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Theoretical Study on Structural and Electronic Properties of Polypyrrole: Ammonia Gas Sensor

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Polypyrrole (PPy) have been considered as one of the most promising conducting polymers for gas sensor application due to it can operate efficiently at room temperature, light weight, thermal stability and high sensibility. In this research, we have been reported the geometric and electronic structure of PPy based on B3LYP/3-21G*, B3LYP/6-31G* and SCC-DFTB methods. The effects of polymer chain length of PPy on structural and electronic properties including bond length, bond angle, torsion angle, the highest occupied orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and energy gap have been studied from the optimized PPy oligomers (n=1-10). The results show that the bond length, bond angle and torsion angle from SCC-DFTB method are C-N = 1.38 Å, N-H = 1.04 Å, C-C = 1.45 Å, N-C-C = 122 ^{o}, C-C-C = 131^{o}, N-C-C-C = 179^{o} and C=C-C=C = 179^{o}, respectively. The HOMO and LUMO are ranging from -5.49 to -4.23 eV and -0.078 to -1.92 eV, respectively. The energy gap decreased with increasing polymer chain length from 5.41 to 2.31 eV. Furthermore, the results based on B3LYP/3-21G*, B3LYP/6-31G* and effects of PPy ammonia gas sensor have been investigated and discussed in more detail.

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