MorphCT Results - PAHs

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1 Latest Jobs, 11/17

Based on the recent changes to the neighbour calculations and fine-graining, I have rerun our PAH stack systems to see if there are any changes.

2 Mobility Results

ID	Simulation Name	Density ($g\,cm^{-3}$)	Anisotropy (Arb. U.)	Anisotropy (Shape)	Stacks (Arb. U.)	Mobility ($cm^2\,V^{-1}\,s^{-1}$)
1	PE_MultiStack_Eclipsed	1.06	0.9456	Thin Tube	19	5.87×10^{0}
2	PE_SingleStack_Eclipsed	1.06	0.0206	Spherical	8	1.13×10^{-1}
3	PE_SingleStack_Ordered	1.06	0.1087	Oblate Spheroid	16	5.44×10^{-1}
4	PT_MultiStack_Eclipsed	1.01	0.0581	Spherical	20	8.80×10^{-1}
5	PT_MultiStack_Ordered	1.01	0.1414	Oblate Spheroid	20	2.49×10^{-2}
6	PT_SingleStack_Eclipsed	1.01	0.7264	Thin Tube	1	1.15×10^{0}
7	PT_SingleStack_Ordered	1.01	0.0575	Sphere	1	4.91×10^{0}

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

The mobility results are effectively the same, although some of the anisotropy values have changed from previously.

2.1 Conclusions

- Exploring the ΔE_{ij} has shown that some of the systems (namely PE_MultiStack_Eclipsed, PT_SingleStack_Eclipsed, and PE_SingleStack_Ordered) contain rigid bodies (delta function for the DoS), whereas others don't. Having a $\Delta E_{ij} = 0$ will strongly affect (increase) the eventual hopping rate and so we are comparing apples to oranges.

- Additionally, while the PT_SingleStack systems are truly one single stack, the PE_SingleStack systems are not. They certainly have fewer stacks, but they are not on massive periodic structure like in the PT_SingleStack case, and so a direct comparison can not really be drawn there either.

- The carrier termination (anisotropy) graphs in panel **5)** show that carriers have not moved very far out of the simulation volume in the PT_MultiStack, and PE_SingleStack_Eclipsed cases. All of the MSD fits are excellent, however, so this might not be an issue.

- All of the flexible PT_MultiStack and PE_SingleStack systems shown Gaussian DoSes with the maximum breadth permitted by the Gaussian map that we perform in MorphCT (which will shrink a distribution with $\sigma > 100meV$ down to $\sigma = 100meV$, but leave distributions with $\sigma \leq 100meV$ alone). The breadth of the Ordered system is significantly greater than the Eclipsed system, in both cases. This makes sense - in the Eclipsed case, the molecules are azimuthally in-register and so are squeezed into planarity by the molecules closely packed around it. This makes each molecule structurally indistinct, which manifests as an energetic indistinction and the $\Delta E_{ij} \to 0$.

I think there are too many variables here that we are unable to resolve with just these 7 simulations. This makes it impossible to draw any conclusions about the presence and orientation of the stacks other than "it matters and can affect the mobilities by an order of magnitude". Given the strict mathematical constraints on how the stacks can form and still produce a coherent structure without morphological defects, I am not convinced that this is something we can adjust our mobilities for either. Instead, I think it's something that we just have to be aware of when submitting our simulations to KMC, consider when drawing conclusions, and disclose fully when we present results.

