# First Principal and QM/MM study of Dopamine Adsorption on Single Wall Carbon Nano Tubes and Single Wall Boroan Nitride Nano Tubes

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## ABSTRACT

In the brain, dopamine functions as a neurotransmitter a chemical released by neurons (nerve cells) to send signals to other nerve cells. The brain includes several distinct dopamine pathways, one of which plays a major role in reward-motivated behavior. In this work we have calculated our systems based on the Dopamine binding with various diameters of SWBNNTs and SWCNTs. In this work, the electron density profile in the composition of the Dopamine binding to SWCNTs and SWBNNTs have been calculated.

**Keywords**: Dopamine, Adsorption on SWCNTs and SWBNNTs, LOL, ELF.

## INTRODUCTION

Dopamine is an organic chemical of the catecholamine and phenethylamine families that plays several important roles in the brain and body. it is an amine synthesized by removing a carboxyl group from a molecule of its precursor chemical L-DOPA, which is synthesized in the brain and kidneys. Dopamine is also synthesized in plants and most multicellular animals.

In the brain, dopamine functions as a neurotransmitter a chemical released by neurons (nerve cells) to send signals to other nerve cells. The brain includes several distinct dopamine pathways, one of which plays a major role in reward-motivated behavior. Most types of reward increase the level of dopamine in the brain, and most addictive drugs increase dopamine neuronal activity. Other brain dopamine pathways are involved in motor control and in controlling the release of various hormones.

Outside the central nervous system, dopamine functions in several parts of the peripheral nervous system as a local chemical messenger. Several important diseases of the nervous system are associated with dysfunctions of the dopamine system, and some of the key medications used to

treat them work by altering the effects of dopamine. Parkinson's disease, a degenerative condition causing tremor and motor impairment, is caused by a loss of dopamine-secreting neurons in an area of the midbrain (called the substantia nigra).

Its metabolic precursor L-DOPA can be manufactured, and in its pure form marketed as Levodopa is the most widely used treatment for the condition. There is evidence that schizophrenia involves altered levels of dopamine activity, and most antipsychotic drugs used to treat this are dopamine antagonists which reduce dopamine activity. Similar dopamine antagonist drugs are also some of the most effective anti-nausea agents. Restless legs syndrome and attention deficit hyperactivity disorder (ADHD) are associated with decreased dopamine activity. Dopaminergic stimulants can be addictive in high doses, but some are used at lower doses to treat ADHD. Dopamine itself is available as a manufactured medication for intravenous injection: although it cannot reach the brain from the bloodstream, its peripheral effects make it useful in the treatment of heart failure or shock, especially in newborn babies[1,2].

The carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter.

Carbon nano cone has a high asymmetric geometry that in our simulations, classical non-equilibrium molecular dynamics method is adopted. The cone is entirely characterized by its cone angle. When one pentagon is introduced into a hexagonal carbon network, a 60 declination defect is formed; leading to the formation of a nano cone with cone angle of 118 and the equilibrium carbon-carbon bond length is 1.418 Å. In this work, we focus on the cone with the cone angle of 180, which is the largest angle observed experimentally and theoretically.

Moreover, in all theoretical models so far, the rectification efficiency decreases quickly as the structure length increases Its structure, which is in the form of a hexagonal mesh, resembles a graphite sheet and it carries a carbon atom located on the vertex of each mesh. The sheet has rolled and its two edges have connected seamlessly.

Although it is a commonplace material using in pencil leads, its unique structure causes it to present characteristics that had not found with any other materials. CNT can be classified into single-wall CNT, double-wall CNT and multi-wall CNT according to the number of layers of the rolled graphite.

