

MorphCT - 1K P3HT 15mers

Matthew Jones

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1 Simulations

The simulations for the systems containing 1,000 15mers of P3HT have completed. There are 4 systems. Those labelled ‘ordered’, ‘disordered’, and ‘semicrystalline’ have been assigned based on the visual order/disorder of the system - no quantification of the level of order has been performed, so these names are subject to change as more data is obtained. The final system contains a blend of p3ht-pcbm. For now, only the hole transport properties are of interest and so reported in this document.

NOTE: The recent improvements in the functionality of MorphCT (namely, Koopmans’ approximation, VRH and simple energy penalties for hopping) were developed after these systems were submitted and so have not been included here. Any combination of these additional mechanisms could dramatically change the resultant mobilities in any number of ways.

2 Observations

- The number of stacks is a good metric for (at least visual) crystalline order
- Intercalating PCBM increases the number of stacks (as expected)

3 Mobility Results

Simulation Name	Density (g cm ⁻³)	Anisotropy (Arb. U.)	Stacks (Arb. U.)	Stack Threshold (Å)	Hole Mobility (cm ² V ⁻¹ s ⁻¹)
large_p3ht_ordered	—	0.1375	12	4.00	2.99×10^0
large_p3ht_semicrystalline	—	0.0175	24	4.00	4.29×10^{-1}
large_p3ht_disordered	—	0.0007	38	4.00	3.02×10^0
large_p3ht_pcbm	—	0.0775	43	4.00	1.47×10^0

Table 1: The results from MorphCT.

