

Can we get useful mobility data from MorphCT after
disabling the Gaussian Mapping subroutines?

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December 13, 2017

1 Mobilities

ID	Simulation Name	Density (g cm ⁻³)	Anisotropy (Arb. U.)	Stacks (Arb. U.)	Stack Threshold (Å)	Mobility (cm ² V ⁻¹ s ⁻¹)
1	nomapP3HT_1.5	1.676	0.1166	1	7.7309	1.29×10^{-4}
2	nomapP3HT_1.75	1.061	0.0295	3	4.8596	2.58×10^{-4}
3	nomapP3HT_2.0	0.892	—	—	—	—
4	nomapP3HT_2.25	0.787	0.0049	5	5.0638	4.27×10^{-3}
5	nomapP3HT_2.5	0.685	—	—	—	—
6	origP3HT_T1.5	1.676	0.1282	1	7.3947	1.17×10^1
7	origP3HT_1.75	1.061	0.0197	19	4.4702	3.48×10^{-1}
8	origP3HT_2.0	0.892	0.0085	1	5.0683	4.46×10^{-1}
9	origP3HT_2.25	0.787	0.0114	5	4.7747	5.52×10^{-1}
10	origP3HT_2.5	0.685	0.0188	25	4.8465	4.03×10^{-1}

Table 1: The results from MorphCT for the usual P3HT morphologies, with Voronoi neighbours. Runs **1-5** are the previous Voronoi systems (where the systems were run for 1E5 timesteps during the final fine-graining phase), whereas runs **6-10** have been equilibrated for 1E7 timesteps during the final fine-graining phase.

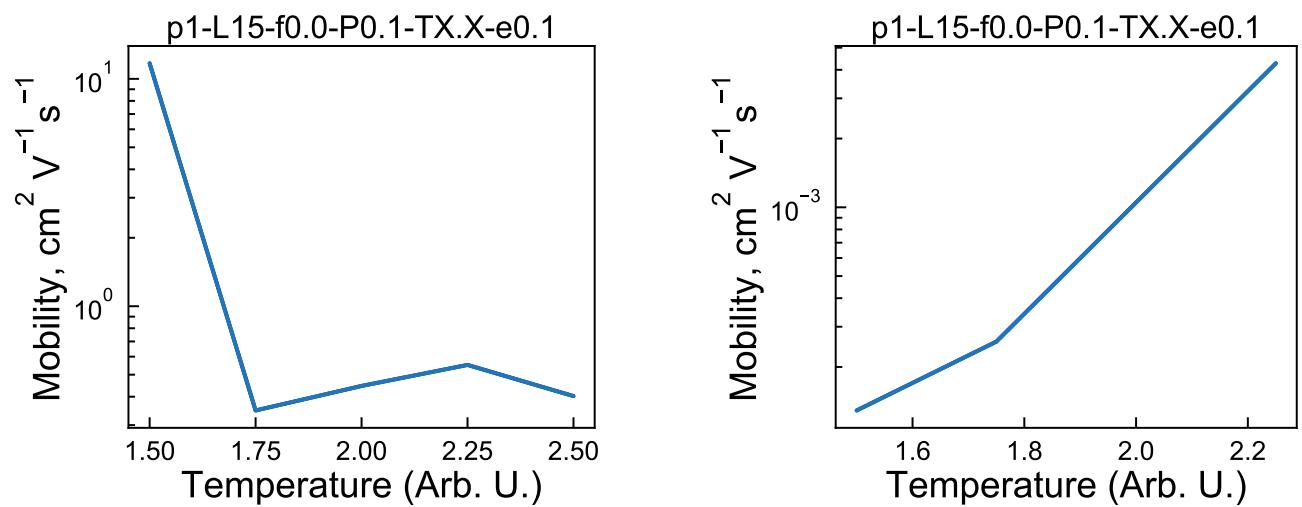


Figure 1: The evolution of the mobility of the p1-L15-f0.0-P0.1-TX.X-e0.5 systems. Left: Original P3HT mobility curve. Right: P3HT mobility curve when the Gaussian mapping is not performed.

