

MorphCT Results - PAHs

Matthew Jones

January 22, 2018

1 Latest Jobs, 01/18

The latest flurry of jobs involve a complete rerunning of the 7 PAH jobs we particularly care about. This time, instead of comparing rigid to flexible and using the old values for the perylene charges that we found in the literature, we have made all of the molecules flexible for better comparisons. Additionally, we have used NWChem running on R2 to determine the partial charges for atoms in both perylene and perylothiophene. The charges for each molecule are shown in figure 1.

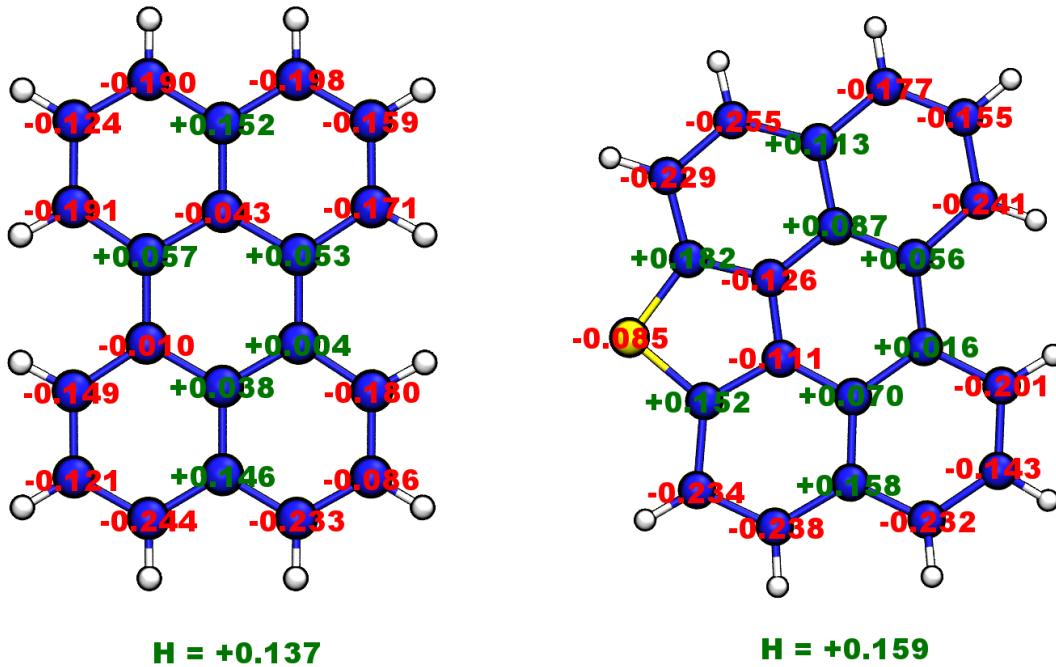


Figure 1: The charges used for the equilibration MD simulations to add charges and molecule flexibility to the previous morphologies

We also explore the affect of variable-range hopping on our systems, by applying a VRH prefactor of the form $k_{ij} \propto \exp\left(-\frac{r_{ij}}{4\text{\AA}}\right)$, which supresses hops over the long-axis of the molecules and stimulates hopping along the π -stacking direction. The VRH decay factor (which is usually associated with the delocalisation length) of $1/4\text{\AA}$ was selected as it corresponds to the π -stacking distance, as well as the approximate chromophore size for P3HT, which we know to work well in the MorphCT pipeline.

2 Mobility Results

Simulation Name	Density (g cm ⁻³)	Anisotropy (Arb. U.)	Stacks (Arb. U.)	Stack Threshold (Å)	Mobility (cm ² V ⁻¹ s ⁻¹)
PE_MultiStack_Eclipsed	1.06	0.5033	20	5.06	7.70×10^0
PE_SingleStack_Eclipsed	1.06	0.1949	71	4.82	7.20×10^{-1}
PE_SingleStack_Ordered	1.06	0.0126	69	4.65	1.64×10^{-1}
PT_MultiStack_Eclipsed	1.01	0.0954	21	5.31	5.54×10^0
PT_MultiStack_Ordered	1.01	0.0058	75	4.83	7.58×10^0
PT_SingleStack_Eclipsed	1.01	0.1018	2	5.14	5.16×10^0
PT_SingleStack_Ordered	1.01	0.0547	6	5.18	5.47×10^0
VRH_PE_MultiStack_Eclipsed	1.06	0.3877	20	5.06	5.33×10^{-1}
VRH_PE_SingleStack_Eclipsed	1.06	0.0935	71	4.82	6.21×10^{-2}
VRH_PE_SingleStack_Ordered	1.06	0.0027	69	4.65	1.33×10^{-2}
VRH_PT_MultiStack_Eclipsed	1.01	0.0861	21	5.31	5.72×10^{-1}
VRH_PT_MultiStack_Ordered	1.01	0.0039	75	4.83	8.35×10^{-1}
VRH_PT_SingleStack_Eclipsed	1.01	0.0344	2	5.14	4.84×10^{-1}
VRH_PT_SingleStack_Ordered	1.01	0.1455	6	5.18	5.47×10^{-1}

Table 1: The results from MorphCT for the various flexible, charged PAH morphologies with variable ranged hopping (VRH) corrections on or off.

