THEORETICAL DESIGN OF CONDUCTING POLYMERS

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Density functional theory is very useful for predicting properties of conducting polymers. The simplest approach to estimate band gaps is to use orbital energies. This is questionable from a theoretic point of view but was shown to work very well by comparison with experimental data. However, it is difficult to improve on the method. Employing TD-DFT, for instance, does not lead to good agreement between calculated and experimental excitation energies for the π–π^*-transition energies. Problems were also encountered in predicting the correct relative energies of structural isomers compared with MP2 results and experimental findings. Data will be presented for polythiophene, polyethylenedioxythiophene and polydifluoroacetylene.