2 Discussion

As expected, a system with a broader density of states will exhibit a lower mobility than one with a less-broad DoS. What is not expected is that it seems that the ordered morphology $T = 1.5$ has a broader density of states than the disordered $T = 1.75$ and $T = 2.25$ systems. As such, the mobility trend is reversed with the ordered system exhibiting a mobility half that of the lowest-temperature disordered system and an order of magnitude lower than the $T = 2.25$ system. I will wait for the results from the $T = 2.0$ and $T = 2.5$ systems to come back before I dig any further here.

P3HT-T1.5-noMap

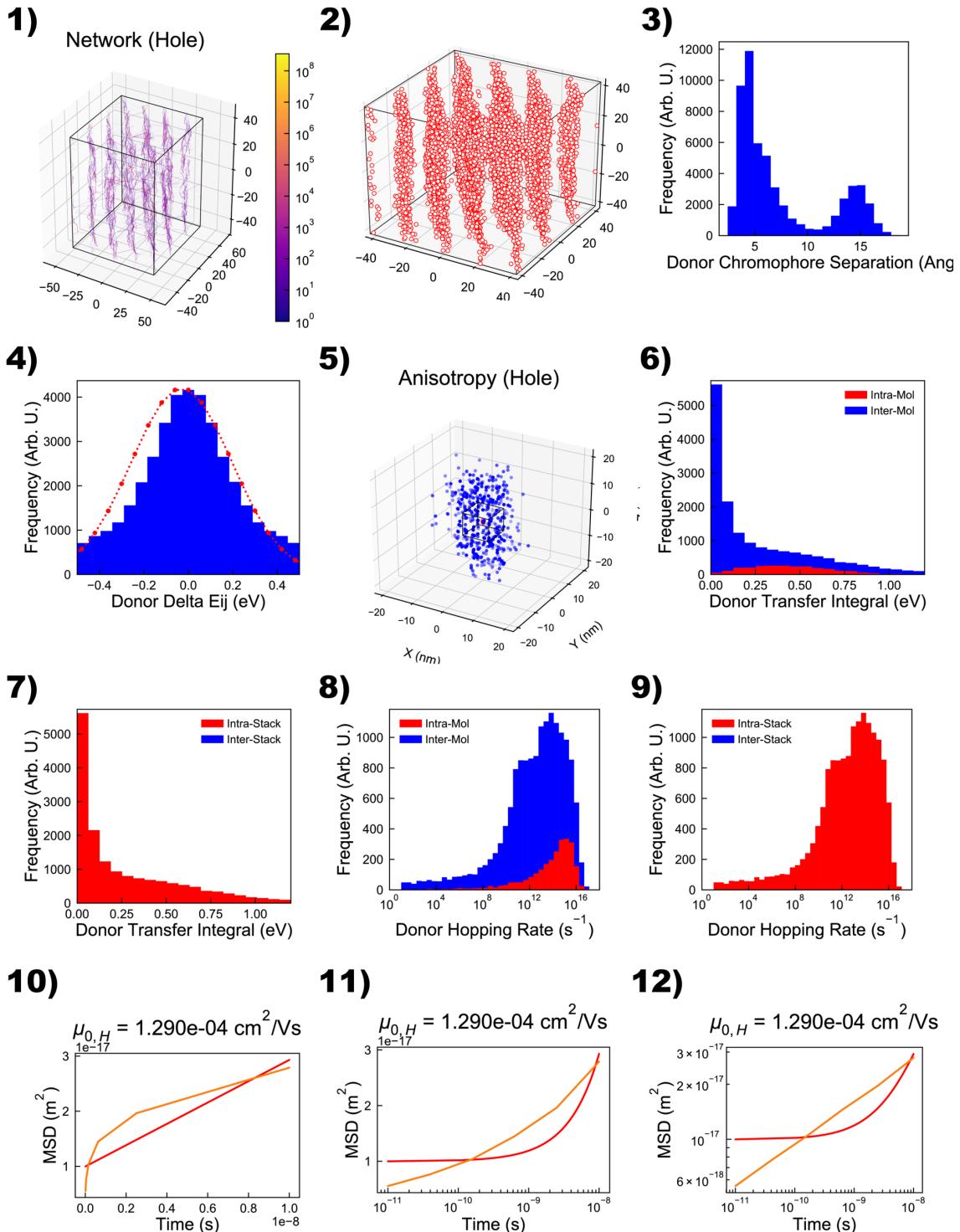


Figure 2: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 7) Histogram of stack transfer integrals, 8) Histogram of molecular hopping rates, 9) Histogram of stack hopping rates, 10) Linear MSD plot, 11) Semi-log-x MSD plot, 12) Logarithmic MSD plot.