3 Analysis Figures with VRH off

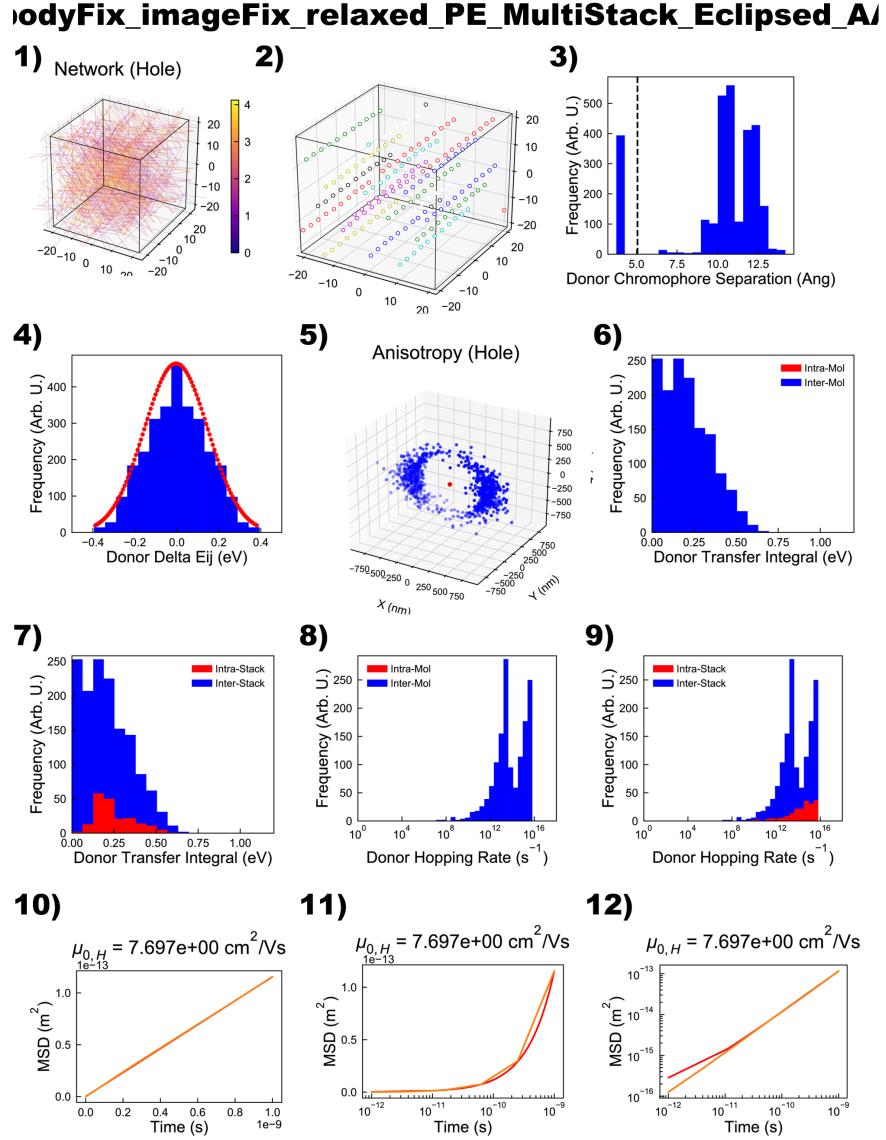


Figure 2: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

bodyFix_imageFix_relaxed_PE_SingleStack_Eclipsed_A

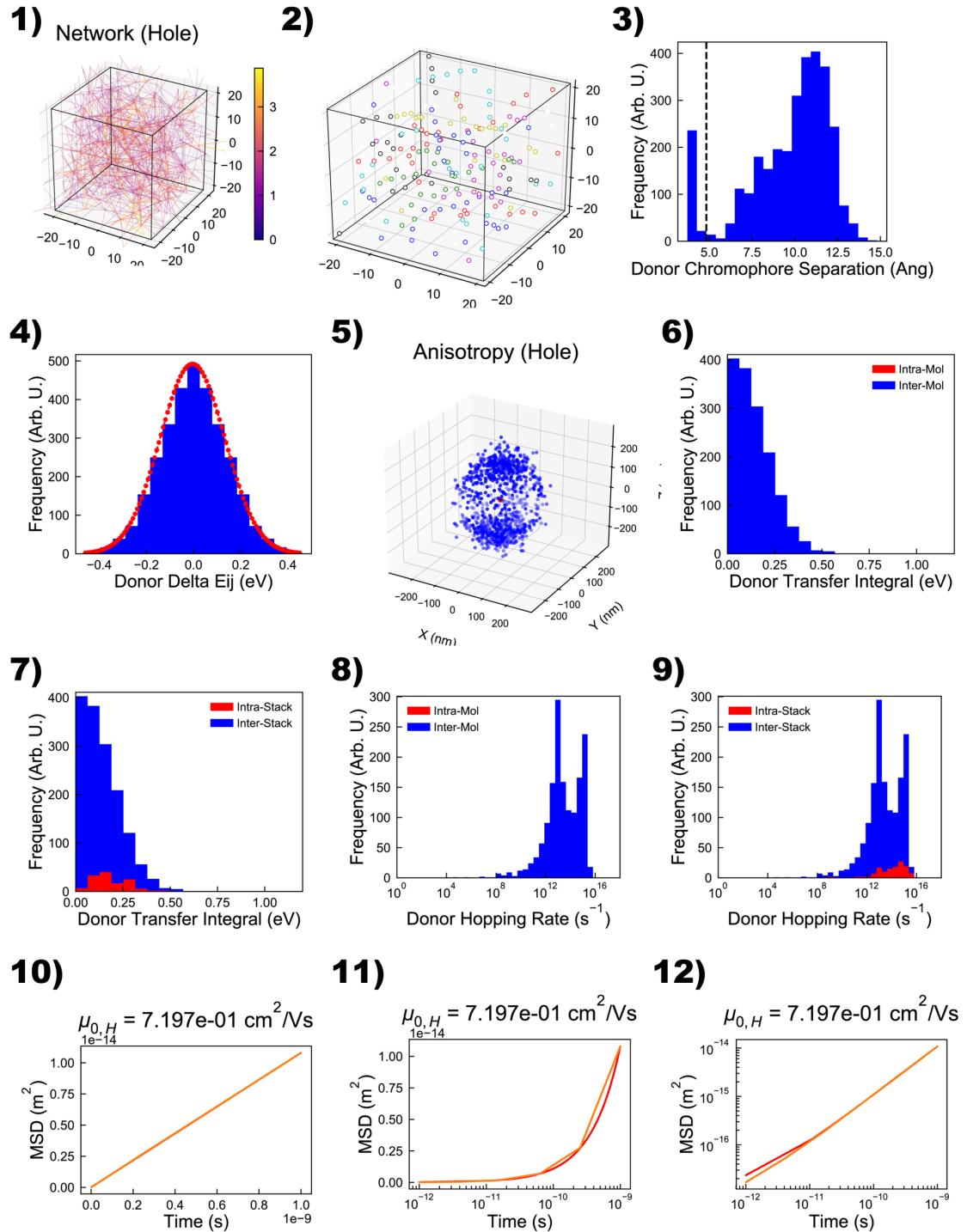


Figure 3: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

odyFix_imageFix_relaxed_PE_SingleStack_Ordered_A

