AB INITIO STUDIES OF FLUOROURACIL AND PYRIDOXINE INTERACTION WITH SINGLE WALLED CARBON NANOTUBES

Maria Ciopata[1]*, Cornel Miclea[1,2], Ciprian Tiberiu Miclea[1]

1 Hyperion University, Physics Department, Popa Nan Str. 90-92, Bucharest, Romania
2 National Institute of Material Physics, P.O Box MG-7, 077125, Bucharest, Romania

***Corresponding author: M. Ciopata; e-mail:** ciopata.maria@infim.ro*

The present work presents some original results concerning the interaction of 5-fluorouracil and pyridoxine (B6 vitamin) with Single Walled Carbon Nanotubes, revealed by first principles calculations. The *ab-initio* calculations were performed in the density functional thory framework and bring some possible advances in drug delivery mechanisms

INTRODUCTION

- It is known that **fluorouracil** is a drug which as a **pyrimidine analogue**, it is transformed inside the cell into different **cytotoxic metabolites** which are then incorporated into DNA and RNA, finally inducing cell cycle arrest and **apoptosis** by inhibiting the cell's ability to synthesize DNA. **In this manner, the proliferation of cancerous cells is stopped**. As all cytostatics, it may have **severe side effects**, damaging both cancerous and healthy cells.

- In order to minimize these side effects, a modern trend is to try sending chemical messages only in target regions through functionalized nanoparticles, though the various toxic effects of drugs may be significantly reduced.

- The interaction of fluorouracil and pyridoxine with SWNT is addressed depending on tube diameter and chirality. We calculated the adsoprtion energy for both metallic and semiconducting nanotubes (armchair (6,6) and (10,10) and zigzag (12,0) and (13,0)).

- These values allows us to extract the optimal energetic configuration in which the adsorption process takes place and also the geometric parameters corresponding to this configuration.

- **On the other hand, there are several studies suggesting that the pyridoxine, an hidrosoluble agent acts itself as an efficient transmitter of biochemical messages by means of selective functionalization[4,5].**

- We focused our attention on its ability to adsorb at tube's surface in order to obtain tunable dimensions of message transporters as it may be useful if we want to introduce a desired drug inside a virus capsid for example, or in other targeted tissue region with desired dimensional selectivity.

NUMERICAL DETAILS

- **The DFT calculations were performed with SIESTA software [1,2] in local density approximation (LDA) for coordinate relaxation, and with the relaxed coordinates, the electronic properties were subsequently calculated using the generalized gradient approximation (GGA) in Perdew-Burke-Erzenhof (PBE) parametrization of the exchange-correlation functional[3].**
- **In both cases a double zeta polarization (DZP) basis was used for expanding the atomic orbitals.**
- **The SCF iterations were performed until the total energy converged with a precision exceeding e-7.**

RESULTS AND DISCUSSIONS

- **We observed that for both species, the optimal adsorption configuration, corresponding to minimum values of adsorption energies, is parallel with tube axis.**
- **Also, we can see (Fig. 2 right) that as the tube diameter increases, the adsorption energy increases too, suggesting that the adsorption is favored at the small tube diameter case and in a less important measure by their character: metallic or semiconducting.**
- **This may be understood as an effect due to tube curvature which distorts the C-C bond length with respect the conventional one in graphite, thus causing a slight change in the hybridization state of carbon atoms. In this way, the reactivity of SWNT increases as the curvature increases (or equivalently when the tube radius decreases).**
- **We calculated the electronic density of states and we observed that localized levels near the Fermi level may appear.**

RESULTS AND DISCUSSIONS

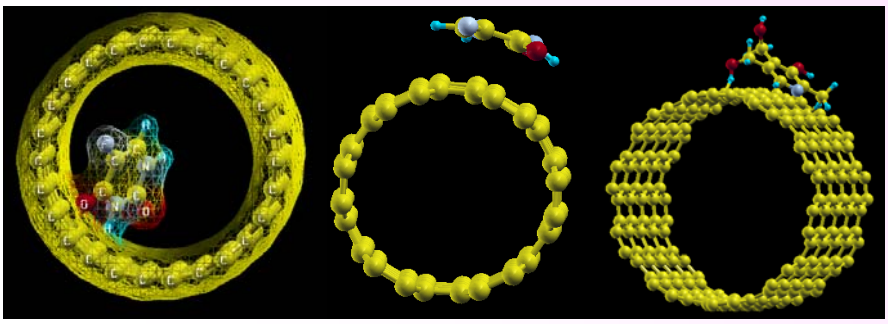


Figure 1
Various geometries used during the simulation procedure: at tube interior: not favorable and at its exterior, in parallel configuration-the most favorable

