Simulations of Organic Field-Effect Transistors by the Combination of Finite Difference Method and Kinetic Monte Carlo Method

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Abstract

Organic field-effect transistors (OFETs) are being actively studied today in a wide range of applications such as e-paper displays, simple circuits, and chemical and biological sensors [1]. Understanding the OFET device physics and their current characteristics is critical in designing new organic materials and optimizing device performance. In this context, 3-dimensional (3D) kinetic Monte Carlo (KMC) simulations have proven useful as they can take detailed account of the microscopic features of organic semiconductors, such as localized electronic states, discrete molecular levels, and the hopping nature of charge transport. Recently, Li. et al. [2] have developed a 3D KMC model that can be used in all operation modes of OFET devices and gives very realistic current characteristics [3]. In these simulations, however, the 2-dimensional (2D) Poisson equation was used to generate the electric potential needed to calculate the charge transfer rates, which means that the electric-potential variations along the device width direction are not considered. Improving accuracy requires the use of the 3D Poisson equation. Ideally, such a 3D Poisson solver must be highly efficient since it will be called multiple times throughout the OFET simulation. To improve the accuracy in OFET device modeling, we present an efficient and accurate 3D Poisson solver, which benefits from multi- and many-core architectures and is applicable to problems with mixed boundary conditions. Through the use of parallel computing, the speed of computation of the electric potential is significantly improved and can outperform earlier methods. For instance, Poisson equation problems with up to 5 million degrees of freedom are solved in less than 1 second on 64-processor elements.

Keywords: Organic field-effect transistors, Finite difference method, Kinetic Monte Carlo, 3D Poisson Equation

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