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Charge Transport in Organic Electronic Materials

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Abstract. Semiconducting conjugated polymers have become the materials of great interest for the use in electronic and optical devices, such as field-effect transistors, light-emitting diodes and solar cells. It is therefore of paramount importance to understand the carrier transport in these materials. Transport in disordered organic materials was until recently modelled only using phenomenological approaches that assume certain spatial and energetic distribution of electronic states and certain form of transition probabilities between them. As such, they lack the predictive power. We have developed an approach that links the atomic structure of the material to its electrical properties without the introduction of any fitting parameters [1]. The approach is based on a multiscale methodology that links the relevant quantities at four length scales. The simulations yield the temperature dependence of hole mobility in amorphous P3HT polymer consistent with experimental results from the literature [1]. Furthermore, using this approach it was possible to test the adequacy of previous simplified models. It was found that the Miller-Abrahams model is not sufficient for describing the hopping probabilities between the states [2] and that the concept of electronic temperature cannot be used to describe carrier heating in electric field [3].

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