

Computational Modeling of Charge Transfer in Nucleobase-Aromatic Amino Acid Complexes

C. Butchosa

When DNA is oxidized radical cations are formed, they are also called electron "holes". These holes can migrate long distances along the stack of nucleobases that conform the DNA string, and then lead to the formation of a mutagenic lesion.

This presentation shows the obtained results for the study of hole transfer (HT) reactions between nucleobases and aromatic amino acids. Thus an electron hole could be transferred from the DNA nucleobase to an interacting protein or peptide avoiding genetic damage.

Although charge transfer reactions on DNA have been widely explored, not much is known about the charge transfer capabilities of the DNA when it interacts with amino acids. Three main questions have been explored:

- NB-interactions with the four aromatic amino acids.¹
- Conformational dependence of electronic coupling for G-Trp and A-Trp systems.^{2,3}
- Utilization of a 3-state model to calculate electronic coupling in G-Trp systems. A multistate study.

¹ Butchosa, C.; Simon, S.; Voityuk, A., Electron transfer from aromatic amino acids to guanine and adenine radical cations in π -stacked and T-shaped complexes. *Org. Biomol. Chem.* **2010**, 8, 1870-1875.

² Butchosa, C.; Simon, S.; Voityuk, A., Conformational Dependence of the Electronic Coupling in Guanine-Tryptophan Complexes: A DFT Study. *International Journal of Quantum Chemistry* **2011**, DOI 10.1002/qua

³ Butchosa, C.; Simon, S.; Voityuk, A., Conformational dependence of the electronic coupling for hole transfer between adenine and tryptophan. *Comput. Theoret. Chem.* **2011**, 975, 38.