large_p3ht_ordered

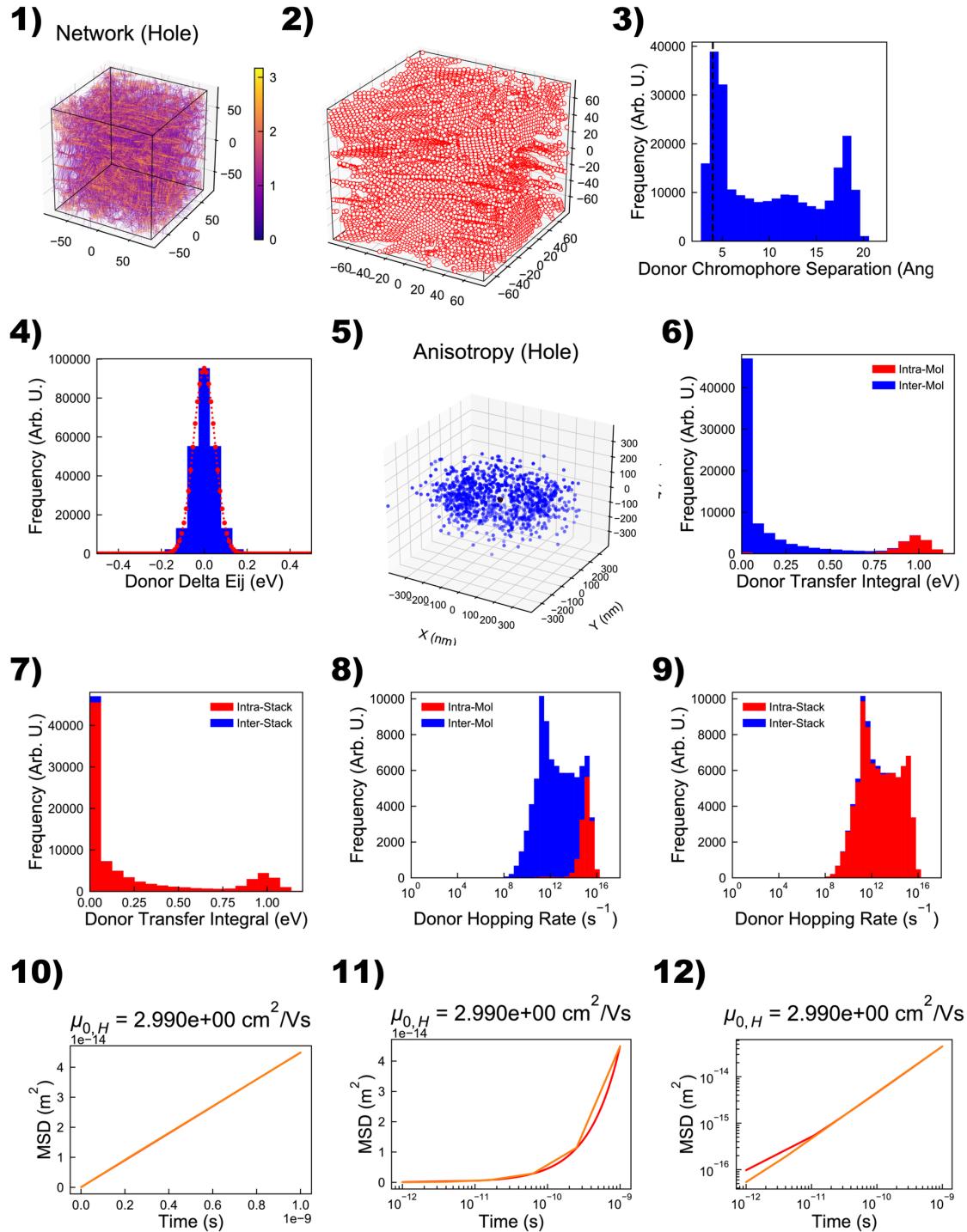


Figure 1: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

large_p3ht_semicrystalline