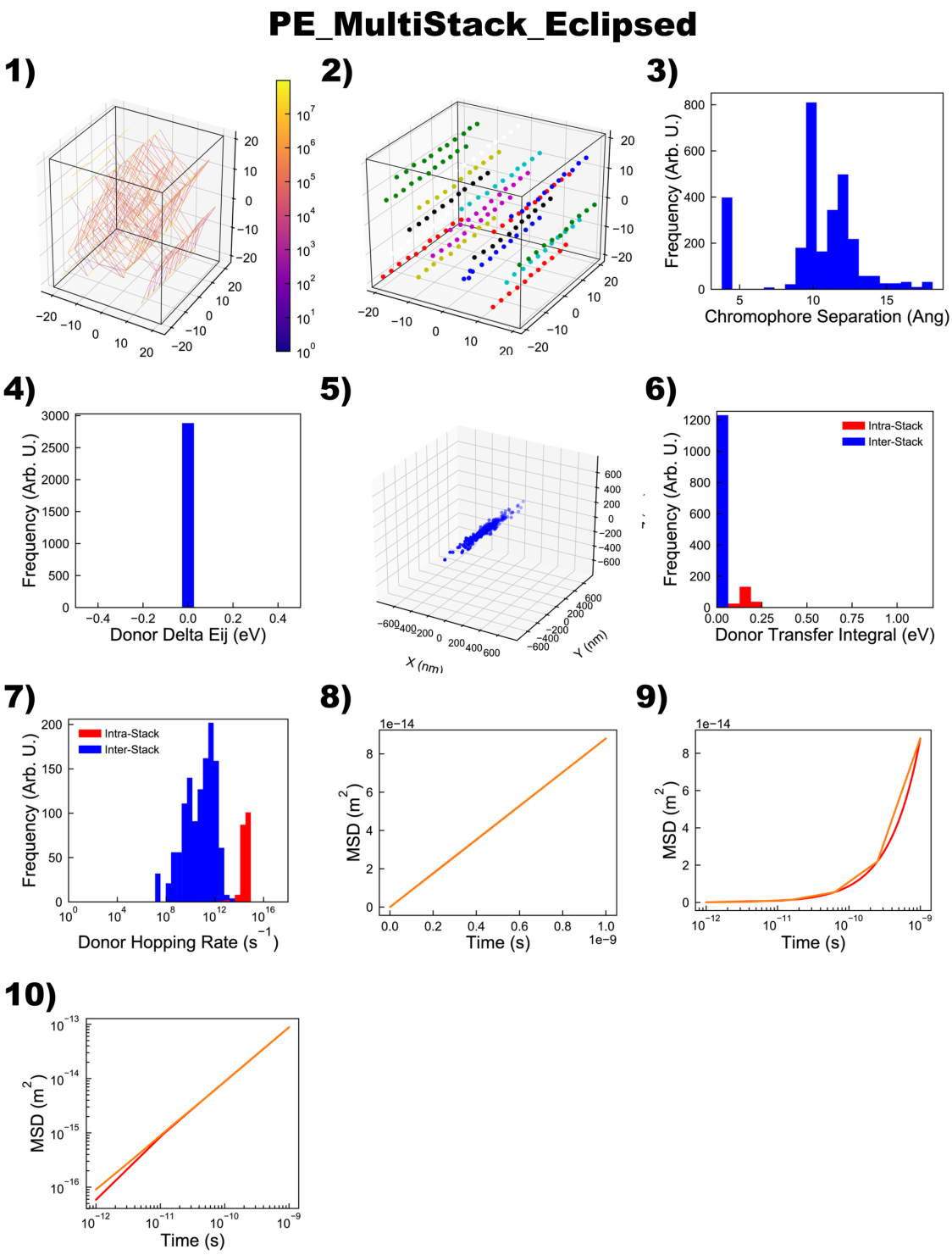

Figure 1: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

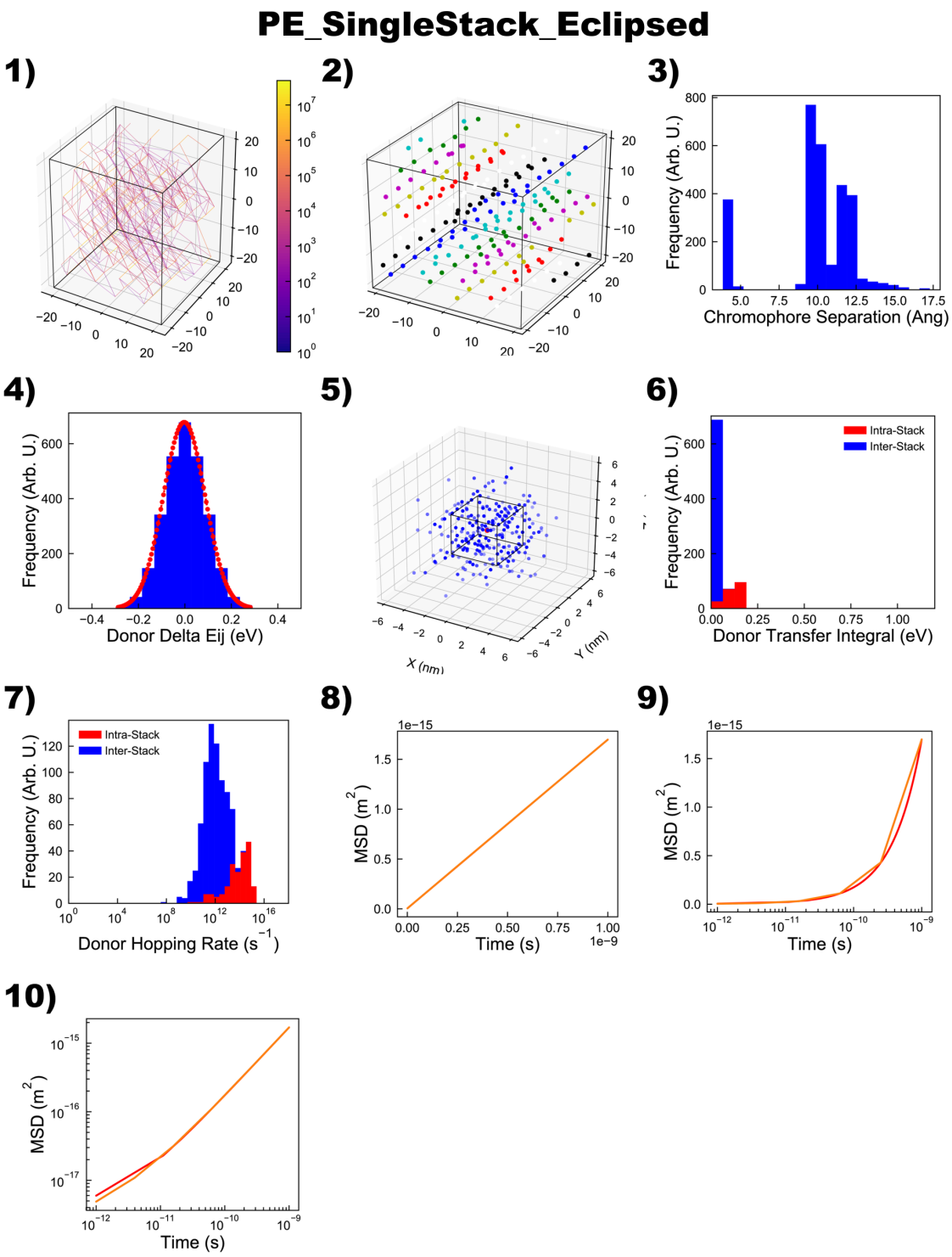

