

Organic electronic materials represent an ecologically friendly and potentially low-cost alternative to conventional inorganic conductors and semiconductors. Such materials are usually constructed from carbon-based molecules and polymers using synthetic organic chemistry and polymer chemistry strategies. Organic electronics is a rapidly developing field of research covering the design, synthesis, characterization, and application of organic molecules and polymers with desirable electronic properties. Examples are conductive organic materials, organic light-emitting diodes, organic field-effect transistors, organic solar cells, and photovoltaics. The development of novel organic devices, materials and building blocks heavily relies on an experimental trial and error approach, which is costly and time-consuming. The computer-aided design and optimization of desired electronic properties using quantum chemistry could shed new light on a better understanding of their electronic structures and structure-to-property relationship, and as a consequence, advance the development of novel organic materials. Unfortunately, a routine quantum chemistry approach, like Density Functional Theory (DFT), to model the electronic structures of such species does not always provide physically correct results. For certain molecules, like long polymer chains, strong electron correlation effects are simply too overwhelming for DFT. Such systems should be modeled with multi-reference methods to provide reliable results. However, the applicability of multi-reference methods is limited to small model compounds usually consisting of few atoms, not polymer chains. A remedy to that problem comes from the pCCD-based methods, which due to efficient parametrization of the wave function, are capable of reliable modeling of large molecules, such as long polymers chains, at low computations cost. Although the unconventional pCCD group of methods available in the PyBEST software package is fairly suitable to the electronic structure modeling of the above-mentioned species, further extensions are necessary to predict electron transport properties. To that end, the main goals of the proposed research project are to design and implement various charge transfer integral models in PyBEST. The main application focus will be set on the prediction of electronic structures and properties of polyaniline and its derivatives, augmented with quantum entanglement analysis of orbital interactions.