The type attracting most attention is the single-wall CNT, which has a diameter deserving the name of "nanotube" of 0.4 to 2 nanometers. The length is usually in the order of microns, but single-wall CNT with a length in the order of centimeters has recently released

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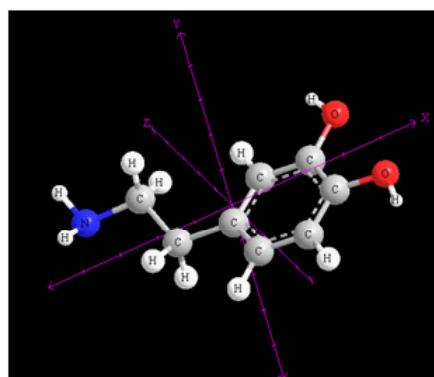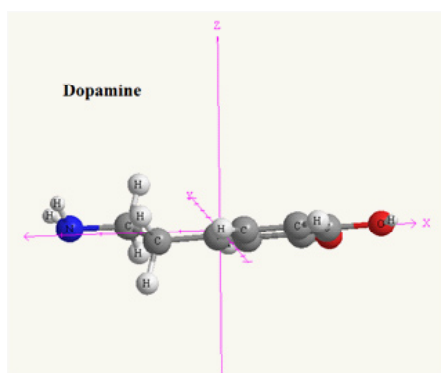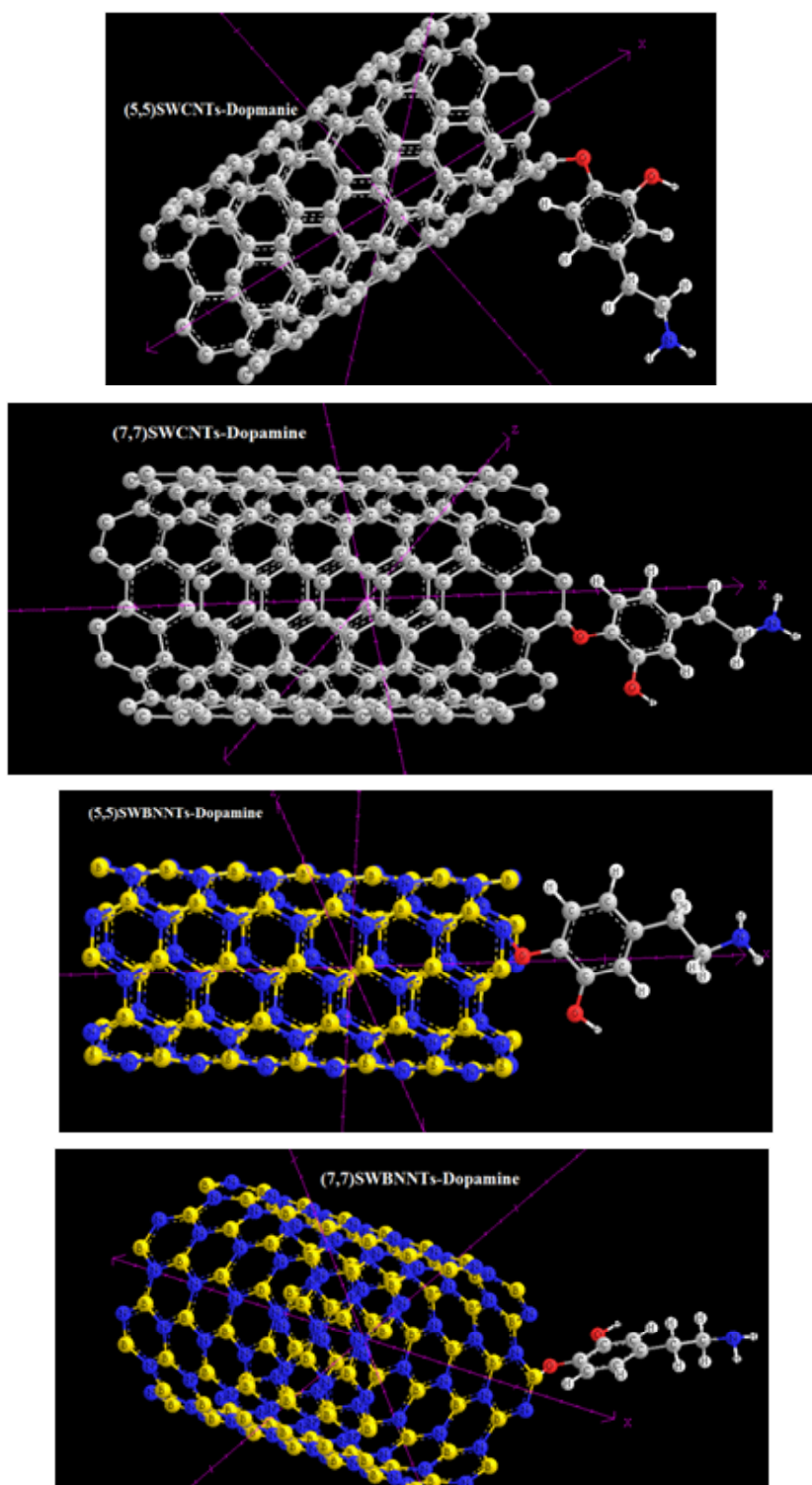


