

MorphCT Results - PAHs

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1 Latest Jobs, 12/17

The latest flurry of jobs involve a complete rerunning of the 7 PAH jobs we particularly care about. In the past, we ran into issues comparing the results because some of the systems contained rigid molecules, which automatically have $\Delta E_{ij} = 0$. Since the Marcus hopping rate equation:

$$k_{ij} = \frac{2\pi}{\hbar} T_{ij}^2 \sqrt{\frac{1}{4\lambda_{ij}\pi k_B T}} \exp -\frac{(\Delta E_{ij} + \lambda_{ij})^2}{4\lambda_{ij} k_B T}, \quad (1)$$

decays exponentially for $\Delta E_{ij} > -\lambda_{ij}$, this suppresses the hopping rate, resulting in lower mobilities (not larger as I said). Either way, we were comparing apples to oranges and at the very least we needed to make everything flexible to make it as realistic as possible.

As an ‘extension task’, we added charges in too, to improve model accuracy. The PE charges were taken from Mitch’s previous work, and the PT charges were calculated from quantum-chemical methods using NWChem. Stacks are assigned automatically using a dynamic distance cut-off between the first maximum and first minimum of the chromophore separation histogram. Periodic boundaries are considered when assigning chromophores to each stack.

How confident are we in the PE charges?

2 Mobility Results

ID	Simulation Name	Density (g cm ⁻³)	Anisotropy (Arb. U.)	Stacks (Arb. U.)	Stack Threshold (Å)	Mobility (cm ² V ⁻¹ s ⁻¹)
1	PE_MultiStack_Eclipsed	1.06	0.0594	1	8.35	8.81×10^0
2	PE_SingleStack_Eclipsed	1.06	0.0893	3	7.36	8.84×10^0
3	PE_SingleStack_Ordered	1.06	0.0471	195	4.51	8.95×10^0
4	PT_MultiStack_Eclipsed	1.01	0.1704	20	6.17	1.92×10^0
5	PT_MultiStack_Ordered	1.01	0.0906	63	4.96	1.27×10^0
6	PT_SingleStack_Eclipsed	1.01	0.0979	4	4.90	5.19×10^0
7	PT_SingleStack_Ordered	1.01	0.0267	63	5.07	1.55×10^0

Table 1: The results from MorphCT for the various PAH morphologies. See the below section for a discussion of the stacks.

TODO: Check the Stack definitions, some of the numbers seem off, especially for the ordered morphologies

