The microscopic origins of charge transport in triphenylene systems
SUPPLEMENTAL MATERIAL

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Figure 1 shows the total change in energy between all pairs of neighbouring sites for a test charge of magnitude $|e|$ as a function of the pair separation in the z direction. This was measured using a steady state distribution of charges obtained from a KMC simulation under a 2V applied bias, and averaged over 6 separate simulations. We also recorded the distribution of ΔG_ω against Δx and Δy and found no difference in the distribution of energies between the two systems despite the presence of structural ordering in the columnar system.

From figure 4(a) in the main text, edges with $\Delta z \approx \pm 0.5$nm possess the highest transfer integrals in the ordered system. Imagining two lobes on figure 1 at the intersection of the line $\Delta G_{ij} = -\lambda$ with regions around $\Delta z = \pm 0.5$nm, the edges that have the highest hopping rates. To achieve transport there needs to be a difference in the population of the positive and negative Δz lobes.

We selected the edges with $\Delta G_{ij} = -\lambda \pm \delta E$ for different values of δE and calculated the histogram of edges with respect to Δz_ω. Figure 1 shows that for $\delta E \gtrapprox 0.5$ the contribution from the lower edge of the distribution does not

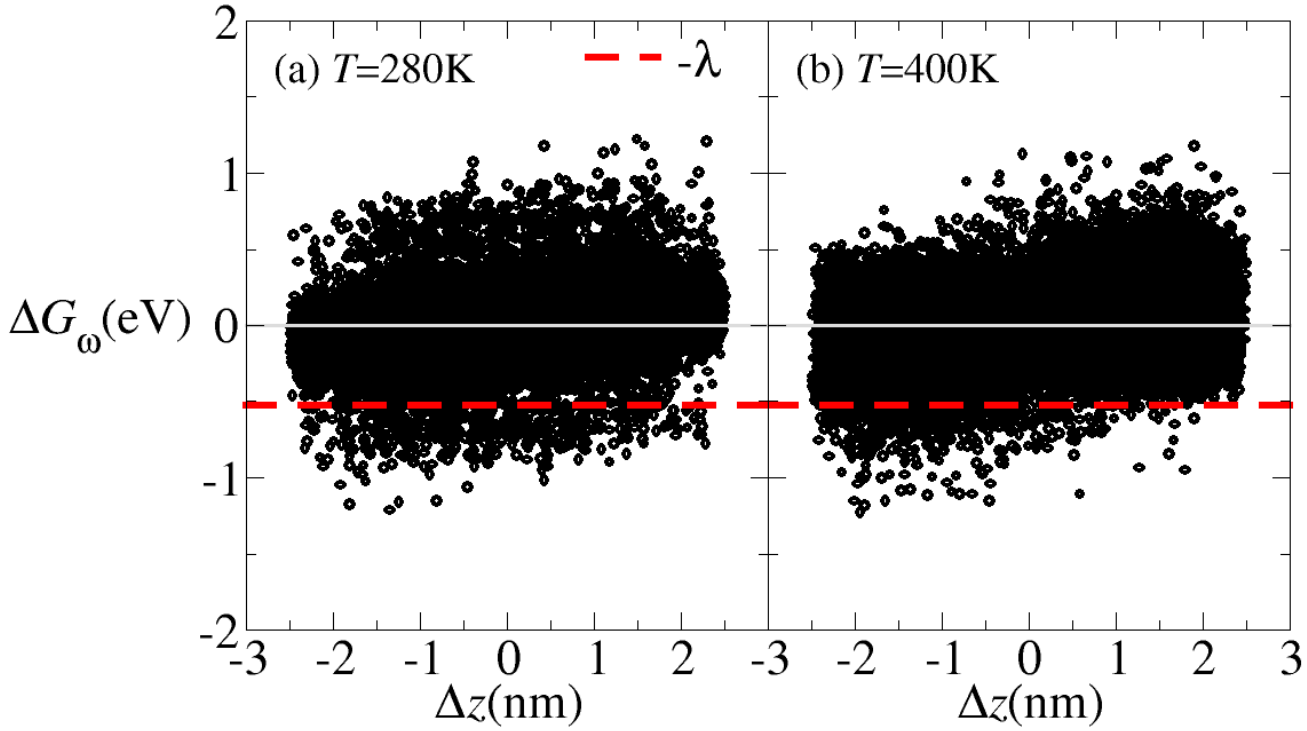

FIG. 1: For each pair of connected sites at an applied bias of 2V we show the change in the z coordinate against the difference in energy for a test charge of magnitude $|e|$. The change in energy with respect to the electric field, and the standard deviation of the site energies are also shown. We can see that the energy landscape is weakly affected by the applied field and that other contributions to the energy dominate.

	$T = 280$K	$T = 400$K
$\mu(\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1})$	1.783×10^{-6}	8.757×10^{-7}
$\mu_z(\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1})$	4.782×10^{-6}	7.938×10^{-7}
N'_e/N_e	1.49×10^{-3}	3.18×10^{-4}
$\tilde{N}_{\mathrm{hops}}/N_{\mathrm{hops}}$	1.54×10^{-4}	5.3×10^{-5}

TABLE I: The precise values of charge transport observables, as defined in the main text, from KMC trajectories at $T_{\mathrm{KMC}} = 300$K under an applied bias of 2V.

increase. We can infer that the most efficient transport properties arise when the applied bias skews the distribution of ΔG_{ij}, relative to a given spatial direction, by an amount that causes the population around $\Delta G_{ij} = -\lambda$ to vary the most.

The difference in the Gibbs free energy between sites is large compared to the effect of the applied field and that the standard deviation in the molecules' HOMO levels. There is a weak asymmetry in ΔG_ω around $\Delta z = 0$ at $T = 280$K, this causes the net electron flow parallel to the z direction although the effect is weak. The asymmetry is also present in the $T = 400$K system, thus this bias is not sufficient to ensure good transport properties.

In the main text we used the measured traffic from KMC trajectories to quantify the degree of rattling motion. The precise values of the qunatities are showin in table I.