P3HT-T1.75-noMap

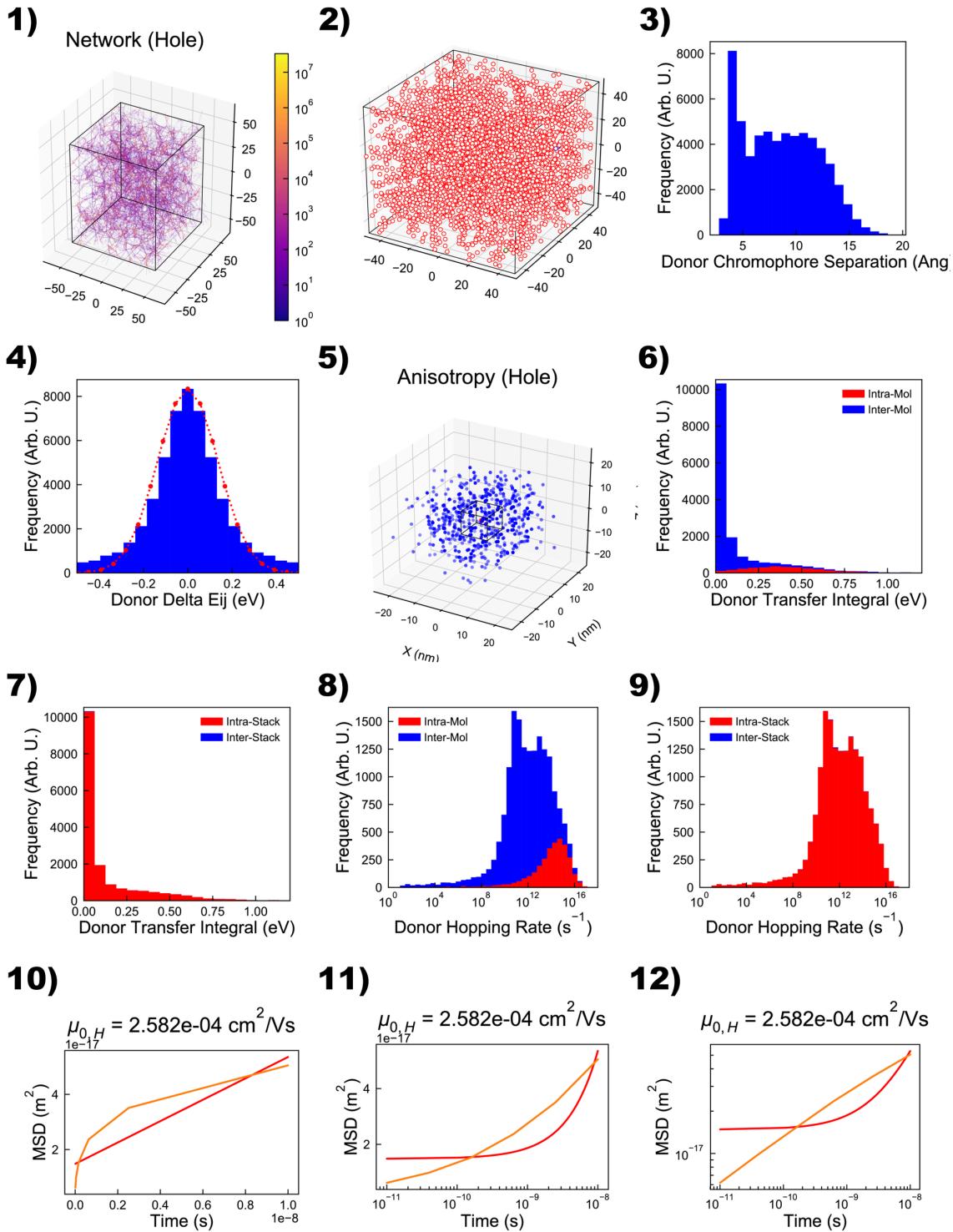


Figure 3: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 7) Histogram of stack transfer integrals, 8) Histogram of molecular hopping rates, 9) Histogram of stack hopping rates, 10) Linear MSD plot, 11) Semi-log-x MSD plot, 12) Logarithmic MSD plot.