dyFix_imageFix_relaxed_PE_MultiStack_Eclipsed_UA

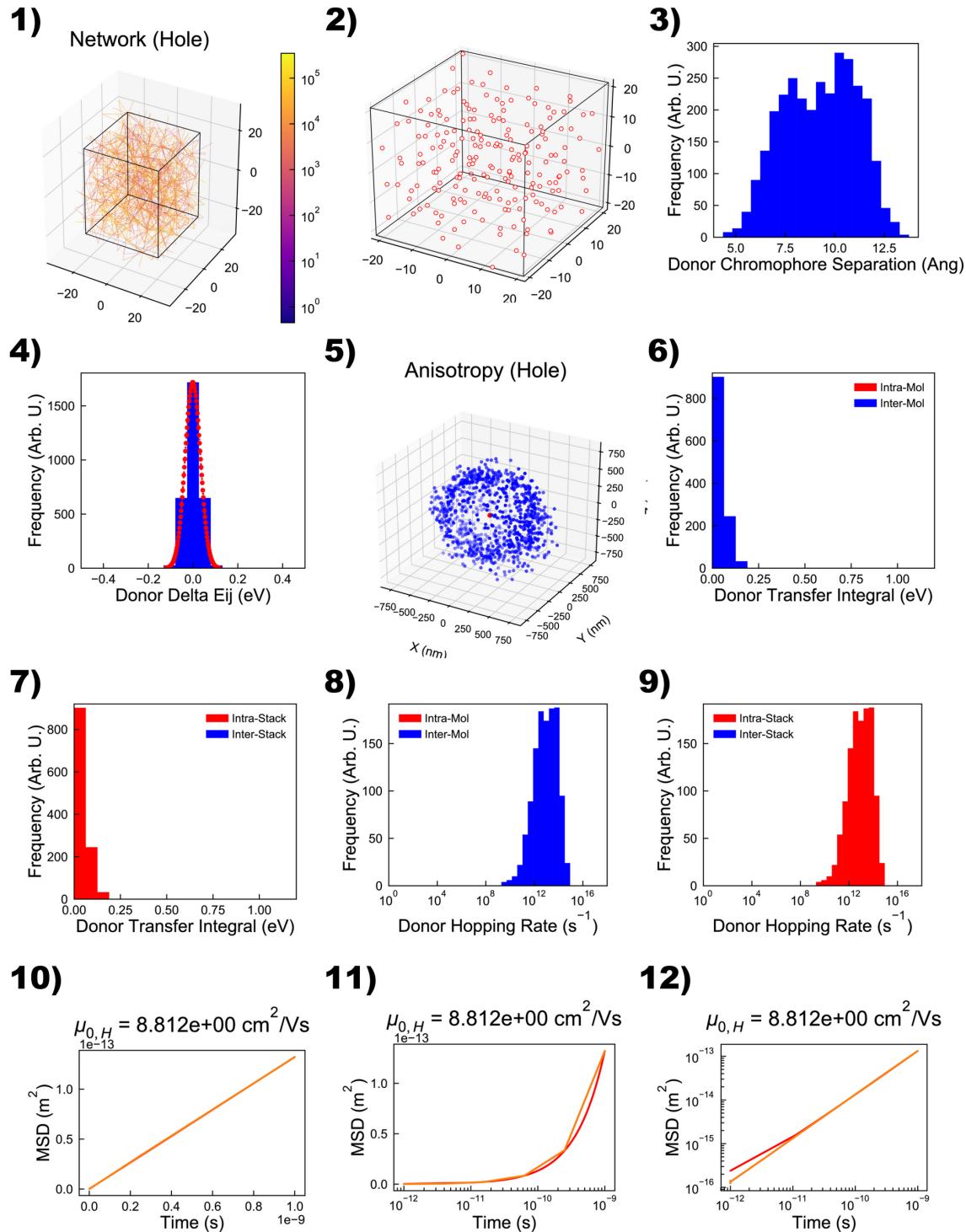


Figure 1: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

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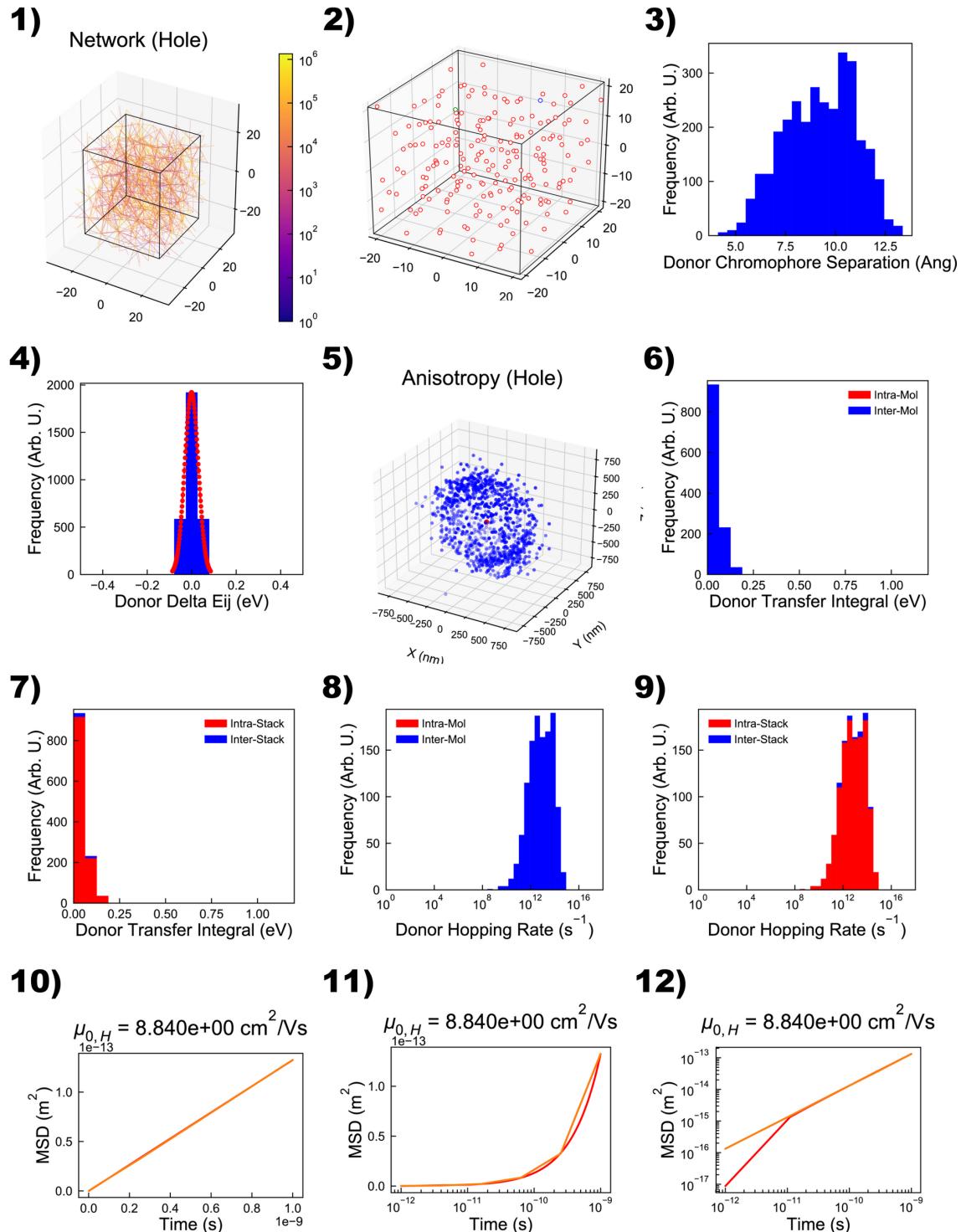


