Supporting Information

Parametrization of extended Gaussian disorder models from microscopic charge transport simulations

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A. Parametrization of Stochastic Model

Center of mass positions are generated using thinning of a Poisson process and validated by comparing the pair correlation function $g(r)$, which is a measure of the density of neighboring points at a distance r. The resulting pair correlation functions for the microscopic and the stochastic model are shown in fig. 1.

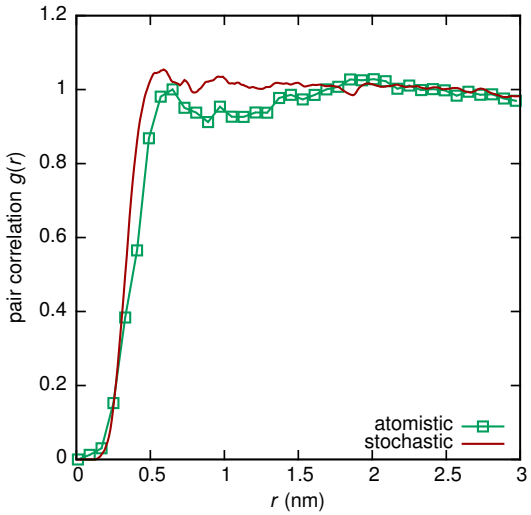

Figure 1: Pair correlation function for the microscopic and the stochastic model.

Analysis of the distributions of transfer integrals, J_{ij}, for all pairs of neighboring molecules shows that $\log_{10}(J_{ij})$ is Gaussian distributed for molecules whose distance r is within a certain fixed interval, with mean and variance of the Gaussian changing with distance, cf. figs. 2(a) and (b). After determining the distance dependence from the microscopic model for each pair, values are drawn following a Gaussian distribution with the respective parameters. Fig. 2(c) shows the overall frequency of rates after plugging in site positions, energies and electronic couplings.

B. Extend Gaussian Disorder Model (EGDM)

The EGDM model[1], parametrized on Monte Carlo simulations (cubic lattice, charges interact via an exclusion principle) postulates a factorization into three terms

$$\mu(T,\rho,F) = \mu_0(T) g(T,\rho) f(T,F), \tag{1}$$

where T is the temperature, ρ the spatial carrier density (carriers per volume), and F the absolute value of the electric field. The functions μ_0, g and f are defined by

$$\mu_0(T) = 1.8\times10^{-9}\mu_0 \exp\left[-C\hat{\sigma}^2\right],\ C = 0.42,$$

$$g(T,\rho) = \exp\left[\frac{1}{2}\left(\hat{\sigma}^2-\hat{\sigma}\right)\left(2\rho a^3\right)^{\delta}\right],$$

$$f(T,F) = \exp\left[0.44\left(\hat{\sigma}^{3/2}-2.2\right)\left(\sqrt{1+0.8F_{\mathrm{red}}^2}\right)\right],$$

$$\delta = 2\frac{\ln\left(\hat{\sigma}^2-\hat{\sigma}\right)-\ln(\ln 4)}{\hat{\sigma}^2}.$$

μ_0 is a material specific property, $F_{\mathrm{red}} = eaF/\sigma$, and $\hat{\sigma} = \sigma/k_{\mathrm{B}}T$.

C. Extended Correlated Gaussian Disorder Model (ECDM)

The ECDM[2] accounts for spatial correlations of site energies. It postulates the following mobility dependence

$$\mu(T,\rho,F) = \mu_0(T) g(T,\rho) f(T,F,\rho), \tag{2}$$

where

$$\mu_0(T) = 1.0\times10^{-9}\mu_0 \exp\left[-C\hat{\sigma}^2\right],\ C = 0.29,$$

$$g(T,\rho) = \begin{cases} \exp\left[\left(0.25\hat{\sigma}^2+0.7\hat{\sigma}\right)\left(2\rho a^3\right)^{\delta}\right], \\ \qquad \rho a^3 < 0.025 \\ \exp\left[\left(0.25\hat{\sigma}^2+0.7\hat{\sigma}\right)\left(2\times0.025\right)^{\delta}\right] \\ \qquad \rho a^3 \geq 0.025, \end{cases}$$

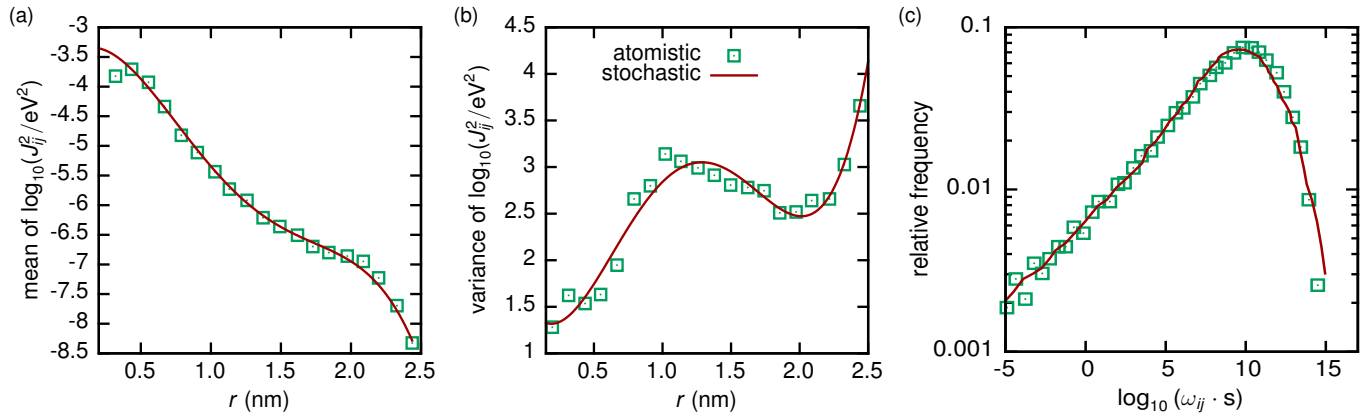

Figure 2: Mean (a) and variance (b) of distributions of $\log_{10}\left(J_{ij}^2/\mathrm{eV}^2\right)$ and (c) distributions of logarithmic transfer rates $\log_{10}\left(\omega_{ij}\cdot\mathrm{s}\right)$.

