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Charge transport in branched conducting polymers: Quantum graphs based approach

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Conducting polymers has attracted much attention recently in the context of organic electronics. Some types of such polymers can have supramolecular (macroscopic) branching. Branched polymers occur when groups of units branch off from the long polymer chain. These branches are known as side chains and can also be very long groups of repeating structures. Branching polymers can be further categorized by how they branch off from the main chain. Polymers with many branches are known as dendrimers, and these molecules can form a webbing when cooled. This can make the polymer strong in the ideal temperature range. Such branched polymer chains can be modeled in terms of so-called quantum graphs, which are the set of nanoscale bonds connected at the vertices. The connection rule is called topology of a graph. Modeling of wave dynamics in branched conducting polymers require developing of effective methods allowing to take into account transition of the waves from one to another branches via the branching points. One of such approaches is based on the use of metric graphs as the models of the branched polymers. Within such approach, exciton dynamics can be modeled in terms of the Schrodinger equation on metric graphs.

In this work we use solve the problem of exciton dynamics and charge separation (via splitting of exciton into electron and hole) by modeling the whole system in terms of quantum graph. The main problem we studied is splitting of exciton from transmission from one branch to another one. Charge separation probability is explicitly calculated.

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