**Fig.1: Molecular geometry of Dopamine**

**Fig. 2: Molecular geometry of (5,5),(7,7)SWCNTs and (5,5),(7,7)SWBNNTs with binding to Dopamine**

The length is usually in the order of microns, but single-wall CNT with a length about centimeters have recently released. The extremities of the CNT have usually closed with lids of the graphite sheet

Boron nitride nanotube (BNNTs) has attracted many interests due to their large gap semi conducting character. Boron nitride (BN) is a structural existing in cubic (diamond-like), hexagonal (graphite-like), turbo static, and amorphous forms .these compounds have been produced by a variety of methods, such as arc melting, high temperature

chemical reaction, carbon nanotube templates, and laser ablating, The most attention has been focused on the development of new methods for the production of nanotube and inorganic fullerene of other materials.

In addition**,** theoretical calculations have been described the possible existence of small BN clusters.

Theoretical studies have been performed for BN doped in CNTs which it has been found that
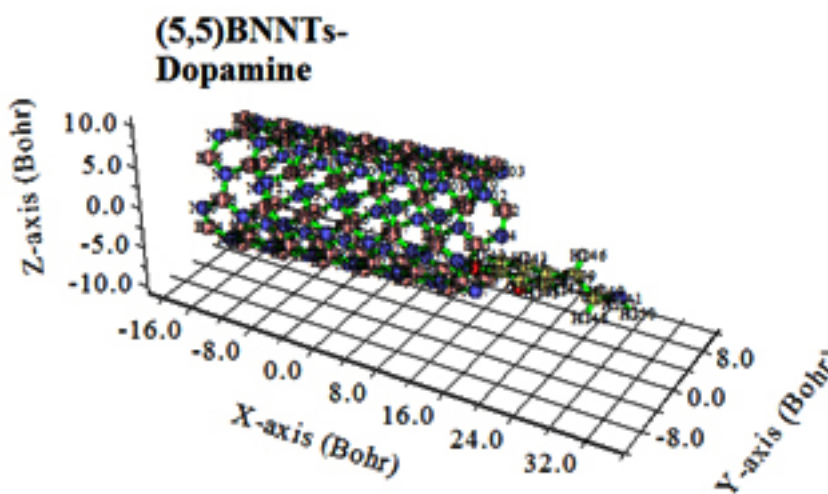


