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Abstract: Organic polymers are promising materials for active layers of chemical sensors. In this context, polyfurane (PF) derivatives have not been extensively investigated due to typical stability problems and low electrical response of these compounds. A recent work have demonstrate that some of these typical drawbacks can be overcome by an appropriate choice of lateral substituents, which could allow the application of PF derivatives in varied areas, including as chemical sensors [1]. In order to better evaluate possible sensory features of these materials, in this report we employed electronic structure calculations to identify and analyze reactive site on the main chain of eight polyfurane derivatives with distinct side ramifications (R). Oligomeric structures with 9 units were fully optimized in vacuo in a Hartree-Fock approach by using the PM6 hamiltonian [2] implemented in the MOPAC2016 computational package [3,4]. The identification of more susceptible sites for analytes adsorption was performed via Condensed-to-atoms Fukui indexes (CAFI) [5] calculated in the Density Functional Theory framework, employing the B3LYP exchangecorrelation functional and 6-31G basis set for all the atoms. CAFI calculations were performed with the aid of Gaussian 09 computational package [6]. Hirshfeld partition method was employed for the evaluation of electronic populations in order to avoid negative CAFI values [7,8]. The obtained results indicate the derivatives PF-C=CH and PF-NO₂ as the most promising materials for the development of chemical sensors. These compounds present high reactivity in the lateral ramifications (more accessible sites for analyte adsorption) and more stability to oxidation in relation to PF. Adsorption studies guided by the reactivity results are currently in progress.

Key-words: polyfuran, Condensed-to-atoms Fukui indexes, chemical sensors, electronic structure calculations.

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