Figure 2: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

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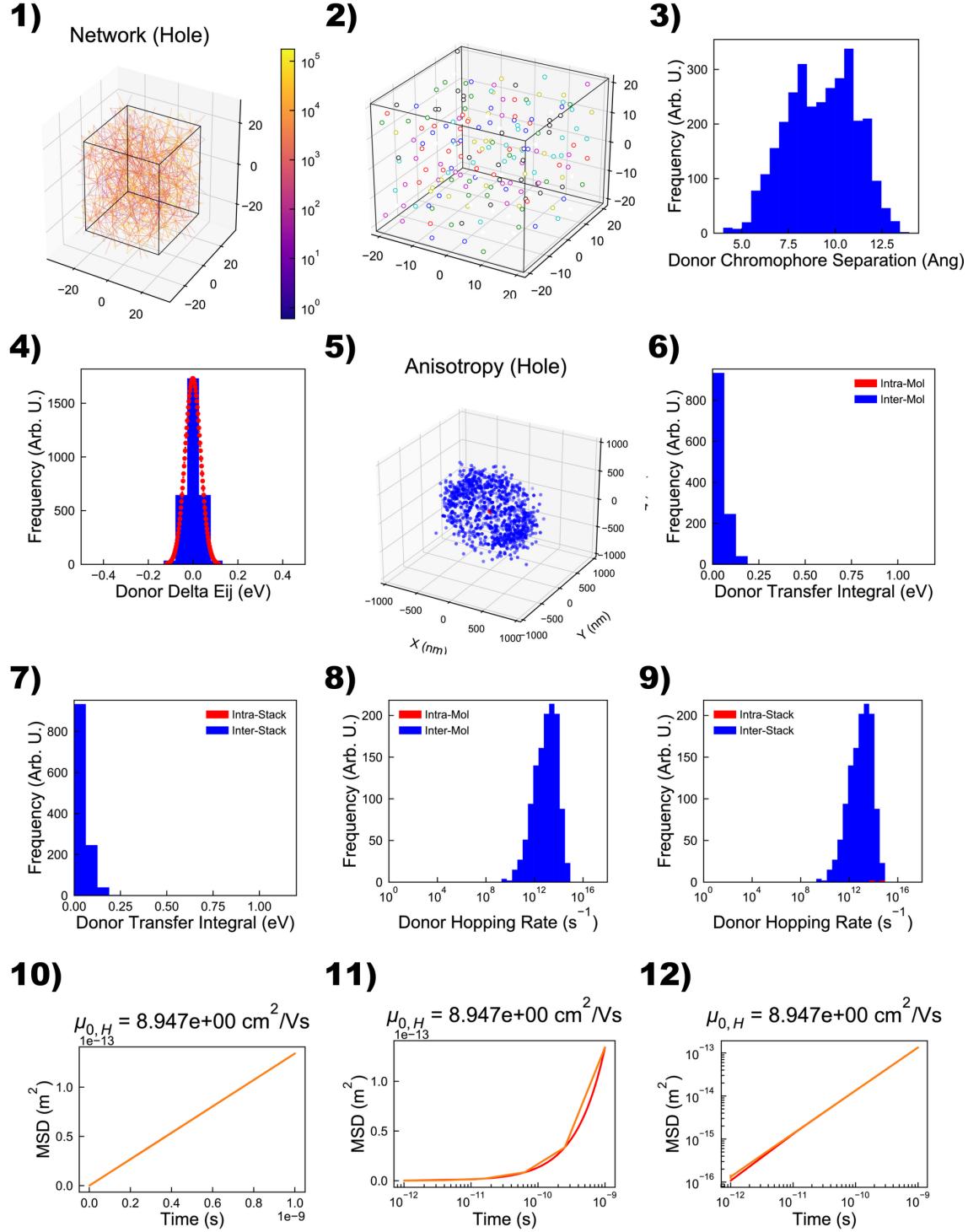


