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Density functional and molecular dynamics study of conducting polymers Y. DAI, E. BLAISTEN-BAROJAS, School of Computational Sciences, George Mason University, Fairfax, VA 22030 — Polypyrrole belongs to the important class of conducting polymers and is a good candidate for photonic devices and chemical sensors. In this work we performed electronic structure calculations of pyrrole oligomers containing 6 to18 rings at the density functional (DFT) level and searched for the charge distribution in the oxidized and neutral phases. The description of bipolaron given in terms of charge localization over domains along the pure polymer chain by semiempirical methods could only be confirmed by DFT studies in the oxidized phase when dopants are present. A model potential for polypyrrole was developed based on the first principles calculations of the structure and charge distribution. Several finite temperature and dynamical properties were studied with molecular dynamics.

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