Figure 2: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

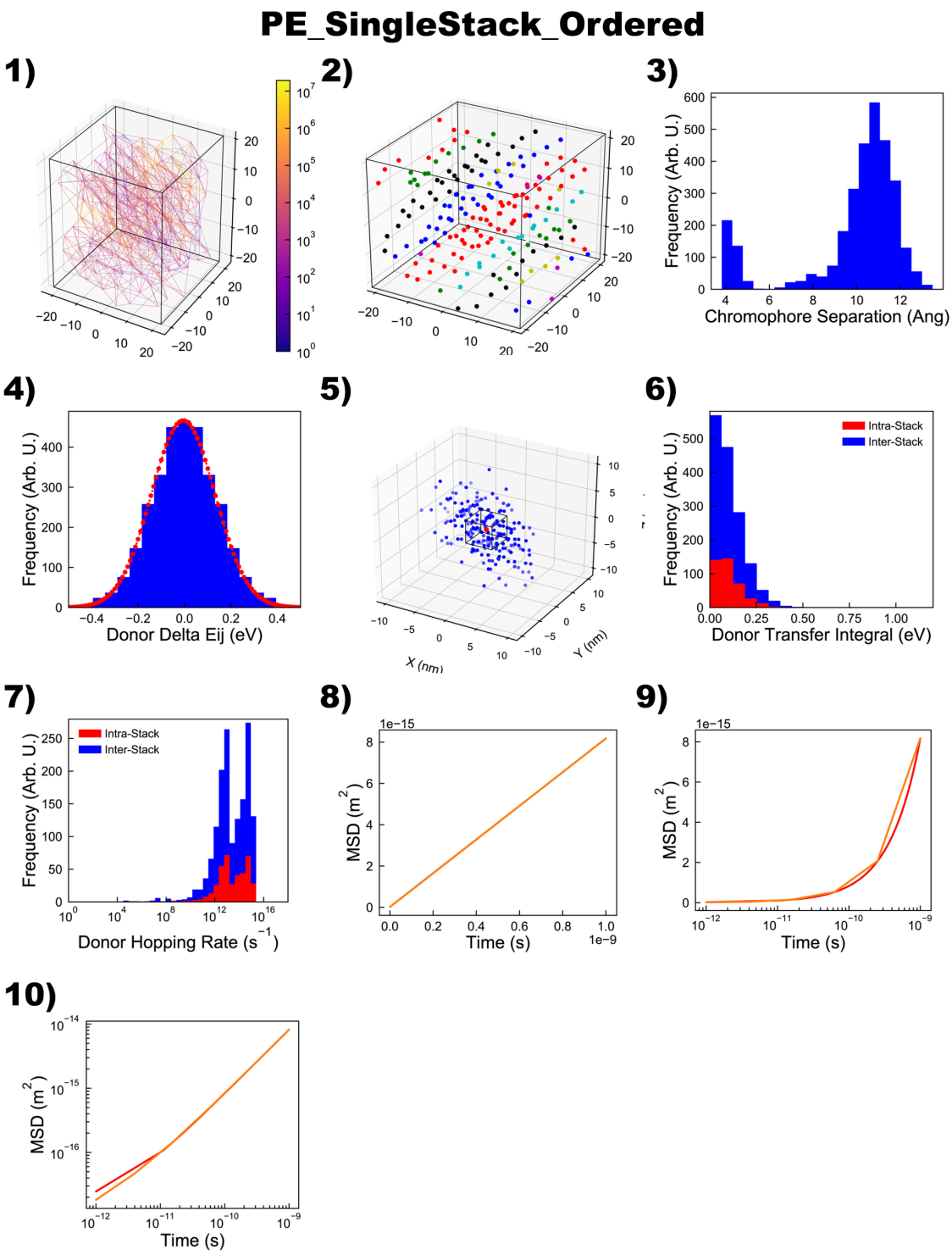

Figure 