure 1).

Table 1. Calculated thermodynamic properties of chemical neurotransmitters in the brain.

| Parameters (kcal/mol) | Dopamine | Epinephrine | Norepinephrine | Histamine | Serotonin |
|-------------------------|-----------|-------------|----------------|------------|------------|
| Total Energy | -46659.62 | -91.85 | -54023.58 | -31900.17 | -50225.38 |
| Binding Energy | -2232.79 | -2612.184 | -2307.16 | -1601.06 | -2585.32 |
| Isolated Atomic Energy | -44426.83 | -55028.1582 | -51716.41 | -30299.11 | -47640.06 |
| Electronic Energy | - | -297296.54 | -269952.75 | -138163.58 | -269970.59 |
| Core-Core Interaction | 176526.12 | 239656.20 | 215929.17 | 106263.41 | 219745.21 |
| Heat of Formation | -60.43 | -105.17 | -75.24 | 61.31 | 34.360 |
| Gradient (kcal/mol/Ang) | 16.70 | 16.25 | 38.49 | 45.51 | 50.03 |

The electronic energy including the core–core repulsion has been calculated by Gaussian09 [26], in analogy with ab initio methods, the total energy relative (as seen in table 1) to a situation where the nuclei (with their core electrons) and the valence electrons have been infinitely separated.

The exact numbers of course depend on which, and how many, compounds have been selected for comparison, thus the numbers should only be taken as a guideline for the accuracy expected (Table 1 and Figure 1).

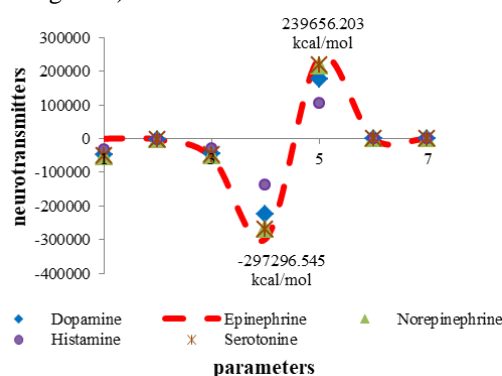


Figure 1. Calculated thermodynamic properties of chemical neurotransmitters in the brain.

Obviously, the IR technique, infrared radiation, has been done on the neurochemical transmitters of DA, EN, NE, HA, ST for unraveling how they do their duties in the brain via different active parts of Nitrogen -Hydrogen, Oxygen-Hydrogen, and etc. (Figure 2).

The vibrational spectral data obtained from IR spectra are assigned modes based on the results of the theoretical calculations as intensity and frequency curves using HyperChem8 [27]. The fundamental vibrational modes were characterized depending on their stability of neurochemical transmitters. It has been investigated the high frequency of normal modes of these structures through variant positions of each molecular basis (Figure 2). Besides, in Figure2, several intensities and frequencies with identified symmetry have been considered for discovering the stable geometry of brain's neurochemical transmitters.

Although, a quantitative description of a potential well requires a more careful approximation, it has been indicated chosen frequencies of the density of states rather well. So, in this paper, it has been presented the main results of the frequencies and intensities of active modes on the neurochemical transmitters of DA, EN, NE, HA, ST [28]. The normal modes of these structures can usually be associated with a certain kind of motion of the molecule (Figure 2).