**Fig. 3: Dopamine Geometry vs 3 axis**

**Table 1: HOMO, LUMO and BAND GAP of some Dopamine-(5, 5) SWBNNT**

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130(N ) --> Charge:  5.000000  x,y,z(Bohr): -16.992276  -3.690291   6.334651
131(C ) --> Charge:  4.000000  x,y,z(Bohr):  19.161190  -1.751256  -2.021016
132(C ) --> Charge:  4.000000  x,y,z(Bohr):  17.396685  -3.306437  -0.591967
133(C ) --> Charge:  4.000000  x,y,z(Bohr):  18.386409  -4.890623   1.430616
134(C ) --> Charge:  4.000000  x,y,z(Bohr):  21.054035  -4.922431   2.048461
135(C ) --> Charge:  4.000000  x,y,z(Bohr):  22.840290  -3.380657   0.646727
136(C ) --> Charge:  4.000000  x,y,z(Bohr):  21.837429  -1.808772  -1.375409
137(O ) --> Charge:  6.000000  x,y,z(Bohr):  18.258621  -0.121521  -4.082932
138(O ) --> Charge:  6.000000  x,y,z(Bohr):  14.678131  -3.306418  -1.172978
139(C ) --> Charge:  4.000000  x,y,z(Bohr):  25.853412  -3.452115   1.403430
140(C ) --> Charge:  4.000000  x,y,z(Bohr):  27.888544  -2.645578  -0.852212
141(N ) --> Charge:  5.000000  x,y,z(Bohr):  30.715208  -3.027033   0.113916
142(H ) --> Charge:  1.000000  x,y,z(Bohr):  16.957798  -6.174428   2.618515
143(H ) --> Charge:  1.000000  x,y,z(Bohr):  21.769244  -6.234974   3.733052
144(H ) --> Charge:  1.000000  x,y,z(Bohr):  23.207116  -0.488306  -2.569197
145(H ) --> Charge:  1.000000  x,y,z(Bohr):  19.806804   0.867065  -4.848321
146(H ) --> Charge:  1.000000  x,y,z(Bohr):  26.143849  -2.067456   3.201443
147(H ) --> Charge:  1.000000  x,y,z(Bohr):  26.383757  -5.550727   2.085596
148(H ) --> Charge:  1.000000  x,y,z(Bohr):  27.579974  -3.941803  -2.686939
149(H ) --> Charge:  1.000000  x,y,z(Bohr):  27.643949  -0.463266  -1.456718
150(H ) --> Charge:  1.000000  x,y,z(Bohr):  32.092055  -2.627767  -1.445195
151(H ) --> Charge:  1.000000  x,y,z(Bohr):  31.051057  -5.036944   0.659517
Note: Orbital   289 is HOMO, energy:  -0.436973 a.u.  -11.890630 eV
      Orbital   290 is LUMO, energy:  -0.339855 a.u.   -9.247929 eV
      LUMO/HOMO gap:    0.097117 a.u.    2.642701 eV    254.981910 kJ/mol
```

a structure built from squares and hexagons is more stable than those built from pentagons and hexagons. This is because in the second case less stable B-B and N-N bonds are formed.

Monajjemi and coworkers have simulated a large range of the nanotube carbons and other molecules via a wide range of methods and basis sets in the field of Physical chemistry, Nano biotechnology, quantum phenomenon, Nano

capacitors, chemical biology, adsorption, and NMR shielding[3-119].

