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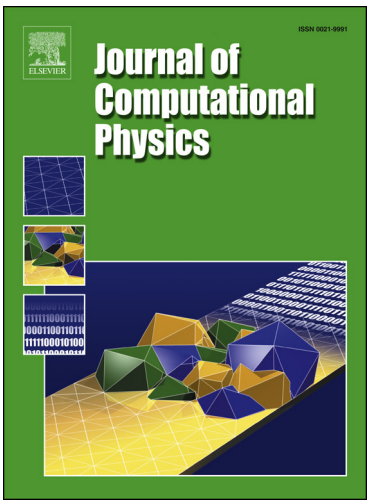

Massively parallel kinetic Monte Carlo simulations of charge carrier transport in organic semiconductors

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Massively parallel kinetic Monte Carlo simulations of charge carrier transport in organic semiconductors

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Abstract

A parallel, lattice based Kinetic Monte Carlo simulation is developed that runs on a GPGPU board and includes Coulomb like particle-particle interactions. The performance of this computationally expensive problem is improved by modifying the interaction potential due to nearby particle moves, instead of fully recalculating it. This modification is achieved by adding dipole correction terms that represent the particle move. Exact evaluation of these terms is guaranteed by representing all interactions as 32-bit floating numbers, where only the integers between -2^{22} and 2^{22} are used. We validate our method by modeling the charge transport in disordered organic semiconductors, including Coulomb interactions between charges. Performance is mainly governed by the particle density in the simulation volume, and improves for increasing densities. Our method allows calculations on large volumes including particle-particle interactions, which is important in the field of organic semiconductors.

Keywords:

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1. Introduction

Kinetic Monte Carlo (KMC) methods are widely used for simulating the time evolution and equilibrium behaviour of systems of particles. These meth-

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