Figure 3: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

dyFix_imageFix_relaxed_PT_MultiStack_Eclipsed_UA

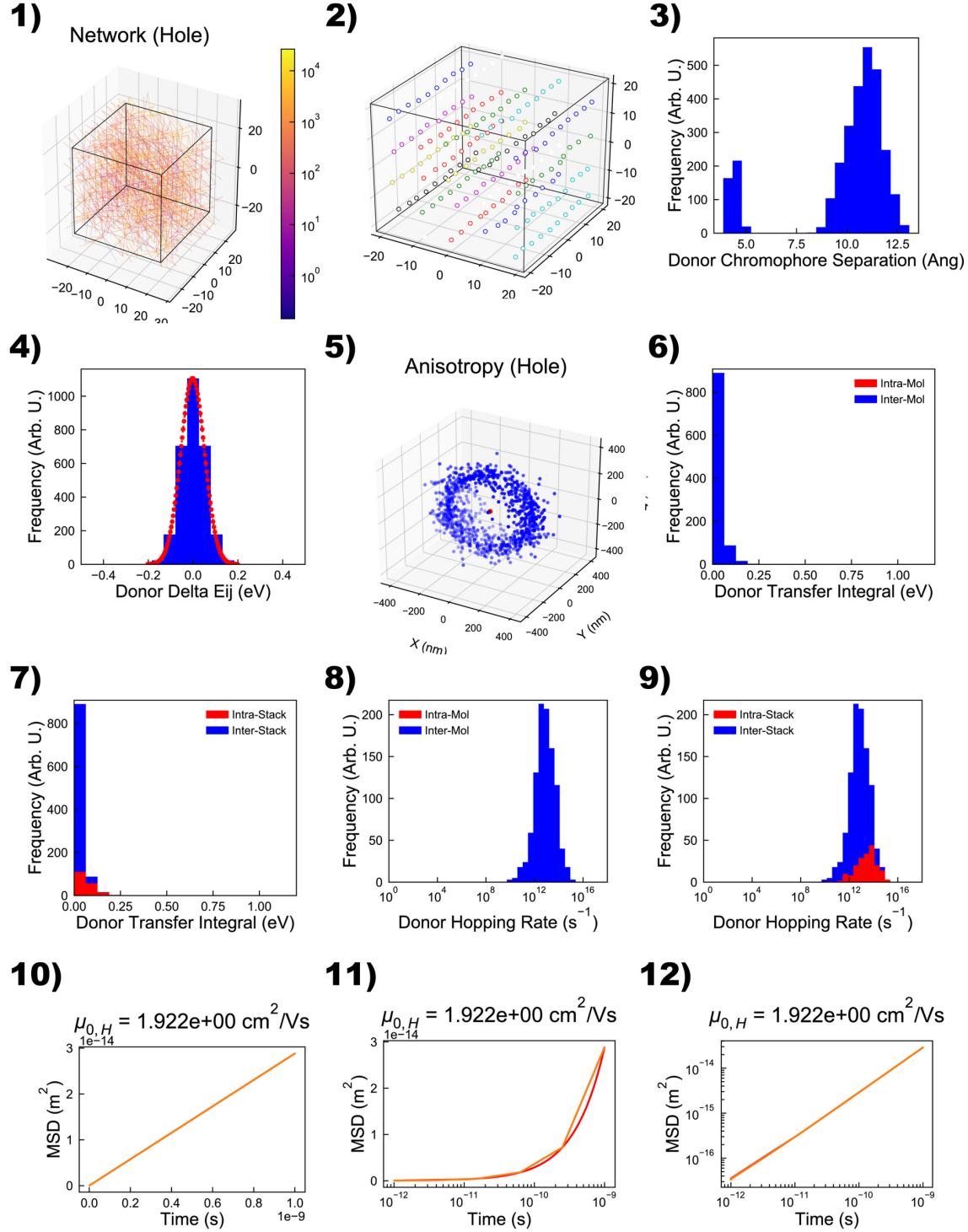


Figure 4: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 6) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer 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.