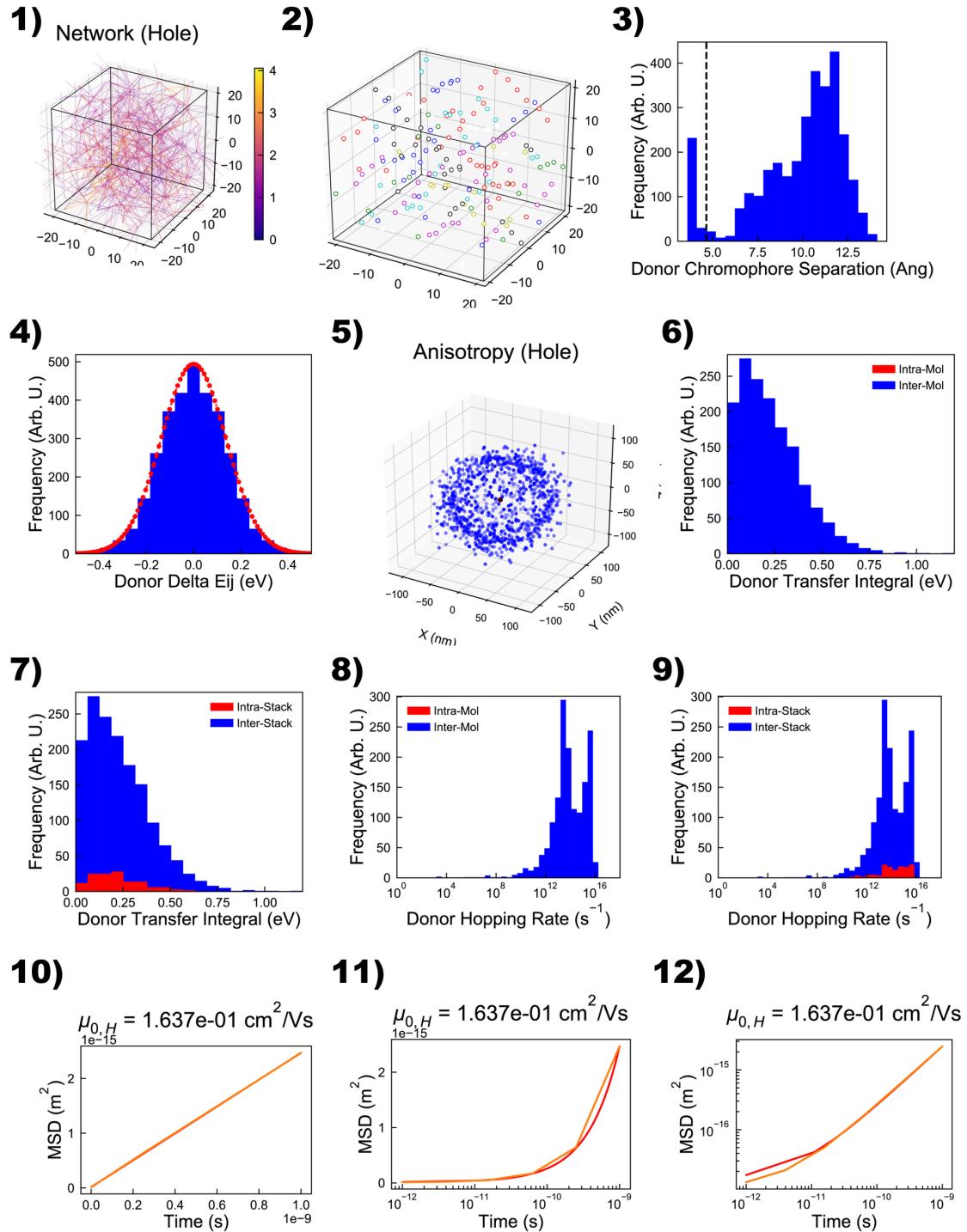


Figure 4: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

bodyFix_imageFix_relaxed_PT_MultiStack_Eclipsed_AJ

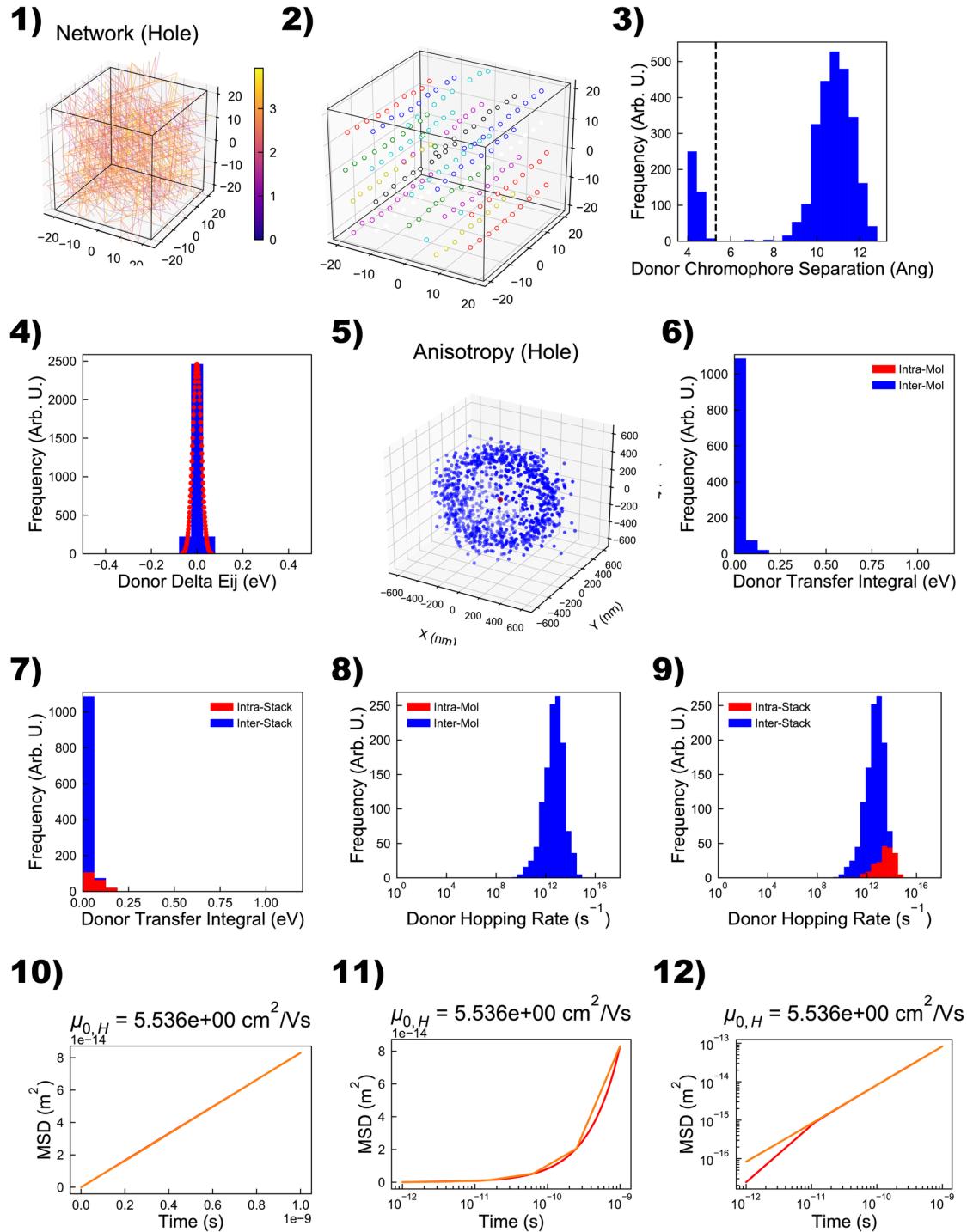


Figure 5: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

bodyFix_imageFix_relaxed_PT_MultiStack_Ordered_AA

