Theoretical Study for Mixed-sequence Oligomer Salt Modeling Doped PEDOT Family

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Organic conductors are divided into two categories: low-molecular-weight and polymer-based materials. Low-molecular-weight materials have well-defined structures but limited control over conductivities. Conductive polymers, on the other hand, have highly conjugated systems but are difficult to control due to their structural inhomogeneity.

To bridge this gap, oligomer-based conductors were developed as intermediate materials. These conductors are made of oligo(3,4-ethylenedioxythiophene), oligoEDOT, and are modeled after the doped PEDOT family 1–4]. The conductivities of these materials were studied by considering counter anion variations, lengths of oligomer donor, and band fillings. Through the study, oligoEDOT analogs were developed with tunable room temperature conductivities by several orders of magnitude, including a metallic state above room temperature [4]. The electronic structural insights were evaluated by first-principles calculations (QUANTUM ESPRESSO, RESPACK, and H-wave packages; Ohtaka, Supercomputer center, ISSP), and it was revealed that the range of Coulomb repulsion between carriers, $\boldsymbol{U}_{\mathbf{eff}}$, is the dominant factor that determines the relationship between the structures and conductivities [5]. The oligoEDOT conductor systems have a unique feature of widely variable $\boldsymbol{U}_{\mathbf{eff}}$, differentiating these systems from strongly electron-correlated systems.

References

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