Microscopic insight into the hopping transport in disordered semiconducting polymers

NENAD VUKMIROVIC, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Charge carrier transport in disordered conjugated polymers has been modeled for decades using simple phenomenological models that assume certain density of electronic states and certain analytical expression for the hopping rates between the states. The density of states is therefore believed to be the crucial property of the polymer material when electronic transport is concerned. We show here that transport properties are also strongly dependent on the proper description of transition rates. We use our recently developed multiscale method [1] for the calculation of electronic transport where transition rates are modeled taking into account the interaction with all phonon modes. Our results indicate that the widely used Miller-Abrahams model of the hopping rates predicts different behavior than our detailed model: a) It gives significantly different dependence of the mobility on temperature. b) It predicts that the concept of effective temperature could be used to describe carrier heating in electric field, in contrast to the results of the detailed simulations. [1] N. Vukmirovic and L.-W. Wang, Nano Lett., in press (2009).

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