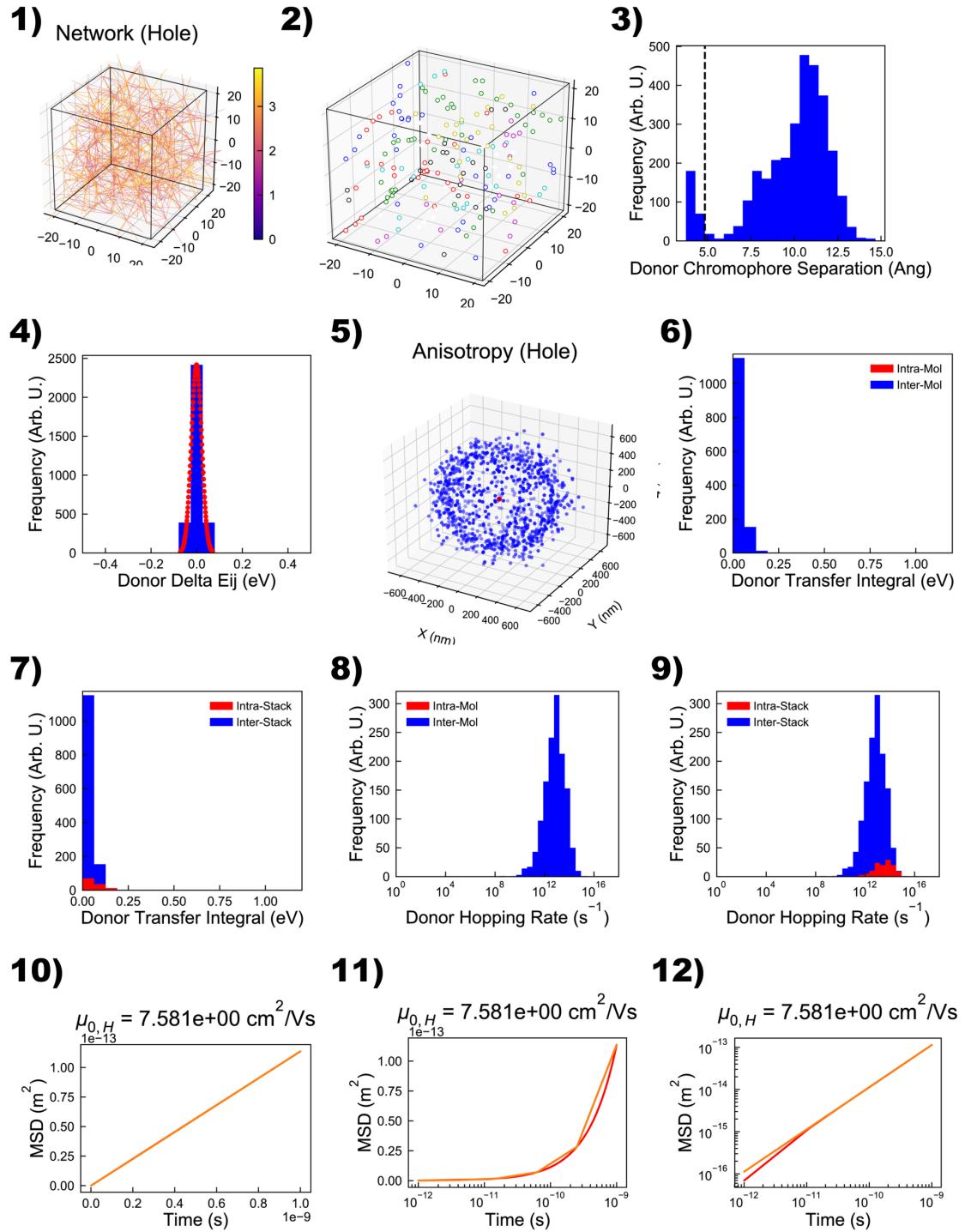


Figure 6: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

bodyFix_imageFix_relaxed_PT_SingleStack_Eclipsed_A

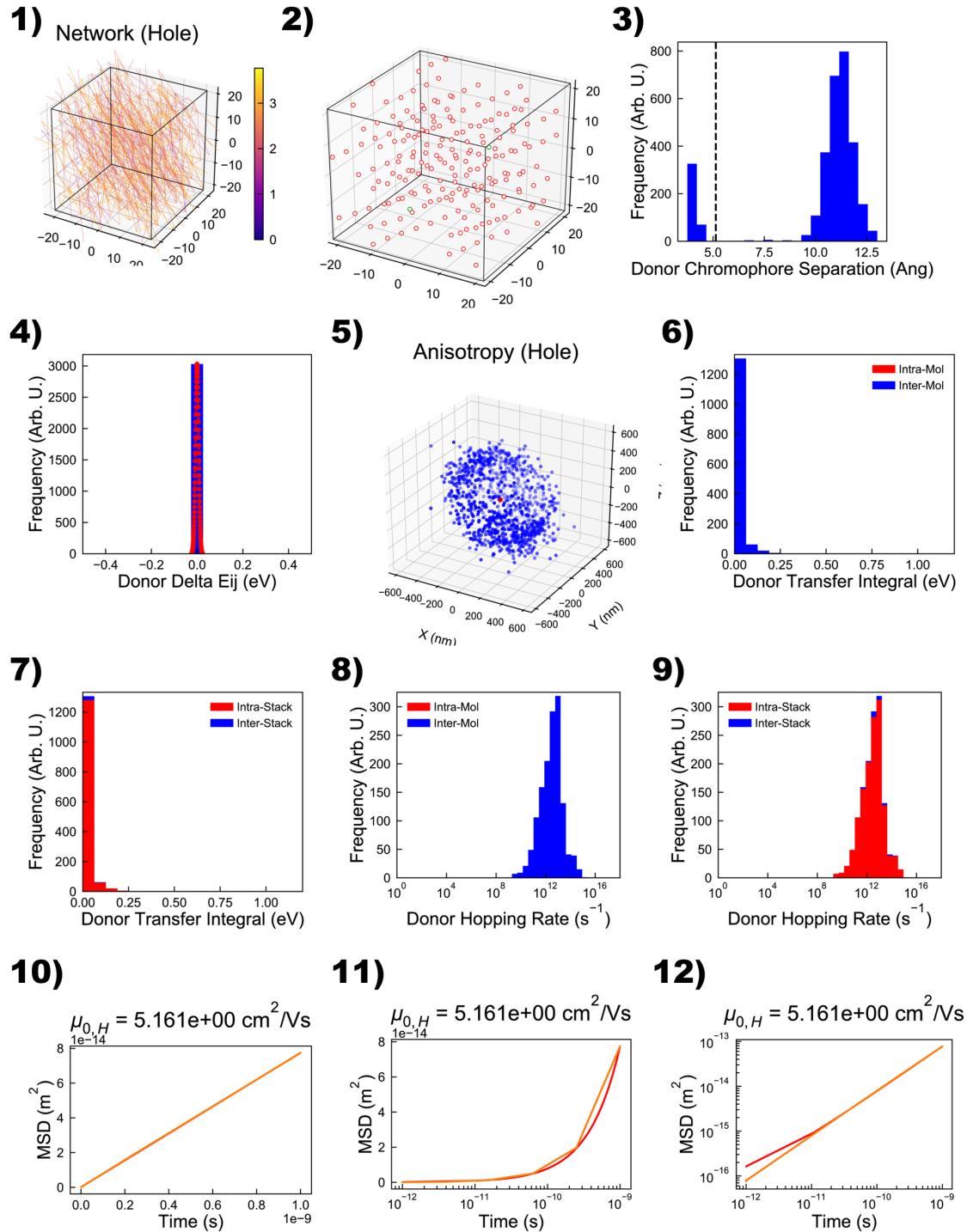


Figure 7: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals,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