dyFix_imageFix_relaxed_PT_MultiStack_Ordered_UA

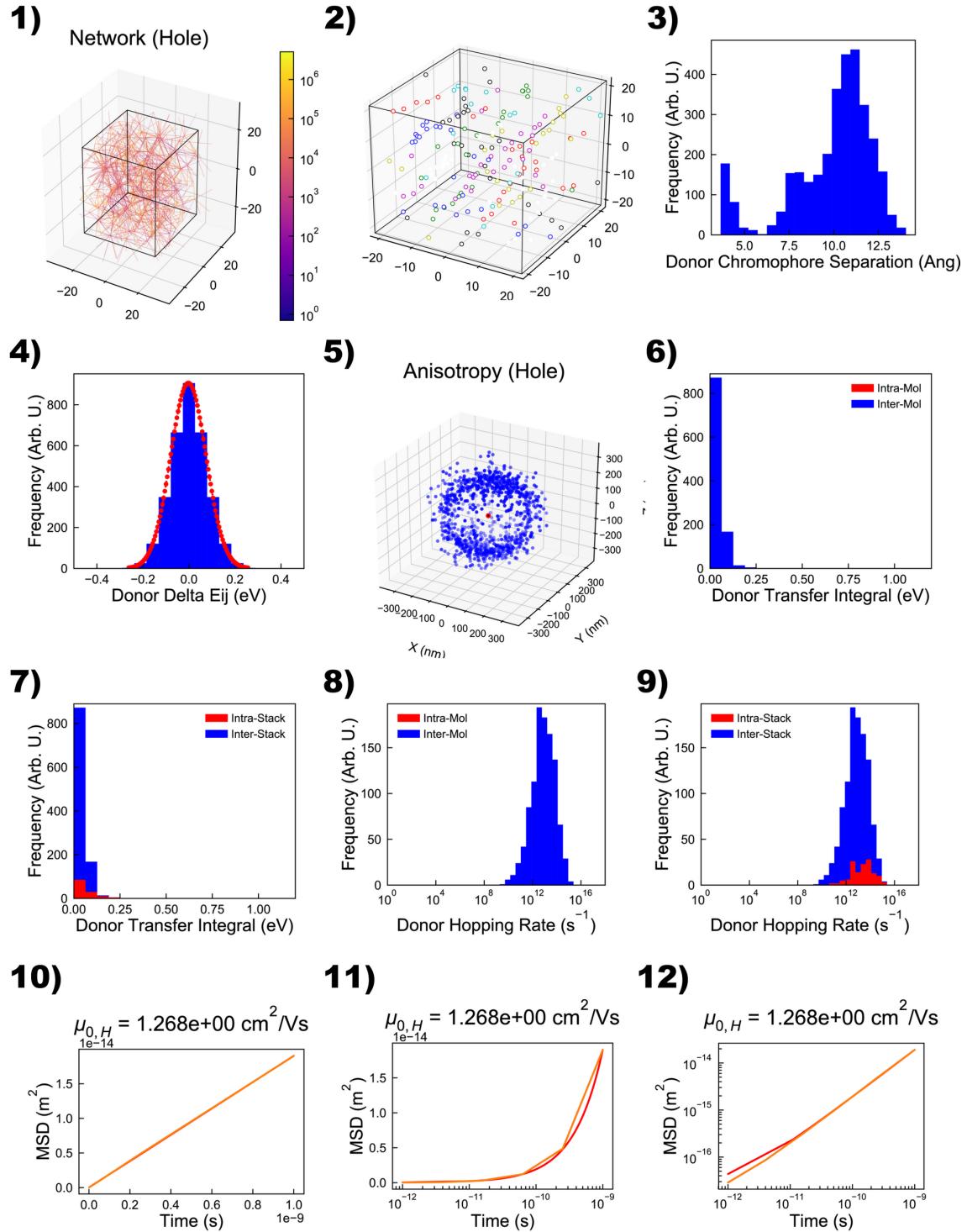


Figure 5: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (δE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