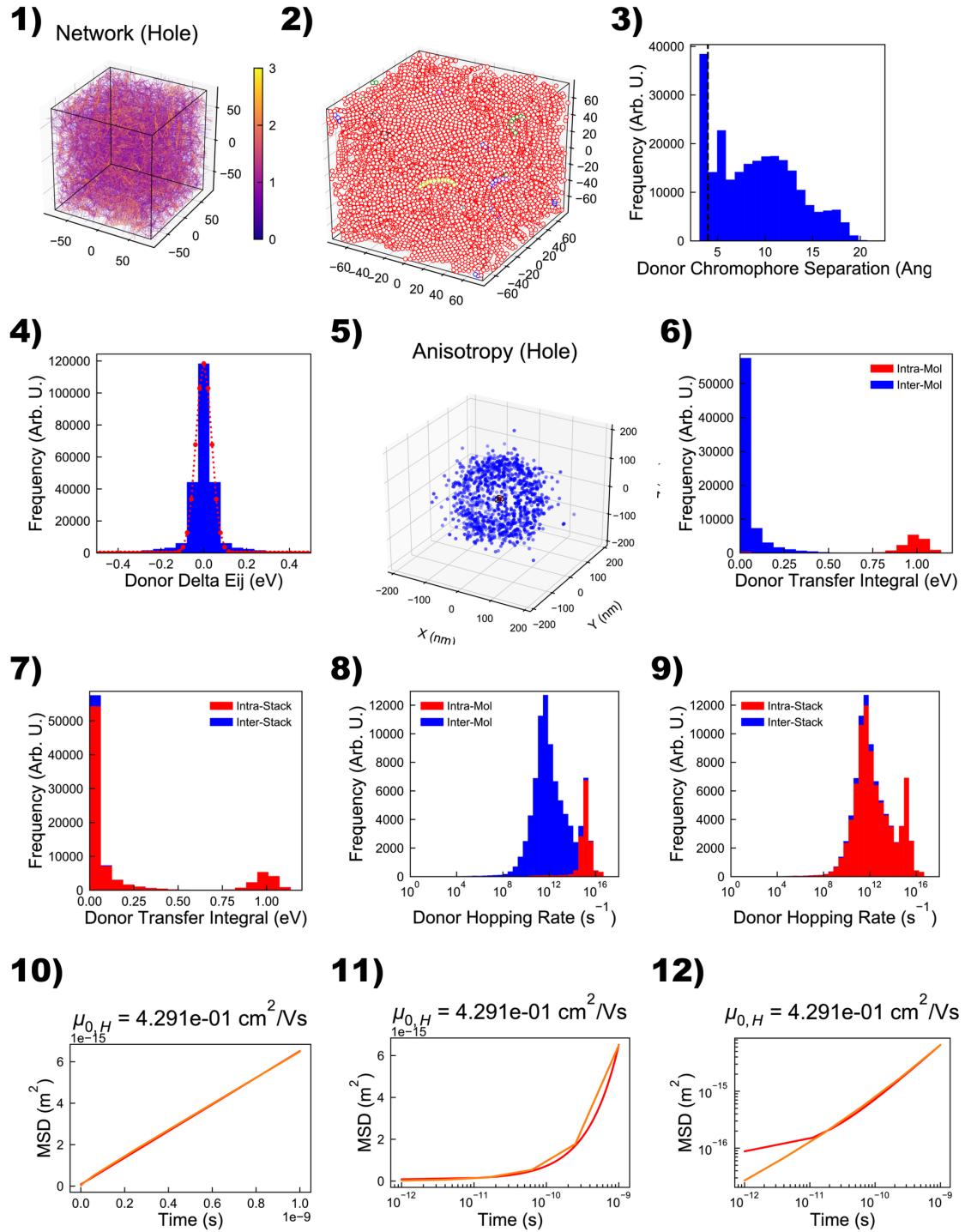


Figure 2: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

large_p3ht_disordered

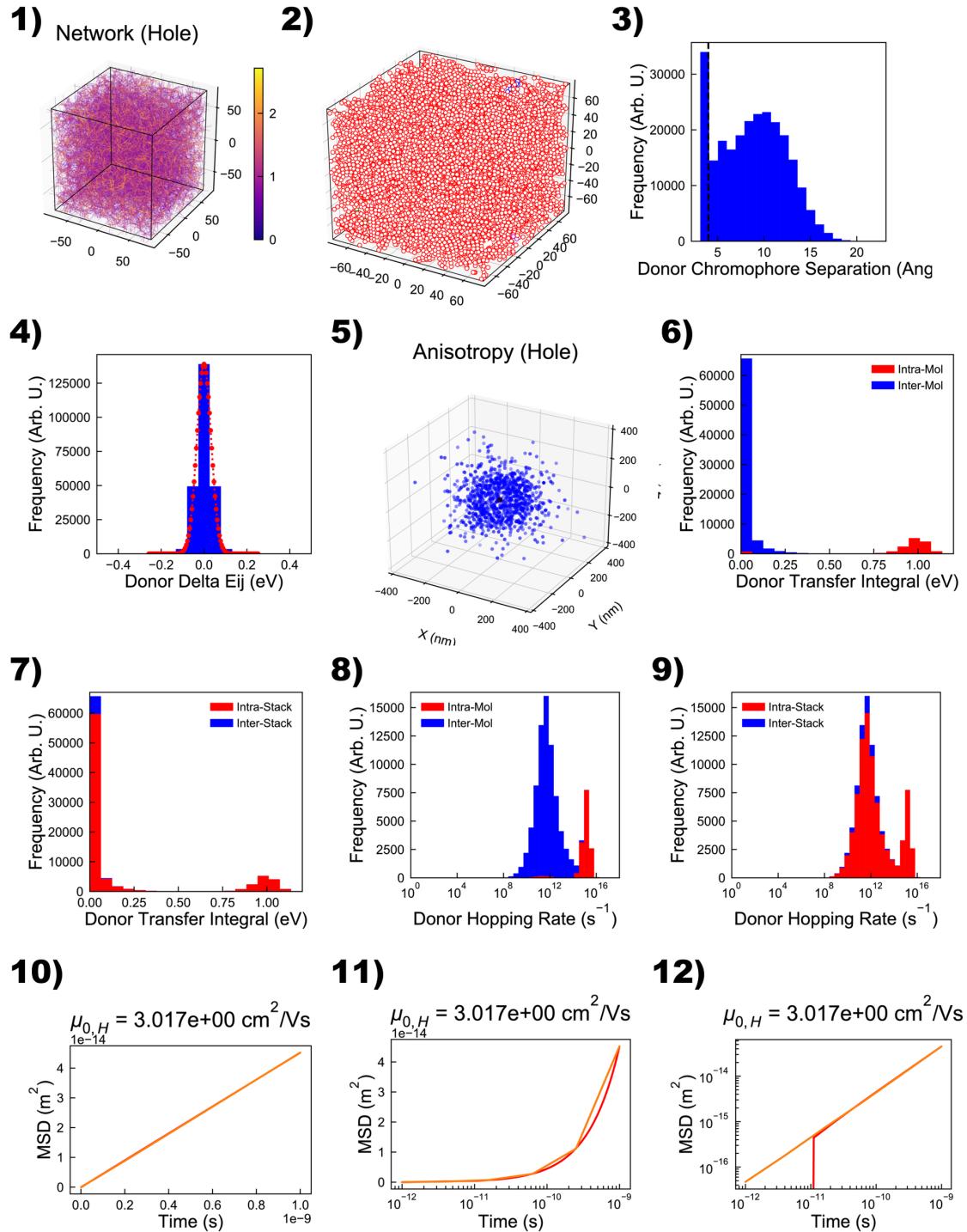