3: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

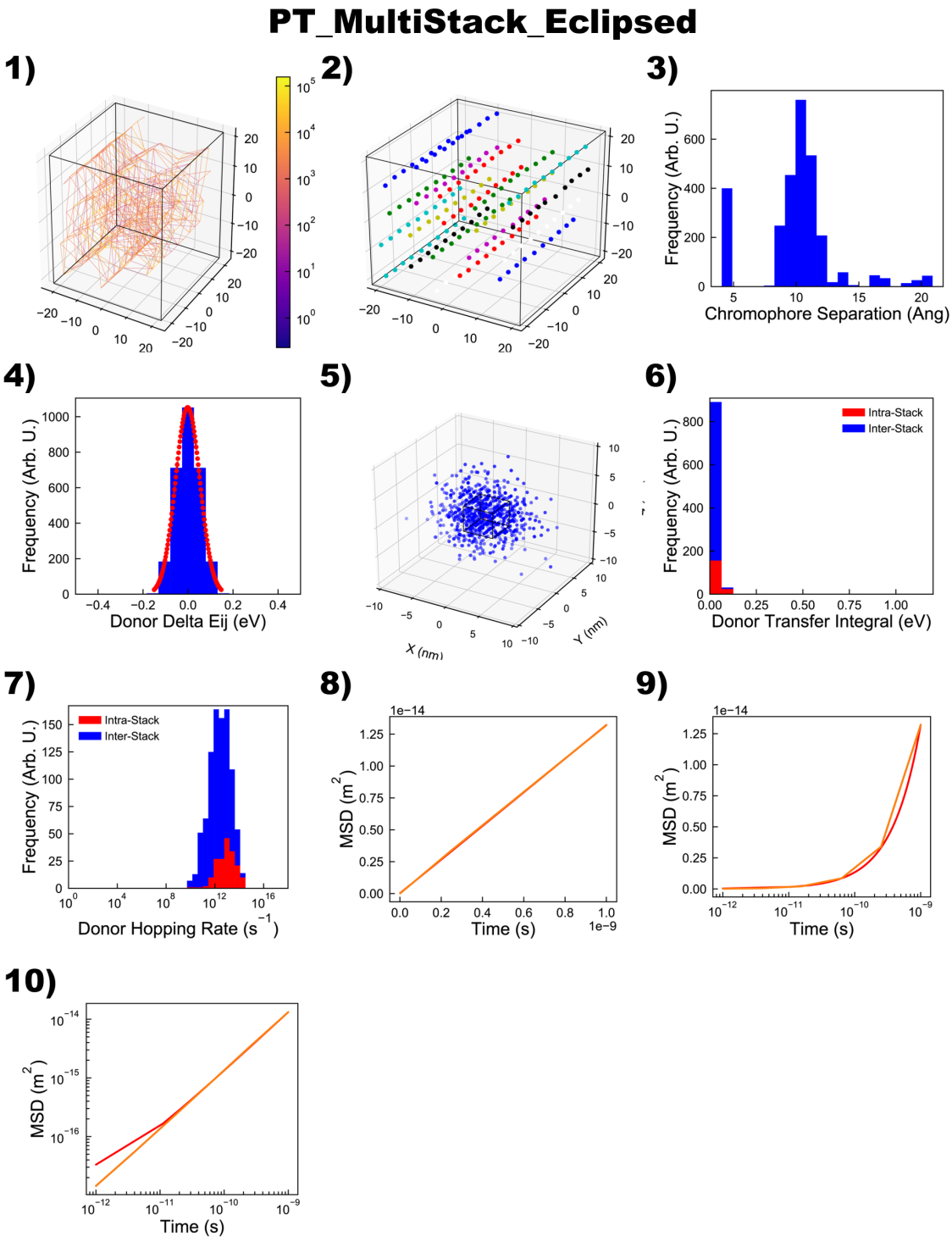

Figure 4: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