$$f(T,F_{\mathrm{red}},\rho)=\exp\left[h(F_{\mathrm{red}})\left(1.05-1.2\left(\rho a^3\right)^{r(\hat{\sigma})}\right)\right.$$
$$\left.\times\left(\hat{\sigma}^{3/2}-2\right)\left(\sqrt{1+2F_{\mathrm{red}}}-1\right)\right],$$

$$r(\hat{\sigma})=0.7\hat{\sigma}^{-0.7},\ F_{\mathrm{red}}=\frac{eaF}{\sigma},\ F_{\mathrm{red}}^{*}=0.16,$$

$$h(F_{\mathrm{red}})=\begin{cases}\frac{4}{3}\frac{F_{\mathrm{red}}}{F_{\mathrm{red}}^{*}}, & F_{\mathrm{red}}<\frac{F_{\mathrm{red}}^{*}}{2}\\ \left[1-\frac{4}{3}\left(\frac{F_{\mathrm{red}}}{F_{\mathrm{red}}^{*}}-1\right)^2\right], & \frac{F_{\mathrm{red}}^{*}}{2}\le F_{\mathrm{red}}\le F_{\mathrm{red}}^{*},\end{cases}$$

$$\delta=2.3\frac{\ln\left(0.5\hat{\sigma}^2+1.4\hat{\sigma}\right)-\ln(\ln 4)}{\hat{\sigma}^2}.$$

D. Extrapolation to Non-Dispersive Transport

The non-dispersive mobilities were extracted by performing simulations at high temperatures (nondispersive regime) and then extrapolating to room temperatures[3]. The minimal temperature at which transport becomes non-dispersive was estimated from an empirical relation

$$\ln N=0.95\left(\frac{\sigma}{k_{\mathrm{B}}T}\right)^2+5.4, \tag{3}$$

where N is the number of molecules (sites), and σ is energetic disorder. For 4096 molecules in the microscopic system with an energetic disorder of $\sigma=0.253\,\mathrm{eV}$ the equation predicts $T_{\mathrm{min}}=1686\,\mathrm{K}$. Simulations at six different temperatures above this value (from 1800 K up to 57600 K) were fitted to the relation

$$\mu(T)=\frac{\mu_0}{T^{\frac{3}{2}}}\exp\left(-\left(\frac{a}{T}\right)^2-\left(\frac{b}{T}\right)\right) \tag{4}$$

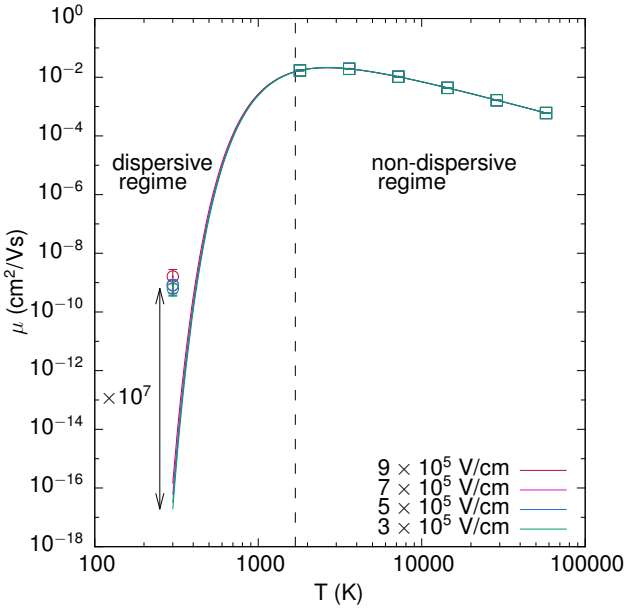

Figure 3: Extrapolation of high temperature mobilities to obtain a non-dispersive mobility at 300 K. Squares represent non-dispersive transport simulations at temperatures from 1800 K to 57600 K, which allow extrapolating down to lower temperatures (solid lines). This was done for four different (small) field strenghts, however, curves lie almost on top of each other. Circles are the uncorrected dispersive values from simulations at 300 K.

which was then used to extract mobility at $T=300\,\mathrm{K}$, see fig. 3. This was done for four different (small) field strengths F, yielding slightly different values in the order of $10^{-17}\,\mathrm{cm}^2/\mathrm{Vs}$. Dispersive transport simulations at 300 K yield values that are around seven orders of magnitude higher (see circles in fig. 3).

[1] Pasveer, W. F.; Cottaar, J.; Tanase, C.; Coehoorn, R.; Bobbert, P. A.; Blom, P. W. M.; de Leeuw, D. M.; Michels, M. A. J. *Phys. Rev. Lett.* **2005**, *94*, 206601.
[2] Bouhassoune, M.; Mensfoort, S. v.; Bobbert, P.; Coehoorn, R. *Organic Electronics* **2009**, *10*, 437–445.
[3] Lukyanov, A.; Andrienko, D. *Phys. Rev. B* **2010**, *82*, 193202.