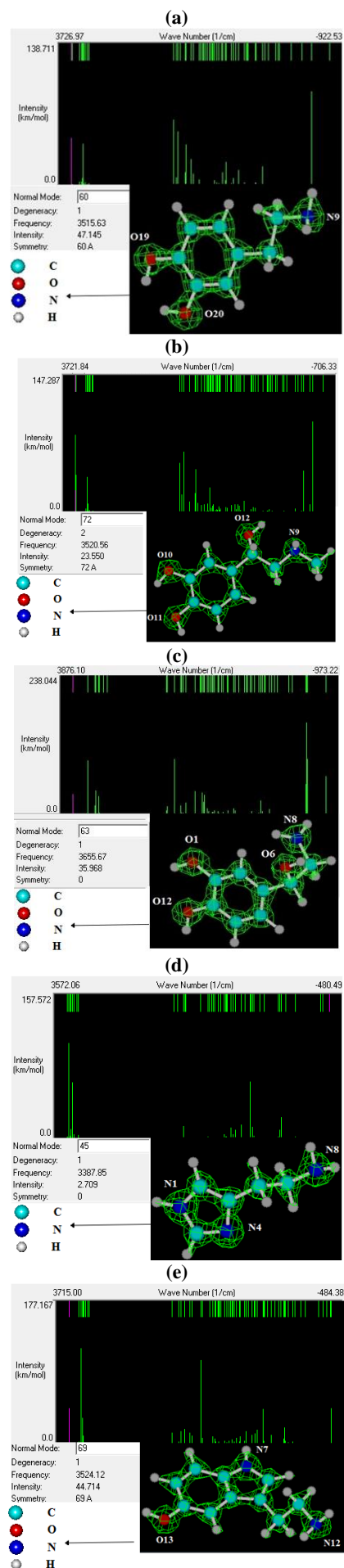


Figure 2. IR spectra of neurochemical transmitters of (a) dopamine (b) epinephrine (c) norepinephrine (d) histamine and (e) serotonin.

Therefore, low-frequency modes are to a very good approximation also low-energy modes, and vice versa. It should

also be considered that at the high frequency end, quantum impacts become significant. However, the transformation to normal mode coordinates remains valid in a quantum description; so, only the dynamic interpretation must be adapted. Moreover, The partial charges and atomic orbital electron population on the compounds have been obtained by fitting the electrostatic potential to fixed charges on the oxygen, nitrogen, carbon and hydrogen atoms for the neurochemical transmitters of DA, EN, NE, HA, ST (Tables 3 and 4).

Table 3. Partial charges of different atoms in DA, EN, NE, HA, ST.

| | DA | | EN | | NE | | HA | | ST | |
|-------|-------|-------|-------|-------|-------|------|-------|-------|-------|--|
| N(9) | -0.29 | N(9) | -0.20 | O(1) | -0.24 | N(1) | -0.49 | N(7) | 0.38 | |
| O(19) | -0.25 | O(10) | -0.24 | O(6) | -0.36 | N(4) | 0.45 | N(12) | -0.29 | |
| O(20) | -0.25 | O(11) | -0.24 | N(8) | -0.26 | N(8) | -0.29 | O(13) | -0.26 | |
| | | O(12) | -0.38 | O(12) | -0.24 | | | | | |

Table 4. Atomic orbital electron population of neurochemical transmitters in brain.

