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Multi-Scale Modeling of Conductive Polymers

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In spite of the tremendous impact of conductive polymers in a number of technological applications, molecular engineering of these materials has not been accomplished yet. One of the main reasons is the lack or limited understanding of the connection between changes occurring at the molecular level and the resulting polymer conductivity. Understanding the influence that local changes to the polymer's structure and chemical composition have on polymer properties, is the key to reach the stage where polymer-based materials and devices can be molecularly engineered with optimum properties. A multiscale model able to predict and accurately describe such a connection is thus a much needed tool to achieve this goal. The main aspect of this project is the bridging between scales in such a way that properties of the polymer at the molecular level are reflected in the observed and measured macroscopic properties. However, to achieve that integration, adapting and improving models at each of the involved scales must be done first. The progress towards improved models at the atomic and at the macroscopic level will be described. The atomic level is dealt with by using quantum mechanics calculations including semiempirical and ab initio methods. A semi-empirical/DFT study of oligomers will be described were extrapolation of electronic properties to an essentially infinite chain show excellent agreement with experimental results. The macroscopic level is addressed with probabilistic models, based on the Monte Carlo Technique, to study the charge transport process. The efforts toward the improvement and implementation of an existing transport algorithm, based on the hopping model, will be described. Existing models consider polymer and polymer devices as a cubic arrangement of sites and incorporate disorder as an ad-hoc parameter, in our model, the use of realistic configurations allows the distinction of intra- vs. inter-molecular conduction and the modeling of polymer devices. In addition, the model is reformulated to incorporate parameters calculated at the atomic level, thus the effect of on macroscopic properties produced by changes at the atomic level can be studied. Plans for the integration across scales, the final step to achieve multiscale modeling, will also be discussed.