

## Electronic structure calculations for the study of polyaniline-based chemical sensors

Larissa Oliveira Mandú, Augusto Batagin-Neto

*Universidade Estadual Paulista (UNESP), Câmpus Experimental de Itapeva, Brazil*

**Abstract:** Conjugated organic polymers represent an important class of materials for varied technological applications, including in active layers of chemical sensors. In this context, polyaniline (PANI) derivatives have been identified as promising candidates, mainly due to their high chemical stability, good processability, versatility of synthesis/polymerization/doping, as well relatively low cost [1-3]. In this study electronic structure calculations were carried out for varied PANI derivatives in order to identify systems with improved sensory properties. Preliminary reactivity studies were performed to identify possible adsorption centers on the oligomer structures via Condensed-to-atoms Fukui indexes (CAFI) [4] employing a DFT/B3LYP/6-31G approach and Hirshfeld partition charge. Adsorption studies were then carried out for selected derivatives employing five distinct gaseous analytes: H<sub>2</sub>, H<sub>2</sub>S, H<sub>2</sub>O, NH<sub>3</sub> and SO<sub>2</sub> [3]. Structural changes, average bond energies, energy level alignments and theoretical optical absorption spectra of the obtained systems were investigated in order to evaluate the influence of the analytes on the oligomers properties. The obtained results indicate the derivatives PANI-NO<sub>2</sub> and PANI-C<sub>6</sub>H<sub>5</sub> as the most promising materials for the development of chemical sensors.

**Key-words:** chemical sensors, polyaniline derivatives, electronic structure.

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