

Fig. 4 shows more detailed simulation results for the configuration of Fig. 3A.

Fig. 5 shows site dependent simulation results for the configuration of Fig. 3A.

Fig. 6 shows location dependent simulation results for the configuration of Fig. 3A.

Fig. 7 is a comparison between local and non-local modeling of recombination.

Fig. 8 shows dependence of simulated J-V curves on disorder energy.

Fig. 9 show dependence of simulated J-V curves on temperature.

Fig. 10 shows mobility enhancement vs. wave function decay length.

Fig. 11 shows the effect of the disorder parameter on  $\mu/\mu_{\text{MMA}}$  as defined in the text.

Fig. 12 shows the dependence of various components of the recombination rate prefactor on the disorder parameter.

## DETAILED DESCRIPTION

### I) Introduction

In the past decades, tremendous progress has occurred in the field of disordered organic semiconductors. For example, organic light-emitting diodes (OLEDs), composed of layers of amorphous organic thin film, have already entered the display and lighting markets. In order to understand the physics and speed up further device development, it is crucial to make use of device modeling techniques which can both describe the essential physics and be computationally efficient.

For unipolar devices, various methods have been applied to disordered organic semiconductor devices, including one-dimensional (1D) drift-diffusion (1D-DD) simulations, three-dimensional Kinetic Monte Carlo (3D-KMC) simulations, one-dimensional master equation (1D-ME) simulations, and three-dimensional master-equation (3D-ME) simulations. 1D-DD modeling is widely used for inorganic semiconductor devices. It has also been **intensively** used to model organic semiconductor devices, because the method is relatively simple and fast. However, the method has various limitations. For example, it assumes the system to be a continuous medium without explicitly including the details at the molecular level. These details are only implicitly