Simulation of Injection Currents into Disordered Molecular Conductors

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We present a three-dimensional Kinetic Monte Carlo simulator which has been designed to simulate the injection and propagation of currents into a disordered molecular conductor.

INTRODUCTION

The gold standard for the numeric simulation of organic semiconductors has been defined by Heinz Bässler[1] and co-workers several decades ago. The established approach to the simulation of polymeric devices since then is based on hopping among "sites" standing for some kind of molecular transport unit like e.g. a single molecule or a chromophore. These sites usually constitute a three-dimensional lattice and have no further inner structure. The transition of carriers from one site to another is facilitated by thermally activated tunneling. Thereby the Miller-Abrahams rate[1], the Marcus rate[2], or similar rate expressions are used. Especially when modeling molecular geometries or spatial disorder effects, Monte Carlo simulations are often enhanced by combining the former mentioned hopping rates with the results of quantum theoretical calculations[3].

EXPERIMENTAL/THEORETICAL STUDY

We implemented a simulator based on a three-dimensional grid of two-level sites, each level hosting two spin-paired electrons, the p-conductive bonding "HOMO" states and the anti-bonding, n-conductive "LUMO" orbitals. Almost all organic devices exhibit contact-dominated behavior. The physics of the organo-metallic interface, however is heavily dependent on the bulk characteristics and thus cannot be viewed isolatedly[4]. Moreover, the material parameters of a heterojunction's constituents as tabulated in literature may usually not be used without reflection to calculate e.g. interfacial band-offsets[5]. As the elaborate work of e.g. Gao[6] or Ishii[5] demonstrates, opaque effects like e.g. shifts in the vacuum level require considering the electronic structure of such heterojunctions *in situ*. Since the results for pure bulk simulations consequently do not tell us much about the performance the whole device, our work focusses on the injection process. The idea to simulate the injection process self-consistently within the Bässler-formalism is indeed very old and dates back to Gartstein and Conwell[7]. Several workers since then, e.g. Wolf[8] and van der Holst[9] applied this idea and simulated the carrier injection/extraction process by hopping from and to the electrode's Fermi-level. In other words, also interfacial tunneling is modeled in the mentioned works by the according static factor in the Miller-Abrahams rate. We altered the Miller-Abrahams rate twofold. First, we calculate and update both the interfacial tunneling probabilities as well as the tunneling rates between localized (bulk-) electron wave functions. Second, throughout the device we include the multi-phonon corrective term which has been derived by Baranovskii[10] decades ago for inorganic disordered materials. While the application of this correction is better justified for excitations in the metal electrodes, the authors are aware that the validity of this step for organic sites has to be evaluated in a subsequent work.

RESULTS AND DISCUSSION

Our software has been calibrated to the electrical characteristics of p-conductive Au/amorphous Zinc Phthalocyanine/Au devices measured by Gao et al.[6]. Simulated J-V characteristics and distributions for current densities and transmission coefficients will be presented.

CONCLUSION

The naive application of the Miller-Abrahams rate to the injection process in *real* space is a much too simplistic approach. Although only the image force but neither space charges nor interparticle interactions were considered, the fairly abstract sampling algorithm of Wolf et al.[8] indeed provides an impressive congruence with experimental data. However, this injection takes place into an abstract *simulation* lattice. Injections into *real* space facilitate the modeling of interfacial, location-dependent electronic and morphologic phenomena governing a device's transport- and injection efficiency.

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