lyFix_imageFix_relaxed_PT_SingleStack_Eclipsed_UA

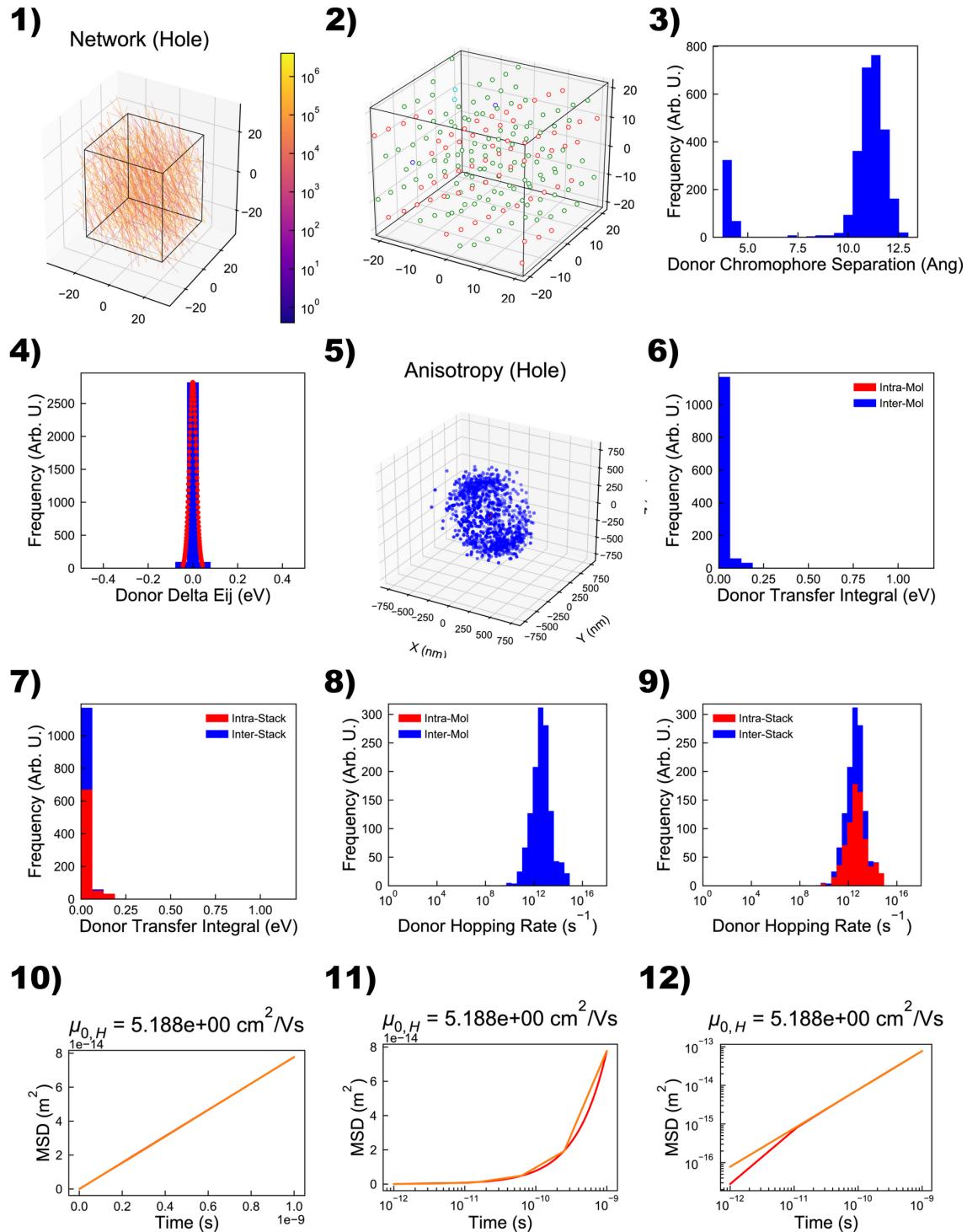


Figure 6: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

