Fragment-Orbital Modeling of Charge Transport in RNA

Juliusz Stasiewicz[1], Janusz M. Bujnicki[1,2]

[1]Laboratory of Bioinformatics and Protein Engineering,
International Institute of Molecular and Cell Biology in Warsaw,
Ks. Trojdena 4, 02-109 Warsaw, Poland

[2]Laboratory of Bioinformatics, Institute of Molecular Biology and Biotechnology,
Faculty of Biology, Adam Mickiewicz University,
ul. Umultowska 89, 61-614 Poznań, Poland

The ability of DNA strands to transport electric charge captured lots of attention over the recent years [1]. It is widely believed that conductivity of DNA may be involved in repair of oxidatively damaged genetic code, i.e. by allowing migration of radicals to non-coding regions. It has also been suggested that positive charge from DNA base stack can oxidize aromatic amino acids in DNA-binding proteins. Although indications do exist that the same issues may arise in RNA [2], the topic of RNA conductivity remains largely overlooked.

According to current state of the art, positive charges are localized mainly on bases, preferably guanine. Guanine posesses the least ionization potential (ca. 0.4 V less than adenine and 1 V less than cytosine and uracil) [3], being the most prone to electron detachment. The hole (unocuppied HOMO) is believed to be the charge carrier, which can do multistep hopping or tunneling between neighbor bases.

In this work we propose a computational scheme for evaluation of hole conductivity in RNA strands. In the scheme we treat all selected fragments (bases, nucleotides or base pairs) on the Density Functional Theory level. The dynamics of system is reproduced by Molecular Dynamics, in the QM/MM spirit. Interactions of the quantum and newtonian parts are accounted for by the means of partial atomic charges. We evaluate the tight binding Hamiltonian as the model for charge movements.

We also present custom C++ codes that perform multiscale modeling with the efficient technique of template metaprogramming.

[1] B. Giese *Annu. Rev. Biochem.* 71:51 (2002)
[2] D. T. Odom, J. K. Barton *Biochemistry* 40:8727 (2001)
[3] T. Kubar *et al. J. Phys. Chem. B* 112:7937 (2008)