odyFix_imageFix_relaxed_PT_SingleStack_Ordered_A

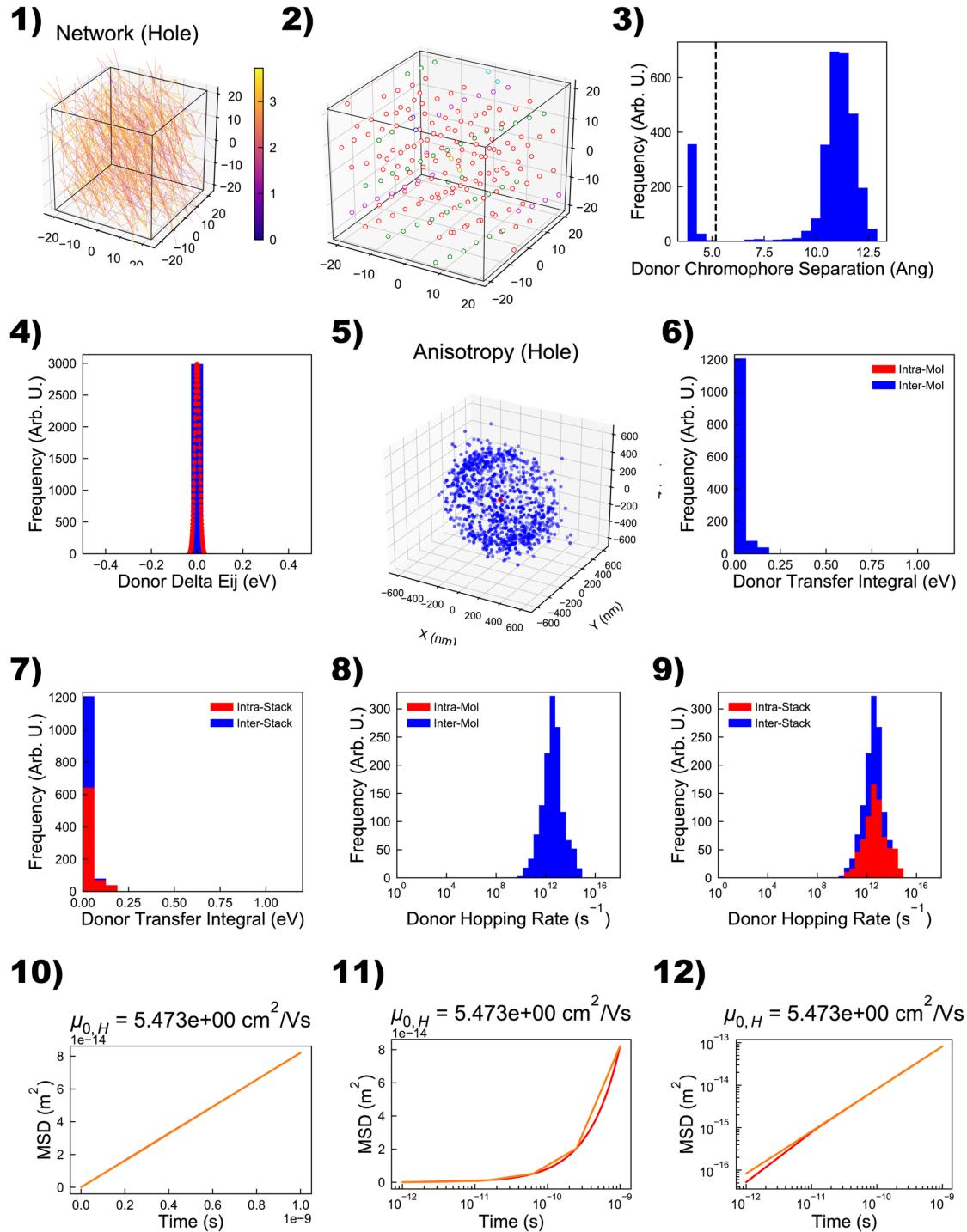


Figure 8: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer 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.

