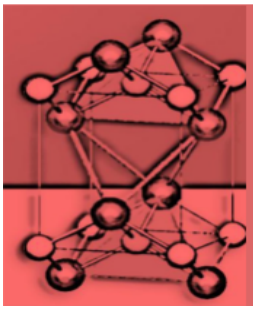

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# Mixed Ionic-Electronic Transport for Crystalline poly(3-hexylthiophene) with both Explicit Lithium bis(trifluoromethanesulfonyl) imide Dopant and dimethoxyethane Additive Assessment Using ab-initio Molecular Dynamics

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Here, we present *ab-initio* molecular dynamics (AIMD) calculations on the mixed ionic-electronic transport for crystalline poly(3-hexylthiophene) (P3HT) using explicit lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) dopant and dimethoxyethane (DME) additive. Up to now, and to the best of our knowledge, AIMD calculations dealing with mixed ionic-electronic transport in a P3HT crystalline supercell including the use of explicit dopants remain unexplored.

Our ionic and electronic conductivities estimations show good correlation with experimental reports of similar mixed ionic-electronic conductors. The use of less artifacts in our calculations allowed us to reveal some interesting behavior due to the presence of explicit dopant on the most relevant parameters associated to mixed ionic-electronic transport in a wide temperature range.

For the electronic transport, our transfer integral (J) and reorientation energies ($\lambda$) values showed an increment respect to typical unexplicit-doped calculations. Furthermore, we also introduce the role of the explicit dopant on the inter-chain, intra-chain, "effective" doping and charge-transfer complex bonding distances and their associated static and dynamic disorder effects on the electronic transport.