PR-1. ACCESSING MOLECULAR PROPERTIES BY EXPERIMENTAL AND THEORETICAL DETERMINATION OF ELECTRONIC STRUCTURE

J. R. Garcia, M. G. Reddy, K. C. C. W. S. Klider, Jr. C. Camilo, S. R. de Lazaro

Department of Chemistry of the State University of Ponta Grossa,
Av. Gal. Carlos Cavalcanti, 4748 – Uvaranas, Ponta Grossa – PR, Brazil, 84030-900

E-mail: jrgarcia@uepg.br

Determination of the electronic structure is a key factor to perform easy and fast estimation of chemical, physical and biological activities of conjugate molecules. Electronic structure of this kind of molecules can be easily determined using UV-vis spectroscopy and electrochemical measurements, so parameters as bang gap energy (*Eg*), ionization potentials (IPs) and electron affinities (EAs) can be estimated [1].

However, when comparing the properties of a series of similar molecules, the influence of specific moieties, on a determined property could be hard to evaluate due to the proximity of the produced experimental results. This problem can be overcome by the application of theoretical models suitable to the evaluation of molecular electronic structure.

In this way, density functional theory (DFT) can be applied to study the electronic structure and the optical properties of series of conjugated molecules. Using this approach it is possible to accurately calculate the *Eg* and the energy values for the HOMO and LUMO orbitals and the influence of each different moieties on those values. Those calculations open the possibility for the prediction of the optical transitions in these materials and the values for EA and IP, which ones are directly related to HOMO and LUMO orbital energy.

DFT calculation of a series of conjugated polymers and molecules are compared to results obtained by UV-vis spectroscopy and by electrochemical measurements to estimate the electronic structure of those compounds accessing the optical and electrical behavior when applied in photovoltaics devices [2, 3].

In addition, theoretical calculations were performed on series of molecules with potential application as antimicrobial drugs. The relative energy position of the LUMO orbital in the series have showed that the biological activities in incremented for molecules with high-energy LUMO orbitals [4].

References

1. Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes / J. A. Frey [et al.] // Chem. Rev. 2016. Vol. 116, № 9. P. 5614–5641.

2. Corrigendum: Effect of hexyl substituent groups on photophysical and electrochemical properties of the poly [(9,9-dioctyfluorene)-2,7-Diyl-alt-(4,7-bis(3-hexylthien-5-Yl)-2,1,3-benzothiadiazole)-2′,2″-diyl] / D. J. Silva [et al.] // J. Polym. Sci. Part B Polym. Phys. 2017. Vol. 55, № 12. P. 964–964.

3. Synthesis and Characterization of a New Semiconductor Oligomer Having Quinoline and Fluorene Units / F. C. Correia [et al.] // J. Braz. Chem. Soc. Brazilian Chemical Society. 2014. Vol. 26, № 1. P. 84–91.

4. Synthesis, antimicrobial activity and advances in structure-activity relationships (SARs) of novel tri-substituted thiazole derivatives / G. M. Reddy [et al.] // Eur. J. Med. Chem. 2016. Vol. 123. P. 508–513.

The author would like to thank the Brazilian Agency Funding: CNPq, CAPES and Fundação Araucária.