4 Analysis Figures with VRH on

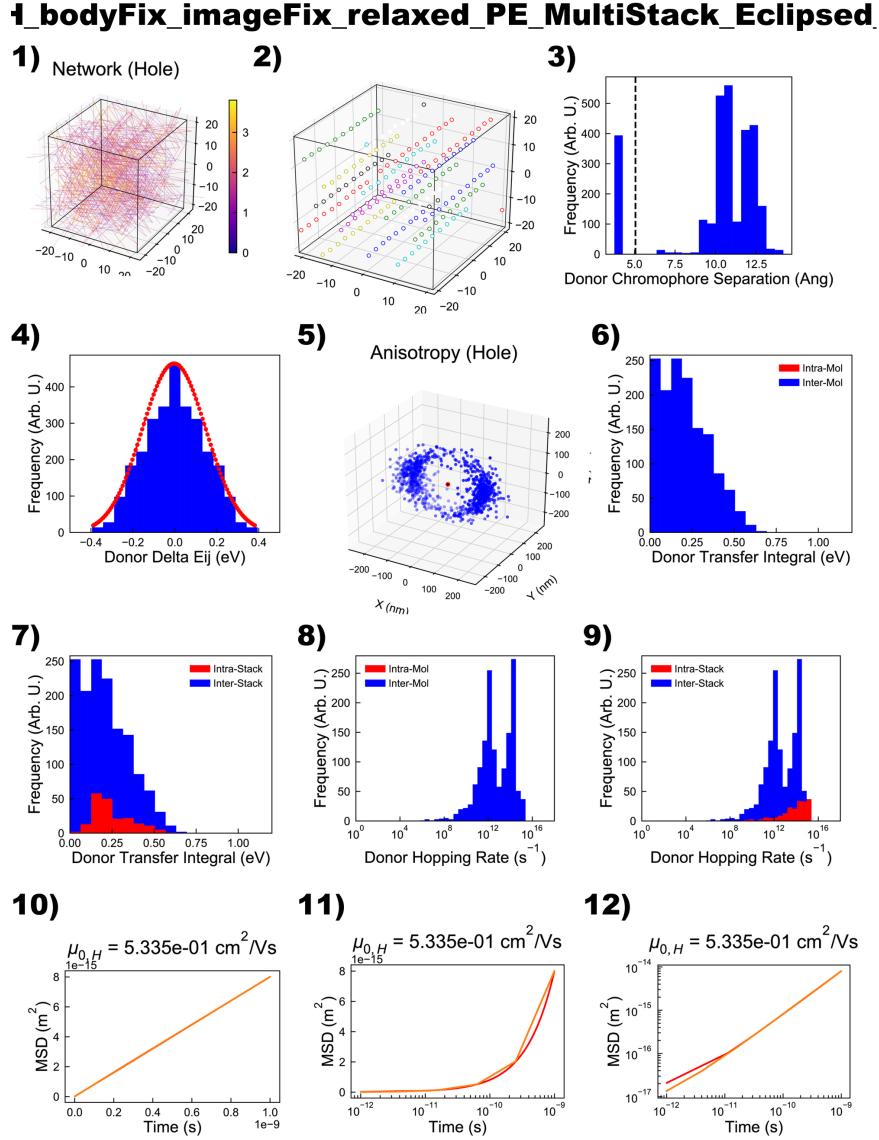


Figure 9: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

_bodyFix_imageFix_relaxed_PE_SingleStack_Eclipsed

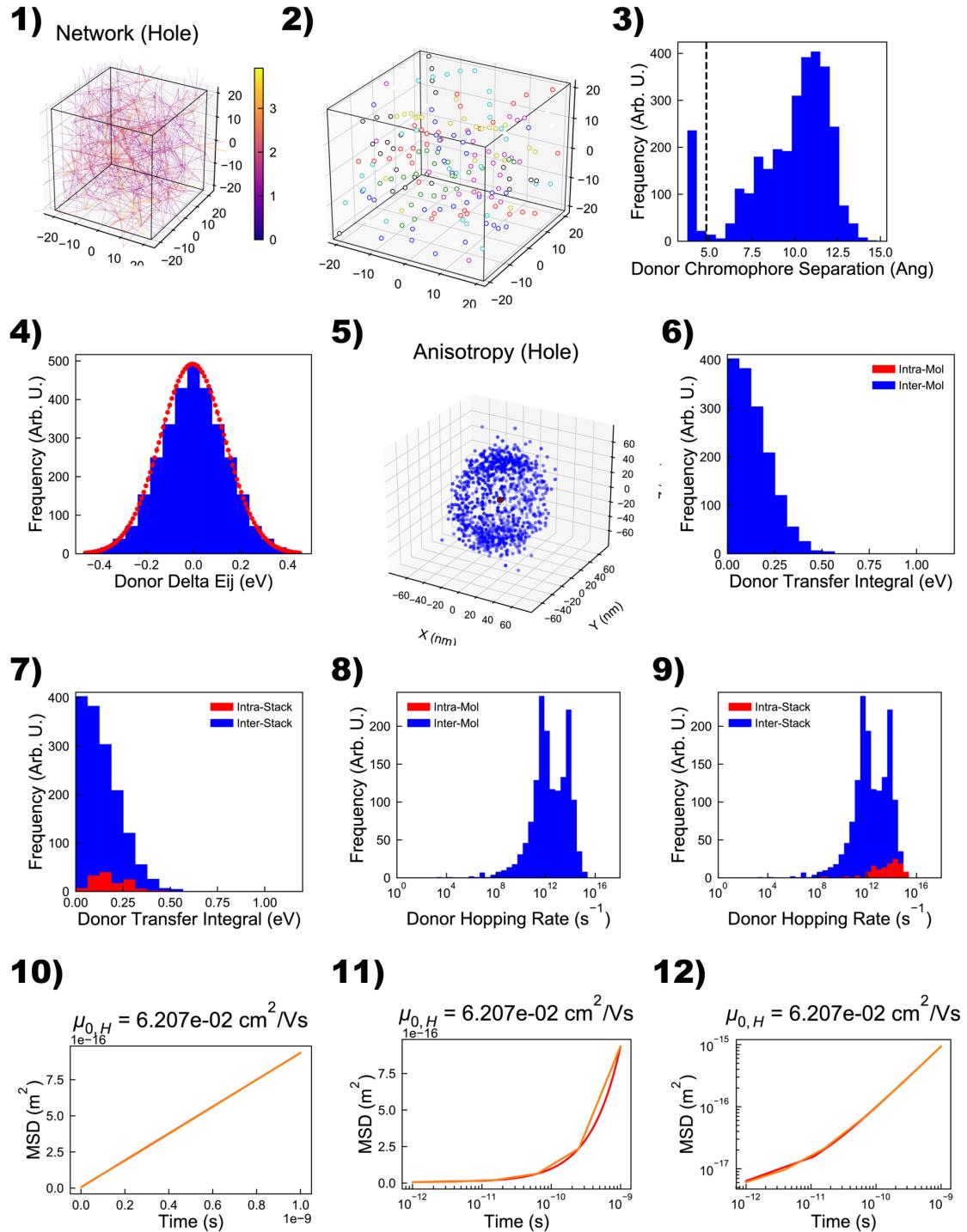


Figure 10: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

I_bodyFix_imageFix_relaxed_PE_SingleStack_Ordered

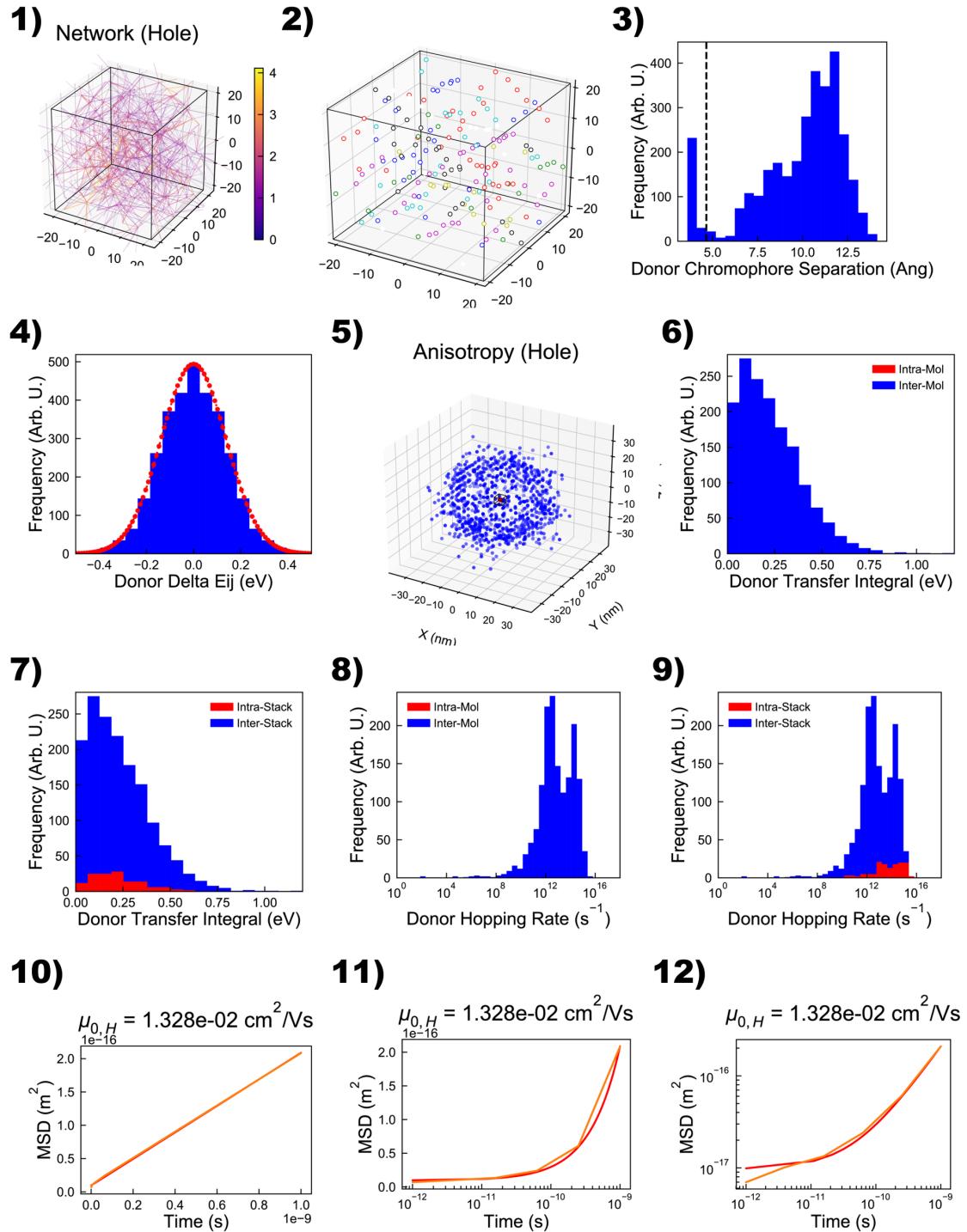


Figure 11: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer 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.

