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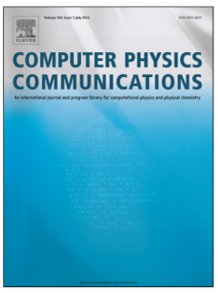

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Kinetic Monte Carlo Simulation of Single-Electron Multiple-Trapping Transport in Disordered Media

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Abstract

The conventional single-particle Monte Carlo simulation of charge transport in disordered media is based on the truncated density of localized states (DOLS) which benefits from very short time execution. Although this model successfully clarifies the properties of electron transport in moderately disordered media, it overestimates the electron diffusion coefficient for strongly disordered media. The origin of this deviation is discussed in terms of zero-temperature approximation in the truncated DOLS and the ignorance of spatial occupation of localized states. Here, based on the multiple-trapping regime we introduce a modified single-particle kinetic Monte Carlo model that can be used to investigate the electron transport in any disordered media independent from the value of disorder parameter. In the proposed model, instead of using a truncated DOLS we imply the raw DOLS. In addition, we have introduced an occupation index for localized states to consider the effect of spatial occupation of trap sites. The proposed model is justified in a simple cubic lattice of trap sites for broad interval of disorder parameters, Fermi levels, and temperatures.

Keywords: multiple-trapping; kinetic Monte Carlo simulation; localized states

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