| Dopamine | | | | |
|----------------|----------|----------|----------|----------|
| 9 Pz N | 19 S O | 19 Px O | 19 Py O | 19 Pz O |
| 1.464658 | 1.856445 | 1.300322 | 1.168003 | 1.920489 |
| 20 S O | 20 Px O | 20 Py O | 20 Pz O | 12 S H |
| 1.856443 | 1.262660 | 1.206071 | 1.919387 | 0.908715 |
| Epinephrine | | | | |
| 9 Pz N | 10 S O | 10 Px O | 10 Py O | 10 Pz O |
| 1.447545 | 1.853712 | 1.257151 | 1.231898 | 1.907599 |
| 11 S O | 11 Px O | 11 Py O | 11 Pz O | 12 S O |
| 1.851921 | 1.330663 | 1.169454 | 1.918999 | 1.869498 |
| 12 Px O | 12 Py O | 12 Pz O | 14 S C | 14 Px C |
| 1.779250 | 1.255853 | 1.421637 | 1.223213 | 0.890332 |
| Norepinephrine | | | | |
| 1 S O | 1 Px O | 1 Py O | 1 Pz O | 2 S C |
| 1.841565 | 1.396689 | 1.341728 | 1.712473 | 1.156196 |
| 6 S O | 6 Px O | 6 Py O | 6 Pz O | 7 S C |
| 1.849293 | 1.378924 | 1.422761 | 1.715343 | 1.223033 |
| 8 Py N | 8 Pz N | 9 S C | 9 Px C | 9 Py C |
| 1.155356 | 1.366124 | 1.188011 | 0.942276 | 0.983844 |
| 12 Px O | 12 Py O | 12 Pz O | 13 S H | 14 S H |
| 1.260658 | 1.456876 | 1.752033 | 0.744254 | 0.842767 |
| Histamine | | | | |
| 1 S N | 1 Px N | 1 Py N | 1 Pz N | 2 S C |
| 1.731848 | 1.161310 | 1.083078 | 1.184771 | 1.218344 |
| 7 Px C | 7 Py C | 7 Pz C | 8 S N | 8 Px N |
| 0.907179 | 0.992943 | 0.958665 | 1.603329 | 1.206377 |
| 8 Py N | 8 Pz N | 9 S H | 10 S H | 11 S H |
| 1.076914 | 1.463339 | 0.858573 | 0.866102 | 0.887369 |
| Serotonin | | | | |
| 7 Px N | 7 Py N | 7 Pz N | 8 S C | 8 Px C |
| 1.079292 | 1.058610 | 1.613956 | 1.208152 | 0.951996 |
| 11 S C | 11 Px C | 11 Py C | 11 Pz C | 12 S N |
| 1.221734 | 0.975488 | 0.912513 | 0.972438 | 1.603230 |
| 12 Px N | 12 Py N | 12 Pz N | 13 S O | 13 Px O |
| 1.077359 | 1.208233 | 1.461991 | 1.854843 | 1.263063 |
| 13 Py O | 13 Pz O | 14 S H | 15 S H | 16 S H |
| 1.220782 | 1.916596 | 0.751031 | 0.860089 | 0.860125 |

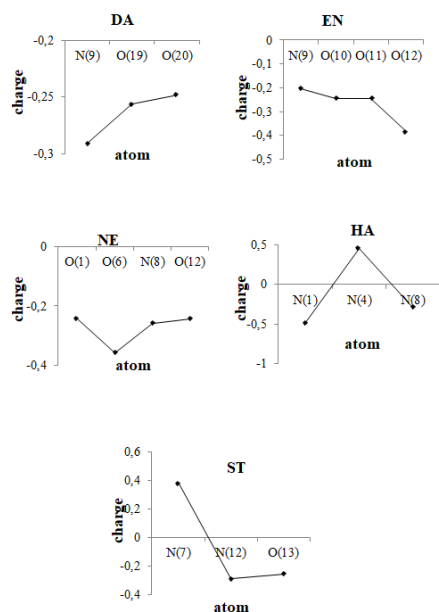


Figure 3. The calculated atomic charge of some active atoms of DA, EN, NE, HA, ST.