1_bodyFix_imageFix_relaxed_PT_MultiStack_Eclipsed

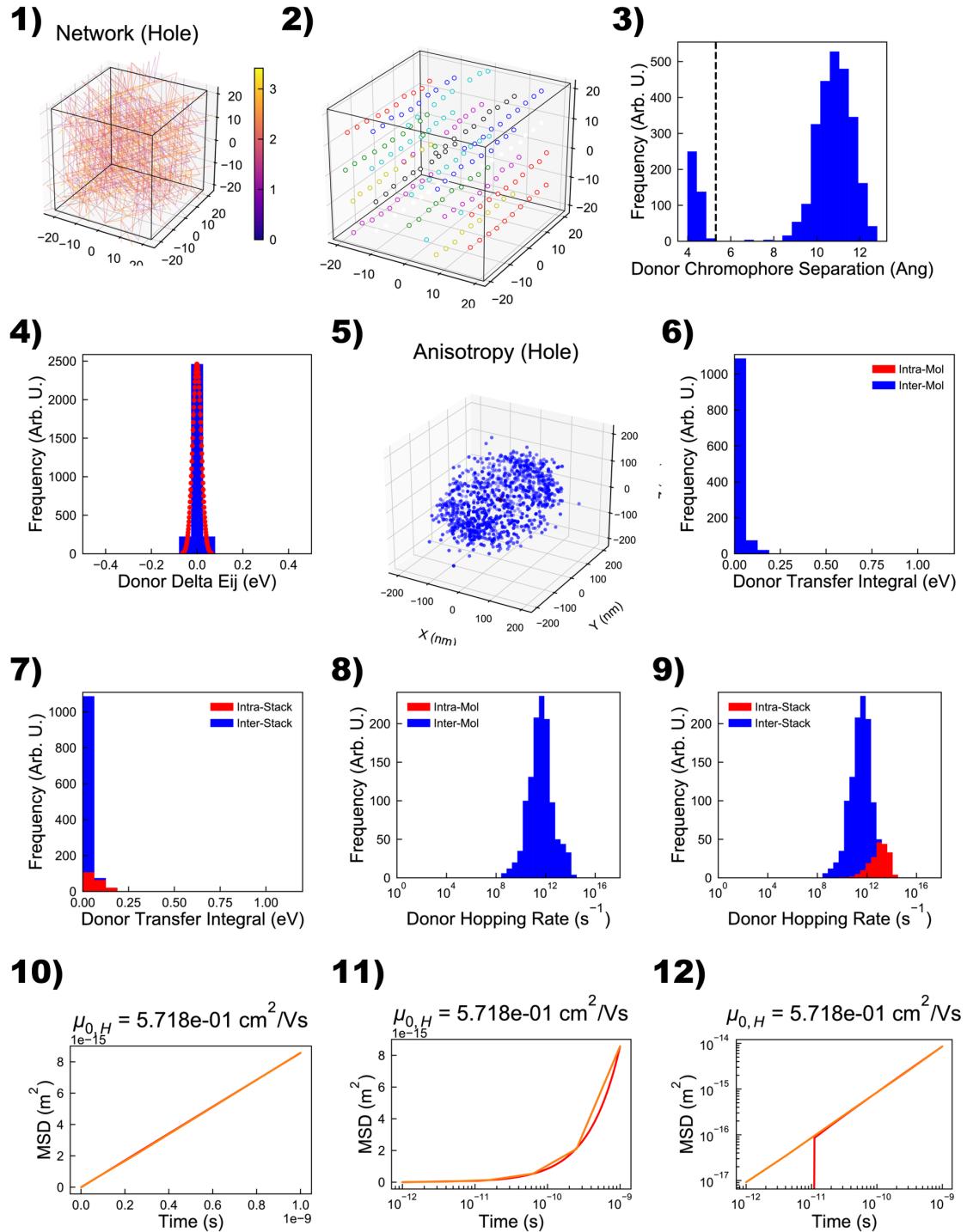


Figure 12: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

H_bodyFix_imageFix_relaxed_PT_MultiStack_Ordered

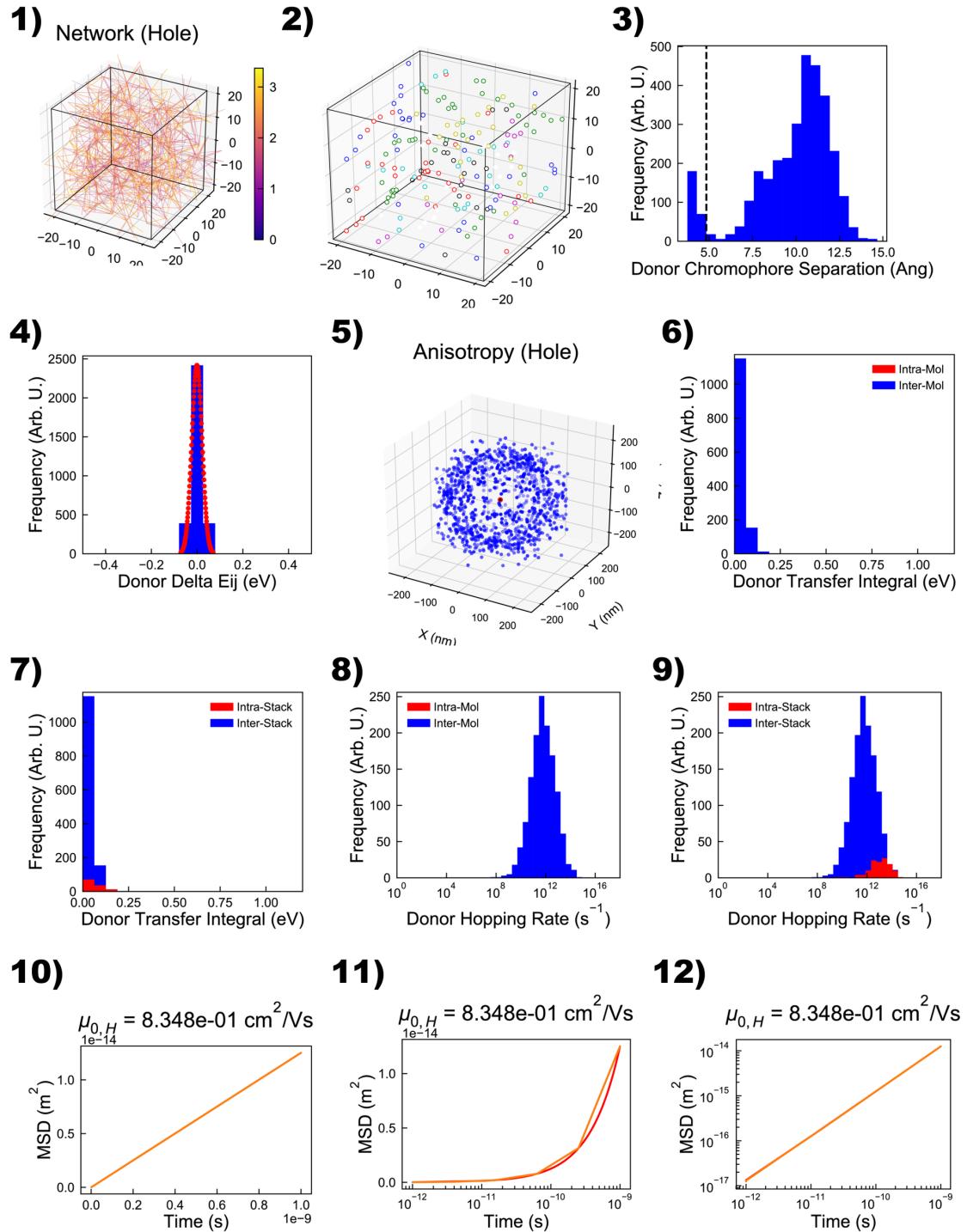


Figure 13: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (ΔE_{ij}), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer integrals, 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.