P3HT-T2.25-noMap

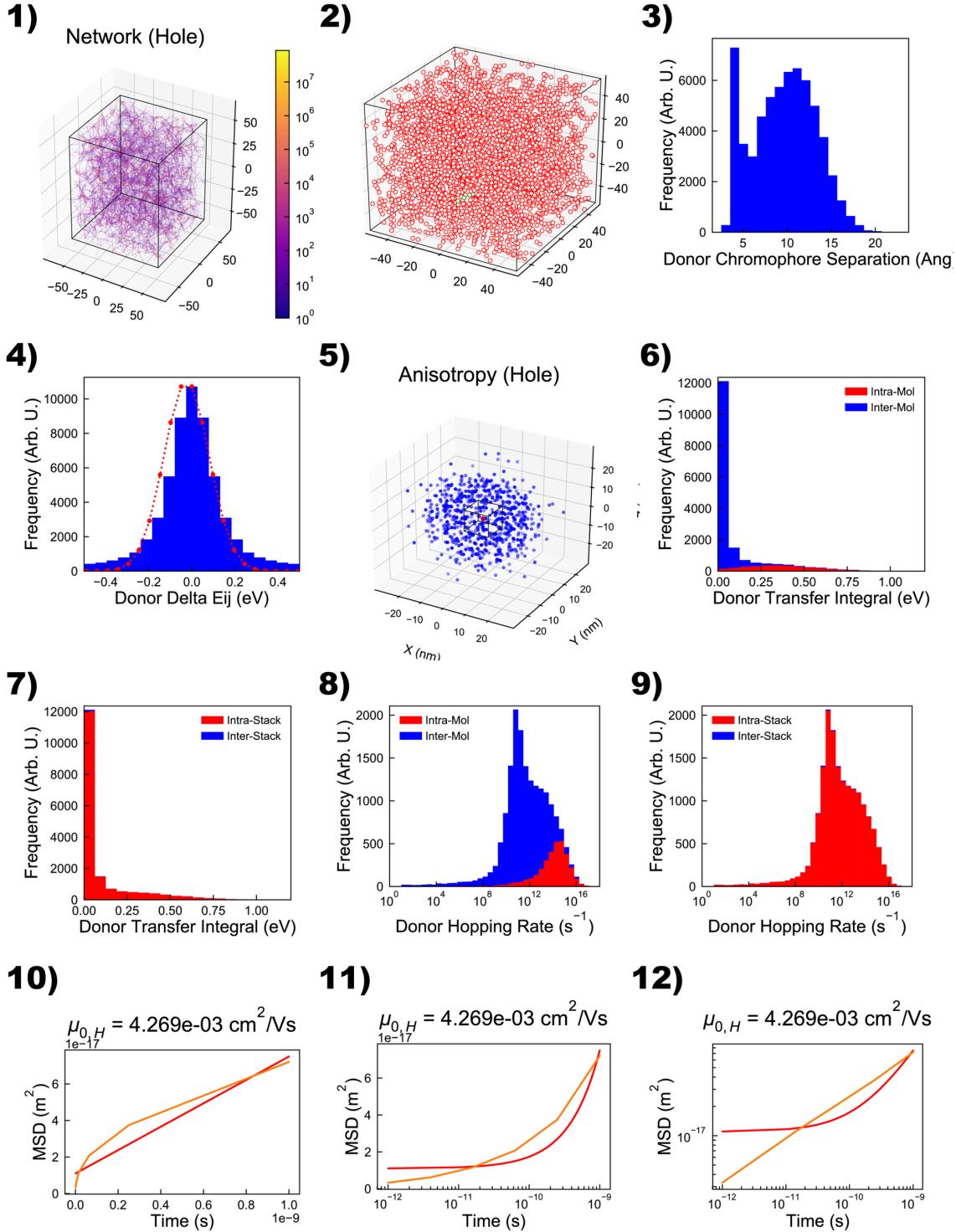


Figure 4: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 7) Histogram of stack transfer integrals, 8) Histogram of molecular hopping rates, 9) Histogram of stack hopping rates, 10) Linear MSD plot, 11) Semi-log-x MSD plot, 12) Logarithmic MSD plot.