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Incorporating Decoherence in the Dynamic Disorder Model of Organic Semiconductors WEI SI, YAO YAO, CHANG-QIN WU, State Key Laboratory of Surface Physics and Department of Physics, — The transport phenomena in crystalline organic semiconductors, such as pentacene, have drawn much attention recently, where the electron-phonon interaction plays a crucial role. An important advance is the dynamic disorder model proposed by Troisi *et. al.*, which is successful in determining the carrier mobility and explaining the optical conductivity measurements. In this work, we aim to incorporate the decoherence effects in the dynamic disorder model, which is essential for the self-consistent description of the carrier dynamics. The method is based on the energy-based decoherence correction widely used in the surface hopping algorithm. The resulting dynamics shows a diffusion process of wave packets with finite localization length, which scales with the decoherence time. In addition, the calculated mobility decreases with increasing temperature. Thus the method could describe a band-like transport based on localized states, which is the type of transport anticipated in these materials.

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