

# MorphCT - 1K P3HT 15mers

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November 27, 2017

## 1 Simulations

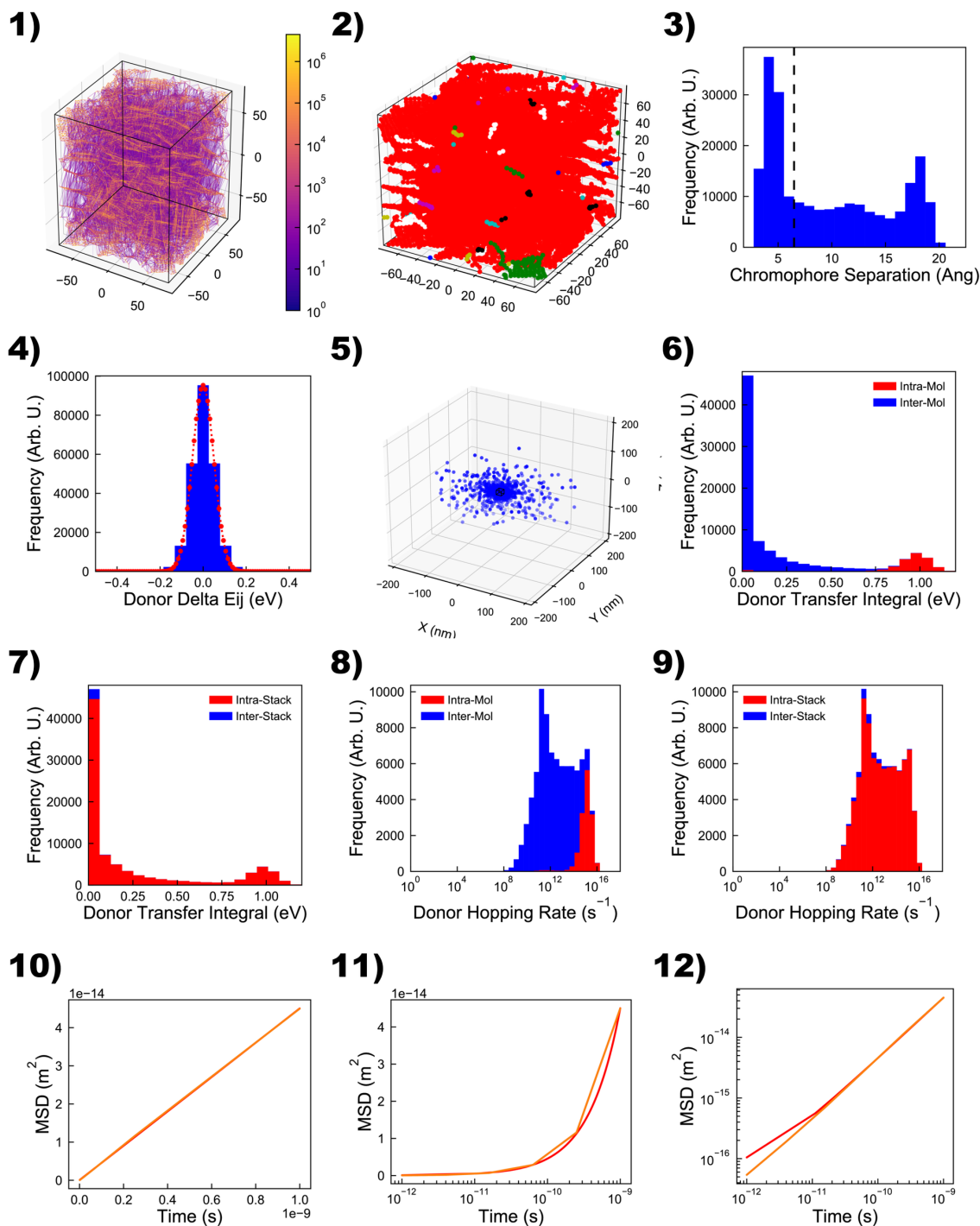
The simulations for the system containing 1,000 15mers of P3HT has completed. The system was UA to begin with, and so no fine-graining was required for this morphology.

## 2 Mobility Results

ID	Simulation Name	Density (g cm <sup>-3</sup> )	Anisotropy (Arb. U.)	Anisotropy (Shape)	Stacks (Arb. U.)	Mobility (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )
1	1k_P3HT	1.11	0.1086	Flat Disk	26	3.00×10 <sup>0</sup>

**Table 1:** The results from MorphCT.

# 1kP3HT



**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.