MorphCT - 1K P3HT 15mers

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1 Simulations

The simulations for the system containing 1,000 15mers of P3HT has compleded. The system was UA to begin with, and so no fine-graining was required for this morphology.

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	1k_P3HT	1.11	0.1086	Flat Disk	477	3.00×10^{0}

Table 1: The results from MorphCT.

Note that chromophores are added to a 'stack' if their CoMs are separated by less than a defined cut-off. As the normal π-stacking distance for P3HT is around 3.9 Å, the stack cut-off was set at 4 Å. Nearly all of the morphology is a single stack, with some of the grains aligned in other directions forming seperate stacks, and many chromophores constituting their own stack. This results in a large number of stacks in the system overall (477). Stack calculations also consider the periodic boundaries.

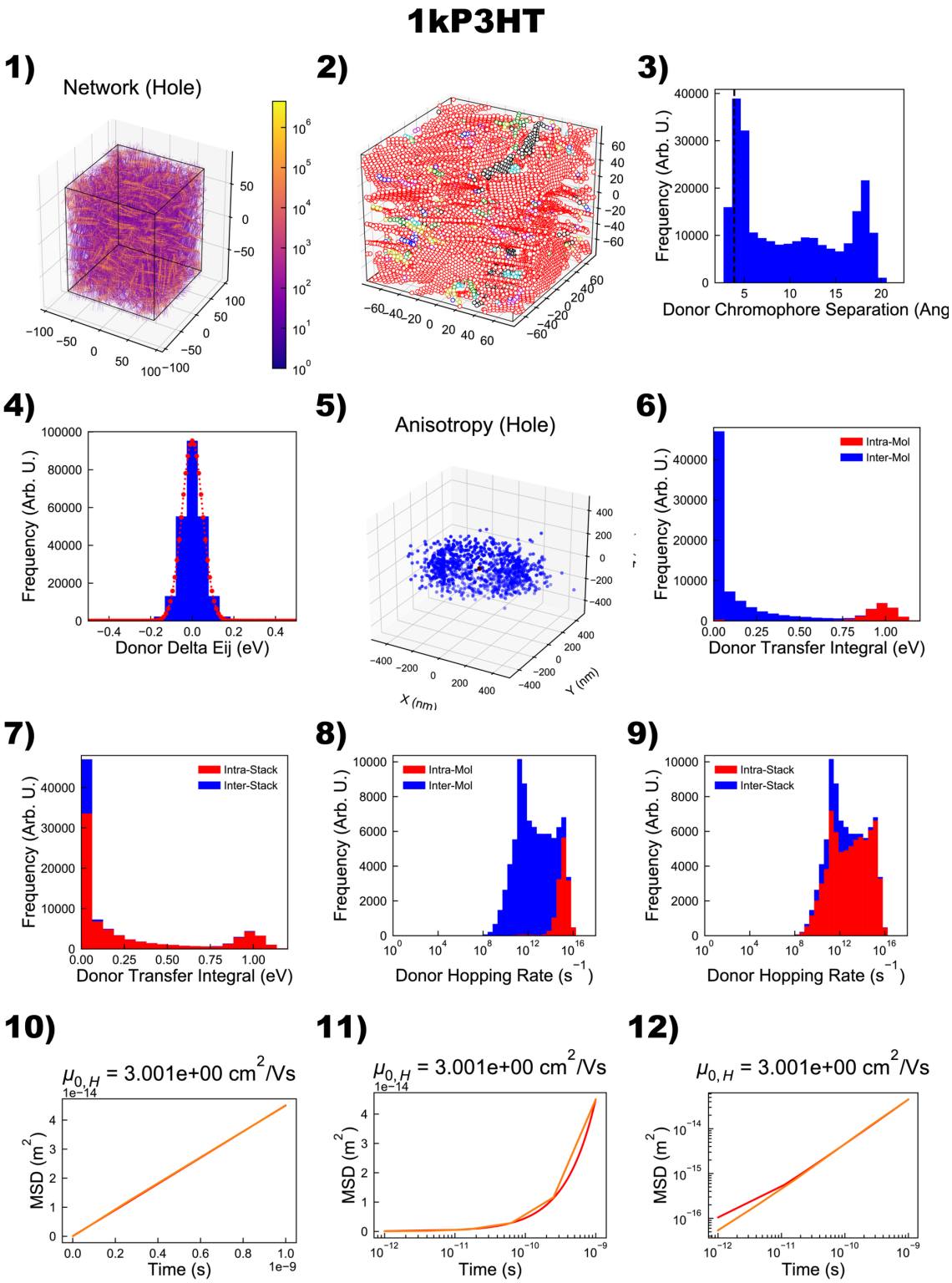

Figure 1: 1) Chromophore connectivity network, 2) Location of 'stacks', 3) Distribution of connected chromophore separations (defines stacks), 4) Density of states of Frontier molecular orbital (delta Eij), 5) KMC Carrier termination locations (defines anisotropy), 6) Histogram of molecular transfer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