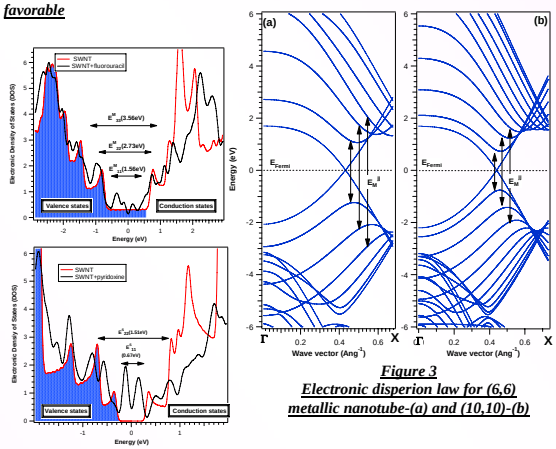


Figure 3
Electronic disperion law for (6,6) metallic nanotube-(a) and (10,10)-(b)

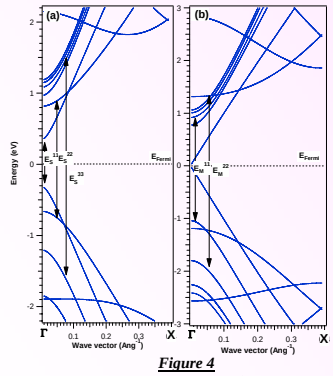
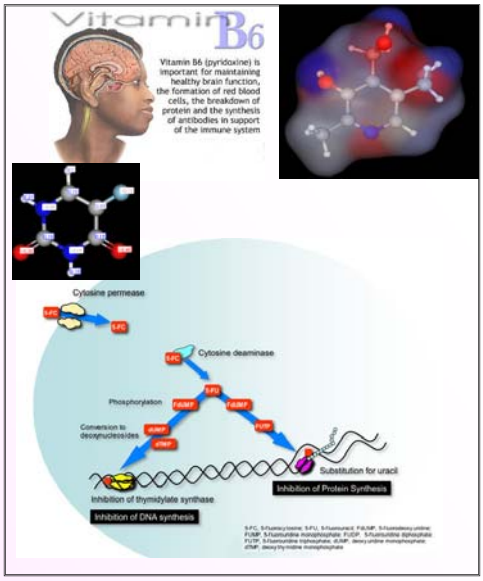
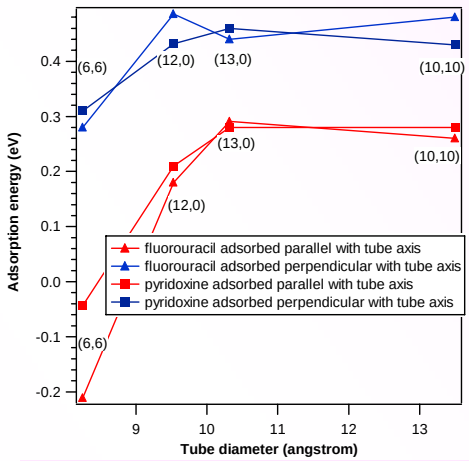


Figure 4
Electronic disperion law for (12,0) metallic nanotube-(a) and (13,0) semiconducting one-(b)





REFERENCES

[1] S. R. Bahn and K. W. Jacobsen, Comput. Sci. Eng. **4, 56 (2002)**
[2] J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J.Junquera, P.Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matter **14, 2745(2002)**
[3] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77, 3865 (1996)**
[4] Ghanshvam V.J *et.al,* Colloid and Polymer Science, **287**, 1071(2009)
[5] Marchand A. *et.al,* Chemistry and Biodiversity, **4 (2007)**

CONCLUSIONS

✓ **We investigated by means of *ab-initio* calculations the interactions between carbon nanotubes of different diameters as well as with metallic or semiconducting character in order to establish the availability of CNT functionalization with this kind of systems.**

✓ **In order to address future advances in drug delivery systems development allowing selective action on target region, we calculated the adsorption energy for each of the above drugs taking into account the interaction with (6,6), (10,10), (12,0) and (13,0) nanotubes.**

✓ **The results show that for small diameter nantubes the reaction is very favorable and as the tube curvature increases its reactivity decreases and the process evolves towards an physical adsorption-like one**