In this work we have calculated our systems based on the dopamine binding with various diameters of SWBNNTs and SWCNTs .The effects of these binding for the drug delivery can also be calculated for any further comparison and discussion.
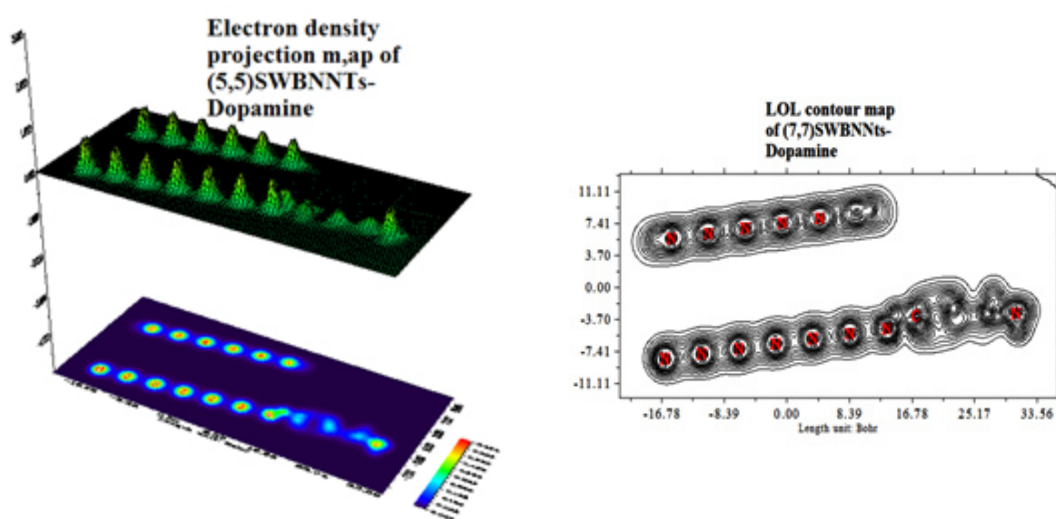


**Fig. 4: Electron density and LOL for (5, 5) SWBNNTs-Dopamine Complex**
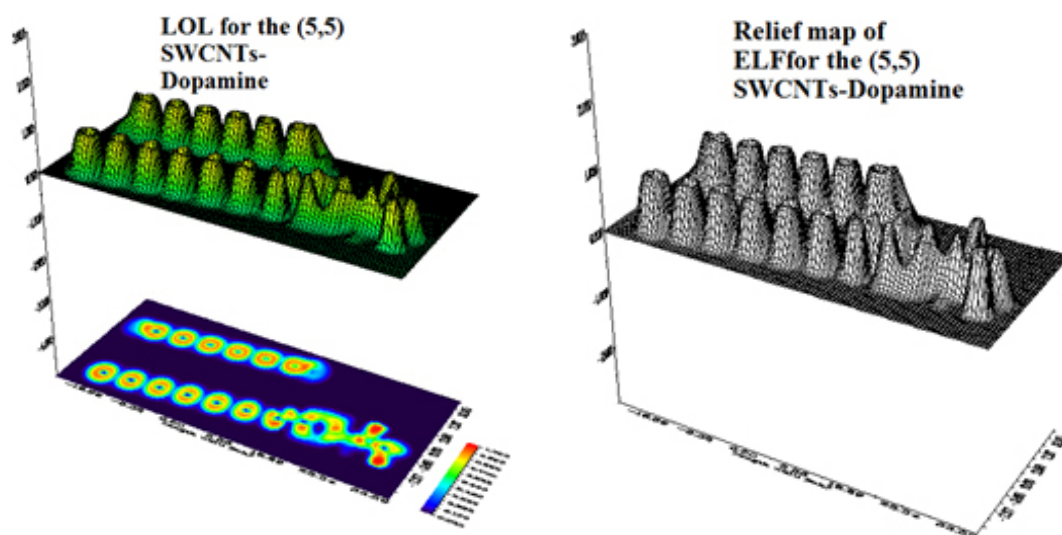


**Fig. 5: LOL and ELF map for (5, 5) SWCNTs with Dopamine**

Zigzag BNNTs (n, 0) are expected to have direct band gap. On the other hand, armchair BNNTs (m, m) will have indirect band gap[120]. Because of their large band gap of (~5 eV), experiments using BNNTs as the conduction channel for field-effect transistors (FETs) showed that BNNTs allowed transport through only the valence band.

Another important feature about the band gaps of BNNTs is that they are tunable by doping with carbon , radial deformation ,or by applying a transverse electric field across the BNNT "so-called giant stark effect"[121].

**Electron localization function (ELF)**
In this work, the electron density profile

in the composition of the Dopamine binding to SWCNTs and SWBNNTs have been calculated.

The electron density has been defined as:

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

...(1)

where $n_i$ is occupation number of orbital $i$, $\phi$ is orbital wave function, $\chi$ is the basis function, $C$ isBader [122] has found that the regions with large electron localization must have large magnitudes of Fermi-hole integration. However, the Fermi hole is a six-dimension function and thus difficult to
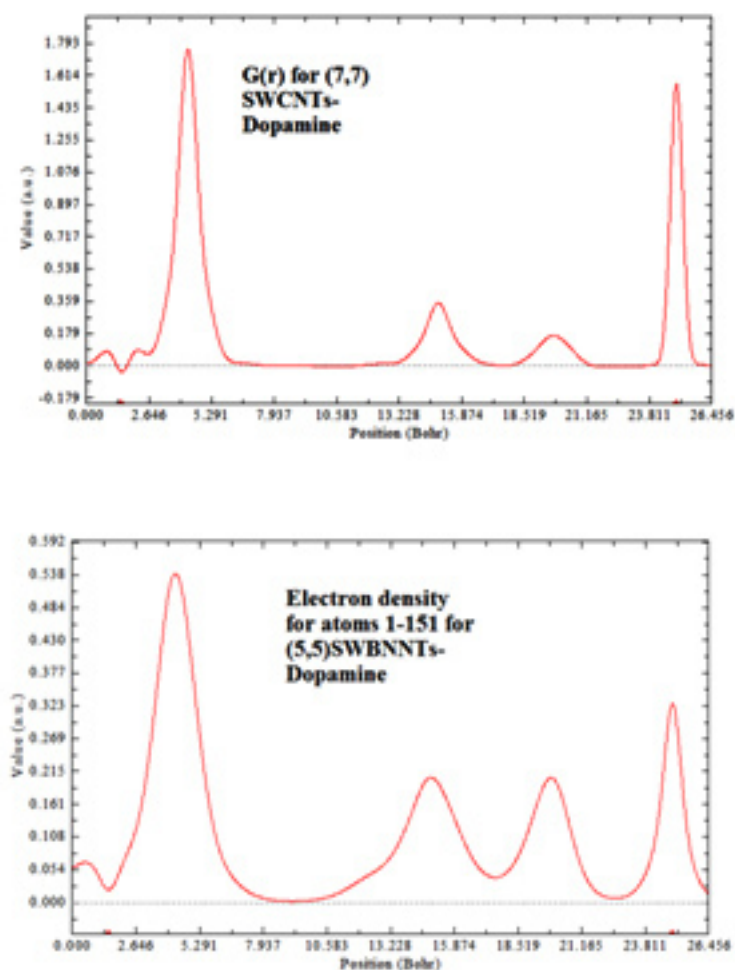


**Fig. 6: G ( r ) for (7,7) SWCNTs-Dopamine and Electron density for (5,5)SWBNNTs Complexes**

be studied visually. Becke and Edgecombe noted that spherically averaged like spin conditional pair probability has a direct correlation with the Fermi hole and further suggested electron localization function (ELF) as:

$$ELF(r) = \frac{1}{1 + [D(r)/D_{0(r)}]^2} \qquad ...(2)$$

where

$$D(r) = \frac{1}{2} \sum_i \eta_i \ |\nabla\varphi_i|^2 - \frac{1}{8}\left[\frac{||\nabla\rho_\alpha|^2}{\rho_\alpha(r)} + \frac{||\nabla\rho_\beta|^2}{\beta(r)}\right] \qquad ...(3)$$

and

$$D_{0(r)} = \frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}] \qquad ...(4)$$

Savin *et al.* have reinterpreted ELF in the viewpoint of kinetic energy,[123] which would make ELF also meaningful for Kohn-Sham DFT wave-function or even post-HF wave-function. They indicated that $D(r)$ reveals the excess kinetic energy density caused by Pauli repulsion, while $D_0(r)$ can be considered as Thomas-Fermi kinetic energy density.