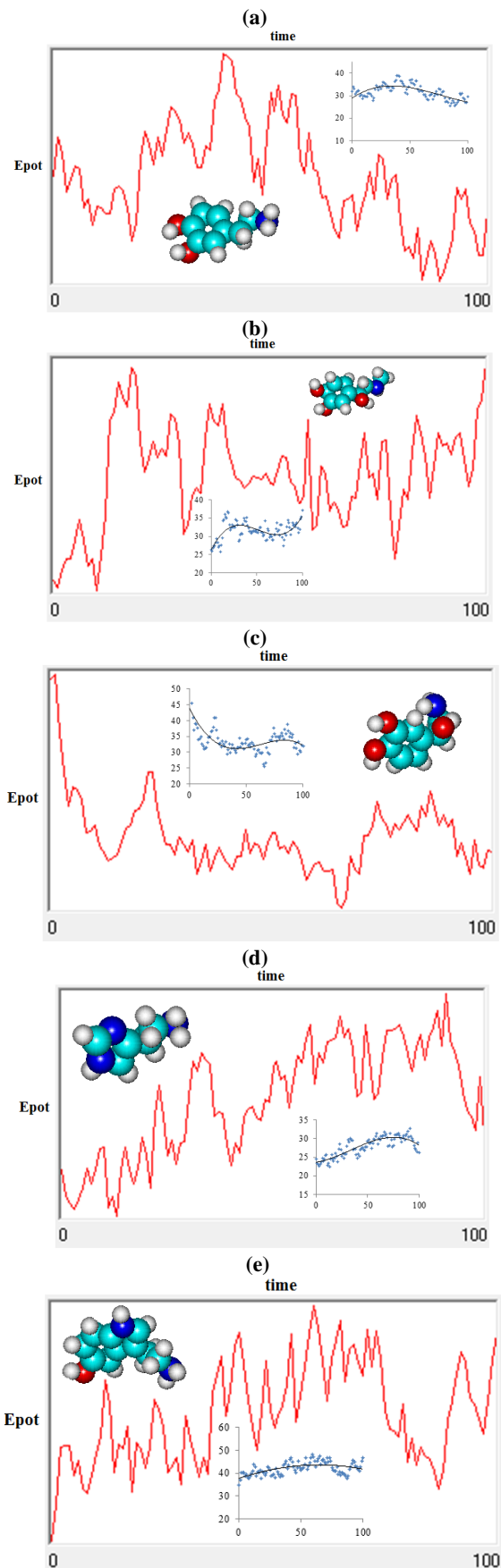


Figure 4. Calculated potential energy graphs via time by Monte Carlo method for (a)dopamine (b)epinephrine (c) norepinephrine (d) histamine and (e) serotonin .

In Figure 3, it has been measured the fluctuation of atomic charge of some active atoms, nitrogen and oxygen, of DA, EN, NE, HA, ST due to the direct electron transfer principle

which leads us to find the reason for the activity and the stability of these structures in the medium of human's brain.

Then, dopamine, epinephrine, norepinephrine, histamine and serotonin have been led to a description of Monte Carlo simulation by potential energy in 300K energy via time scale (0-100). Optimal values are close to 0.5. Varying the step size can have a large effect on the acceptance ratio. The MC Options dialog box permits us to set up the MC simulation parameters. In this work, it has been done a temperature simulation with 100 steps (Figure 4).

Actually, for calculating the desired thermodynamic averages, it is necessary to have some methods available for computation the potential energy by MC simulation, in the form of a function

4. CONCLUSIONS

The power of language learning produced by chemical neurotransmitters in the brain has been studied.

The simulation of dopamine (DA), epinephrine (EN), norepinephrine (NE), histamine (HA) and serotonin (ST) shows that the stabilization energy has been affected by the Monte Carlo force field and the best results have been gained for potential energy vs. time scale. The calculations have demonstrated that

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representing the interaction potential as in molecular mechanics or in the form of direct quantum-mechanical calculations.

Also, it should be noted that constraining potentials have been used at finite temperature, 27°C introducing a constraining potential which enables one to define the neurochemical transmitters of DA, EN, NE, HA, ST. Because the constraining potential is artificial, the dependence of calculated thermodynamic properties on the form and the radius of the constraining potential must be investigated on a case-by-case basis (Figure 4).

The results of Figure4 suggest that the different data observed in DA, EN, NE, HA, ST are predominantly related to the situation of the active site of nitrogen and oxygen atoms in these structures which transfer the electronic charge the molecules (Figures 3 and 4).

such extrapolation schemes significantly overestimate the neurochemical transmitters by active sites of molecules, nitrogen and oxygen linkages, which are the most active points at the indicated structures.

This work can conduct us to find how neurochemical transmitters in the brain can be effective for learning a new language based on a simulated model.

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6. ACKNOWLEDGEMENTS

I would like to express my deepest appreciation to all those who provided me the possibility to complete this paper. A special gratitude I give to the library of Department of French Language and Literature, Science and Research Branch, Islamic Azad University, Tehran, Iran which helped me to coordinate my research.



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