lyFix_imageFix_relaxed_PT_SingleStack_Ordered_UA

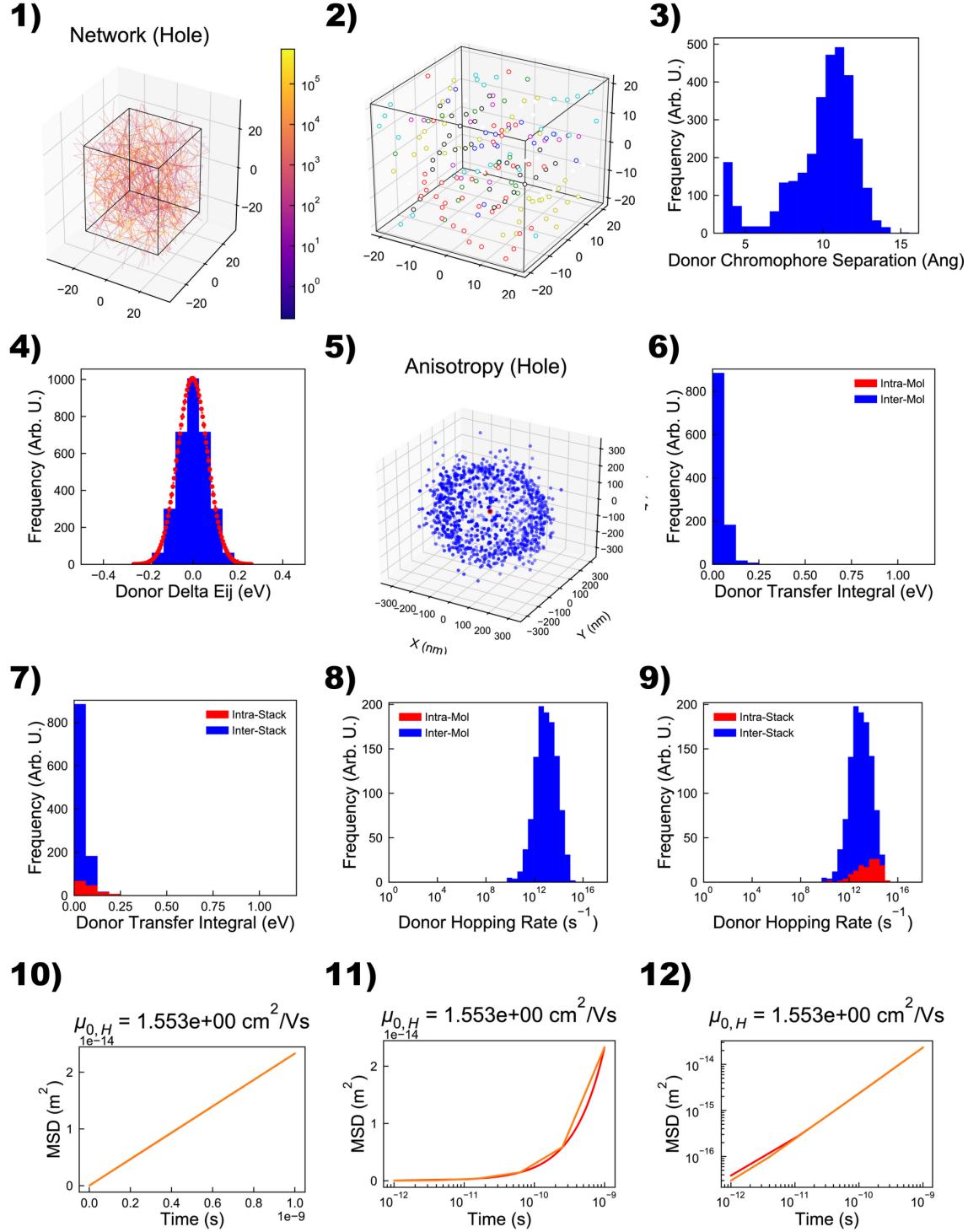


Figure 7: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.