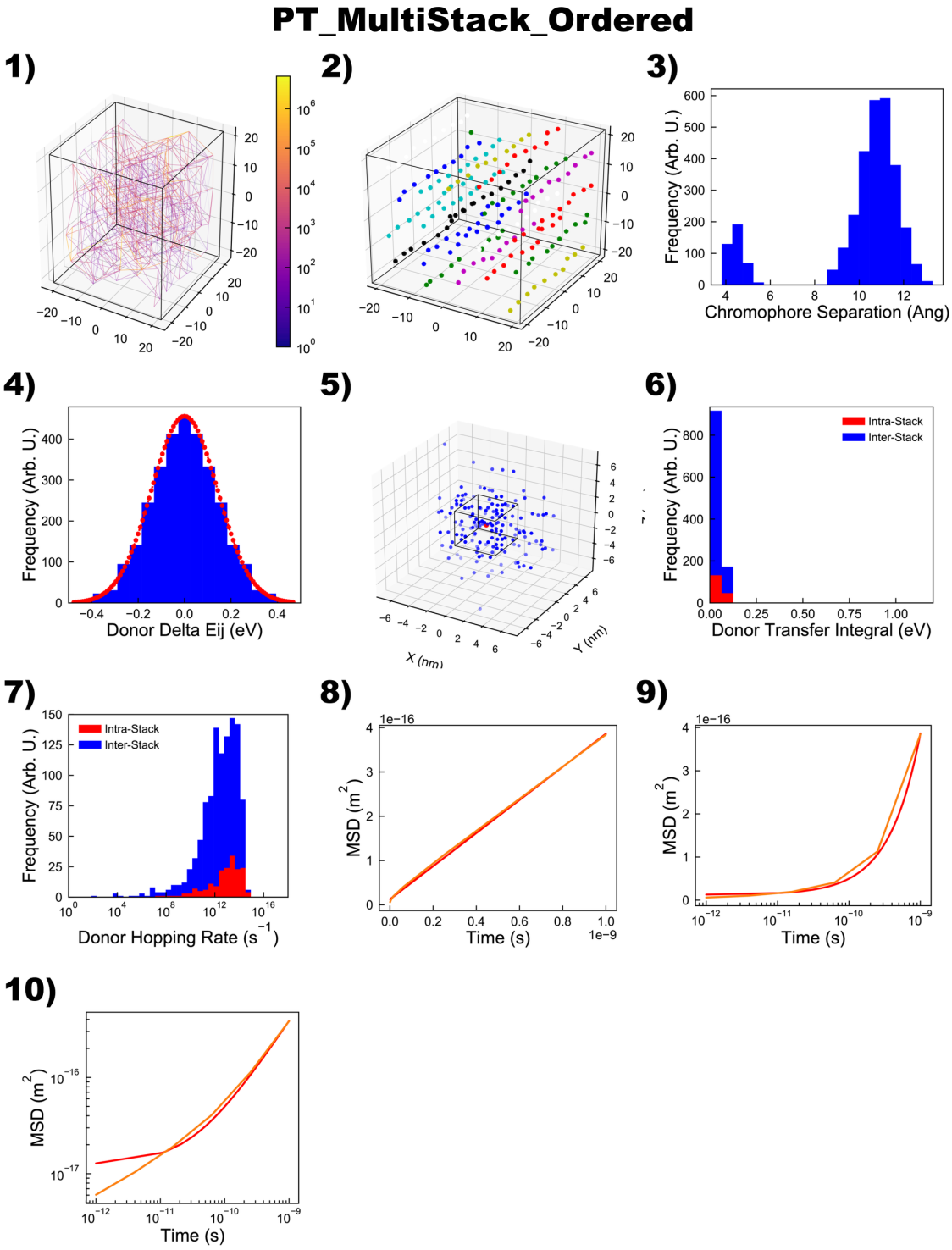

Figure 5: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

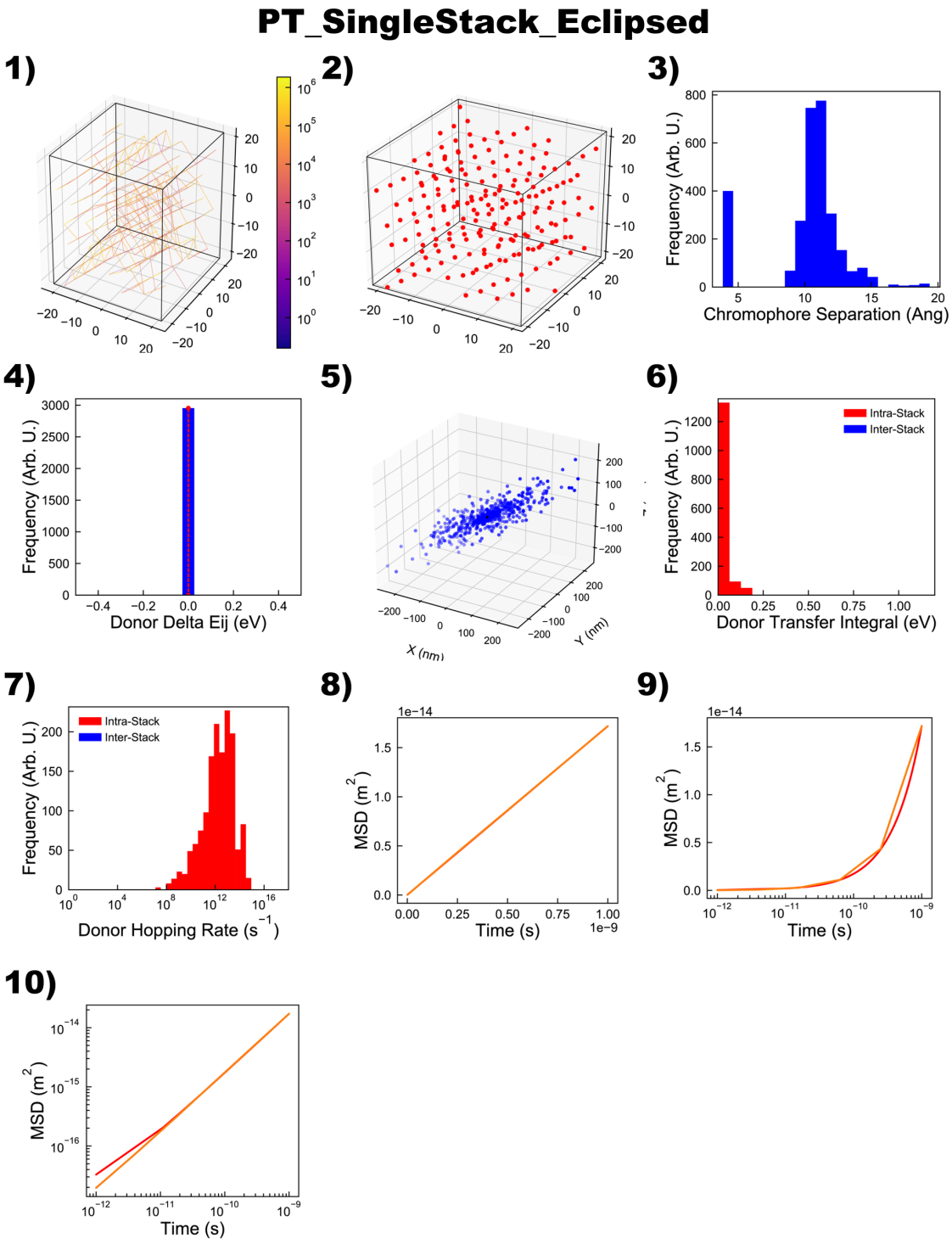

Figure 6: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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