To overcome this problem, Multiwfn automatically adds a minimal value of 10-5 to $D(\mathbf{r})$. This treatment does not really affect the ELF value in interesting regions, in which case, the actual kinetic energy term in $D(\mathbf{r})$ is replaced by Kirzhnits type second-order gradient expansion that is:

$$\frac{1}{2}\sum_i \eta_i \ |\nabla\varphi_i|^2 \approx D_0(r) + \frac{1}{72}\frac{|\nabla\rho|^2}{\rho(r) + \frac{1}{6}\nabla^2\rho(r)} \qquad ...(5)$$

So that ELF is totally independent of the wave-function and can be used to analyze electron density from X-ray diffraction data. It is clear that Tsirelson's ELF can also be used to analyze electron density from quantum chemistry calculation, though, it is not as good as the ELF defined by Becke owing its suitability to the approximation introduced in kinetic energy term; however, qualitative conclusions can still be recovered in general.

Another function similar to ELF is called the localized orbital locator (LOL) which is used to locate high localization regions.

LOL contains a similar expression compared to ELF as well. In fact, the chemically significant regions that highlighted by LOL and ELF are generally qualitatively comparable, while Jacobsen pointed out that LOL conveys clearer and more decisive picture compared to ELF,[123-127]. Clearly, LOL can be interpreted in terms of kinetic energy similar to ELF. However, LOL can also be interpreted in terms of localized orbital. Small or large value of LOL is usually appeared in boundary (inner) region of localized orbitals due to the large of small gradient of orbital wave-function in this area respectively. The value range of LOL is identical to ELF, namely [0, 1].

**Computational details**

Parts of the Nanotubes including dopamine have been modeled with the QM/MM method and the calculations are carried out with the Monte Carlo method.

In this investigation, differences in force field are illustrated by comparing the calculated energy with AMBER and OPLS force fields. Furthermore, a HyperChem professional release 7.01 programs is used for the additional calculations.

The final parameterization of nanotubes was computed using self-consistent field calculations in order to find the optimal starting geometry, as well as the partial charges. The density functional theory with the van der Waals density functional was employed to model the exchange-correlation energies of graphene layers. All optimization of graphene layers were performed by Gaussian 09. The main focus in this study is to obtain the results from DFT methods such as m062x, m06-L, and m06 for the methamphetamine and dopamine. The m062x, m06-L and m06-HF are rather new DFT functional with a good correspondence in adsorption calculations between tubes and methamphetamine and dopamine are useful for the energies and other physical chemistry data.