Figure 3: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

large_p3ht_pcBM

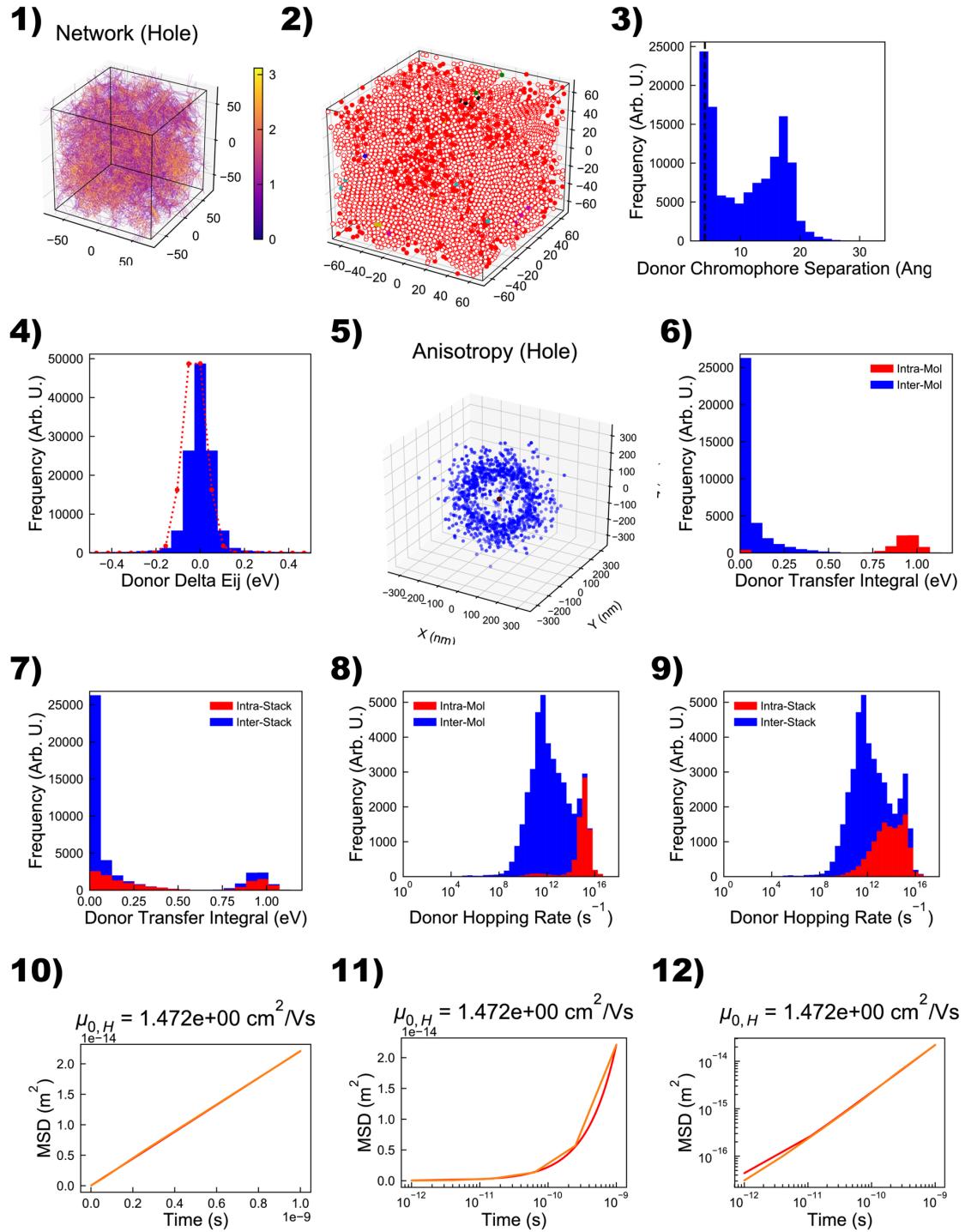


Figure 4: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.