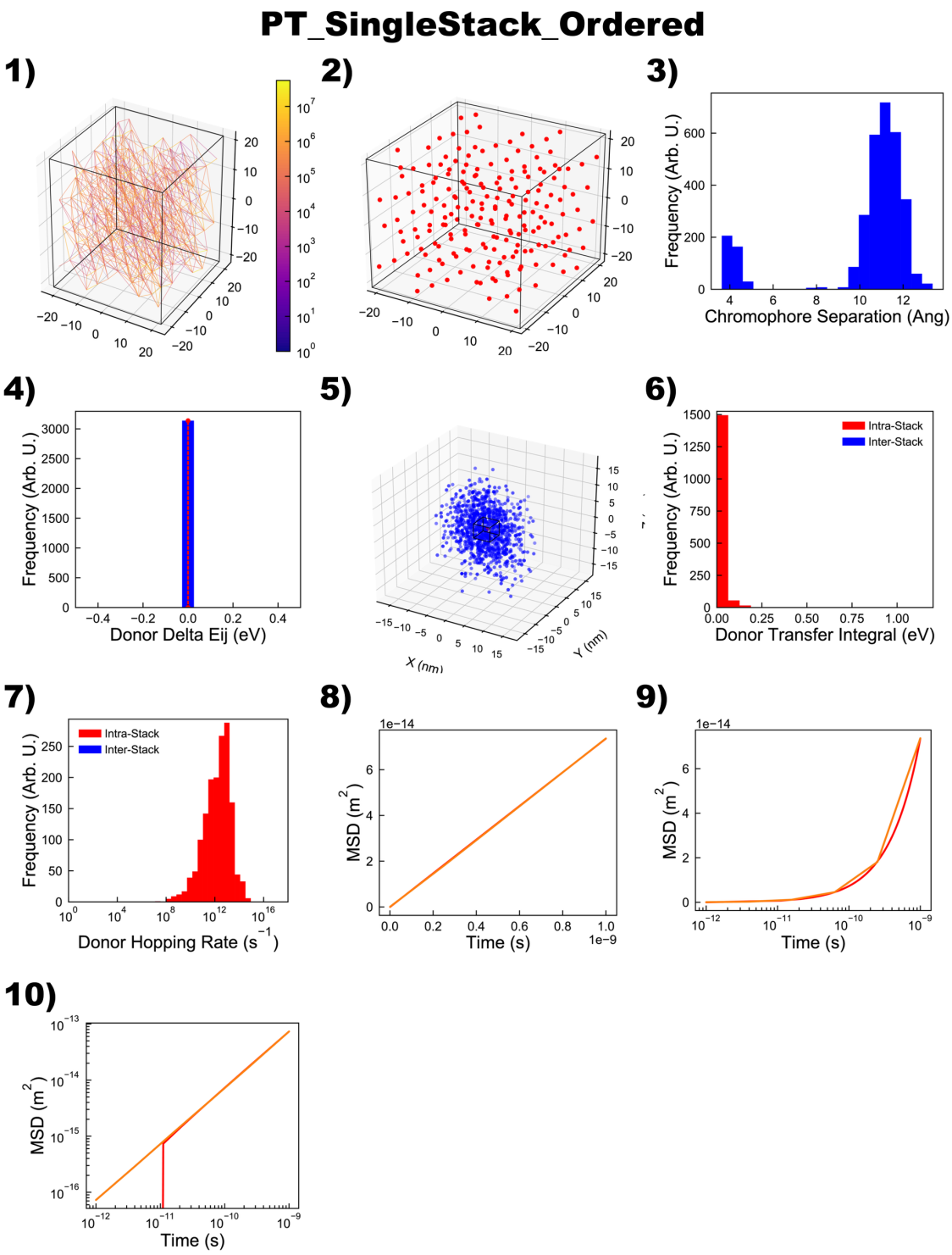

Figure 7: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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