Geometry optimizations and electronic structure calculations have been carried out using the m06 (DFT) functional. This approach is based on an iterative solution of the Kohn-Sham equation[128] of the density functional theory in a plane-wave set with the projector-augmented wave pseudo-potentials.

The Perdew-Burke-Ernzerhof (PBE)[129] exchange-correlation (XC) functional of the generalized gradient approximation (GGA) is also used. The optimizations of the lattice constants and the atomic coordinates are made by the minimization of the total energy.

The charge transfer and electrostatic potential-derived charge were also calculated using the Merz-Kollman-Singh[130], chelp[131], or chelpG[132].

### RESULT AND DISCUSSION

In this study, difference in force field is illustrated by comparing the energy calculated by using force fields, MM+ and OPLS. Also, it has been investigated polar solvent and the temperature effects (between 260K and 400K) on the stability of SWBNNT bonded to methamphetamine and dopamine in various solvents. The quantum mechanics (QM) calculations were carried out with the HyperChem 8.0 program. This study mainly focuses on the electron density of methamphetamine and dopamine in a binding system with (n, n) SWBNNTs surfaces and SWCNTs. The models and situation of molecular structures and binding interaction are shown in figs1- 5. As it is indicated in table HOMO/LUMO and Gap energy shows suitable binding[133,134].

According to the above equations the largest electron localization is located on atoms which are bonded to nanotubes where the electron motion is more likely to be confined within that region. If electrons are completely localized in those atoms, they can be distinguished from the ones outside. As shown in figures1-45 the large density is close to the bonded atoms. The regions with large electron localization need to have large magnitudes of Fermi-hole integration which would lead those atoms towards superparamagnetic. The fermi hole is a six-dimension function and as a result, it is difficult to be studied visually. Based those equations, Becke and Edgecombe noted that the Fermi hole is a spherical average of the spin which is in good agreement with our results in tables and Figs .

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