_bodyFix_imageFix_relaxed_PT_SingleStack_Eclipsed

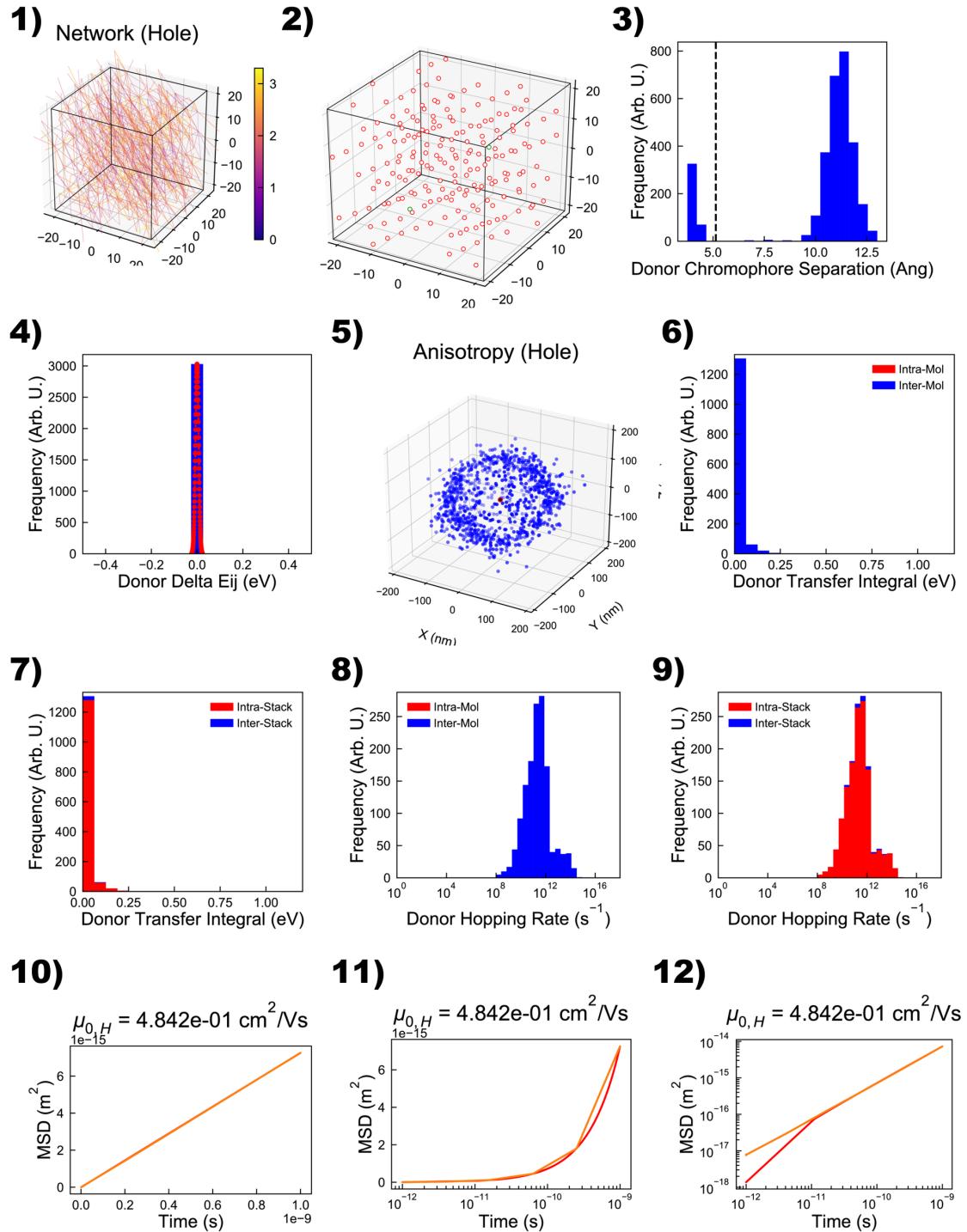


Figure 14: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer 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.

I_bodyFix_imageFix_relaxed_PT_SingleStack_Ordered

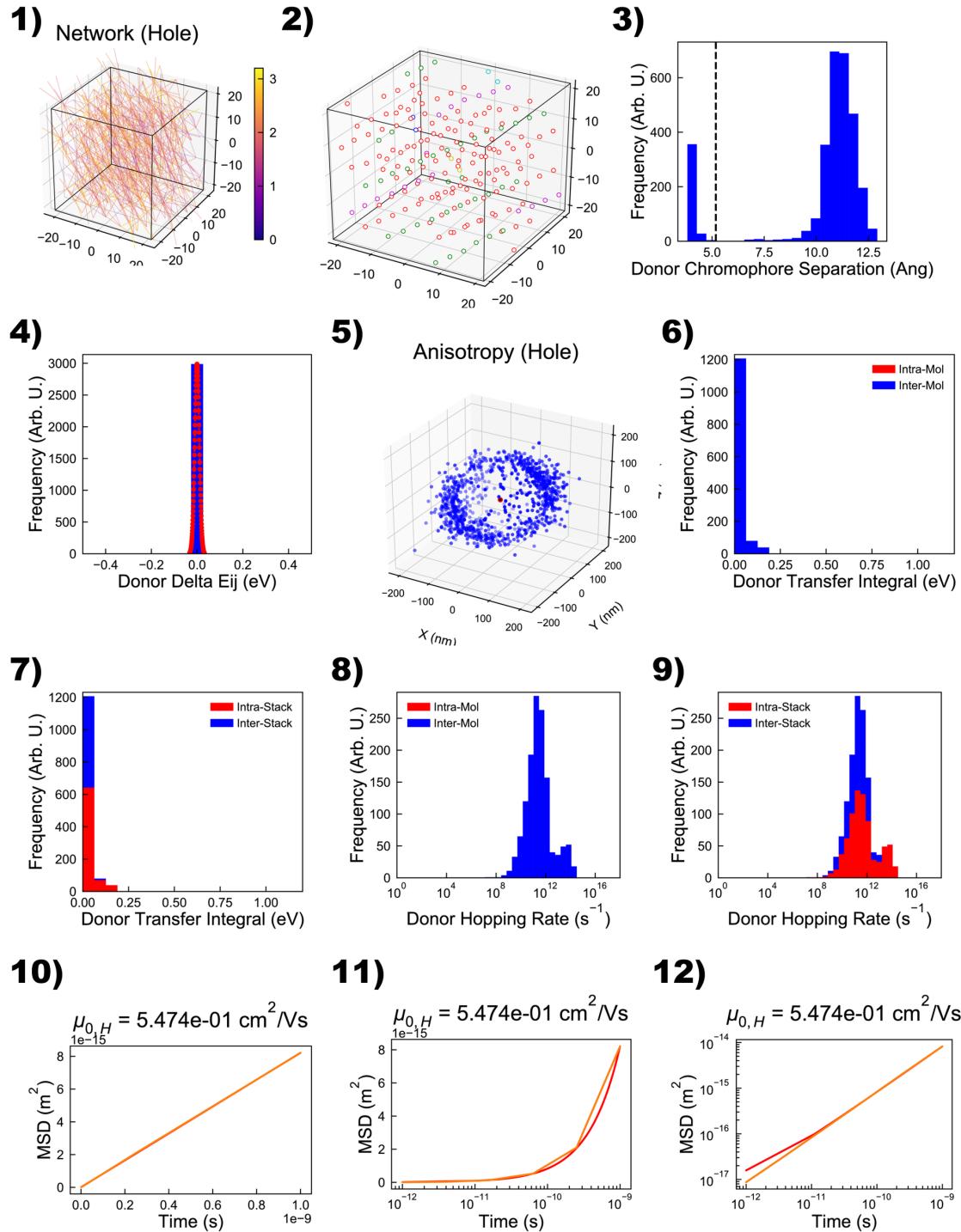


Figure 15: 1) Chromophore connectivity network, 2) Location of ‘stacks’, 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer 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.