MorphCT Results - P3HT

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1 Original Published Results

ID	Simulation Name	Density ($g\,cm^{-3}$)	Anisotropy (Arb. U.)	Anisotropy (Shape)	Mobility ($cm^2\,V^{-1}\,s^{-1}$)	Intra-%
1	0001_withImages	1.061	0.0038	Spherical	1.56×10^{-1}	—%
2	0005_withImages	1.336	0.0046	Spherical	7.19×10^{-3}	—%
3	0010_withImages	1.345	0.0076	Spherical	2.41×10^{-2}	—%
4	0020_withImages	1.428	0.0111	Spherical	1.09×10^{-2}	—%
5	0040_withImages	1.450	0.0114	Spherical	1.74×10^{-2}	—%
6	0100_withImages	1.510	0.0216	Spherical	1.49×10^{-2}	—%
7	0200_withImages	1.550	—	—	—	—%
8	0300_withImages	1.593	0.2135	Disk	5.73×10^{-1}	—%
9	0500_withImages	—	—	—	—	—%
10	1000_withImages	1.662	0.2479	Disk	1.88×10^{0}	—%

Table 1: The results from the new data given a snapshot of the pristine P3HT morphology at a given snapshot during evolution

Representative Values From Literature:

- Density: $1.10\,g\,cm^{-3}$ [1]
- Mobility: 1×10^{-5} - $1\times10^{-3}\,cm^2\,V^{-1}\,s^{-1}$ [2–5]

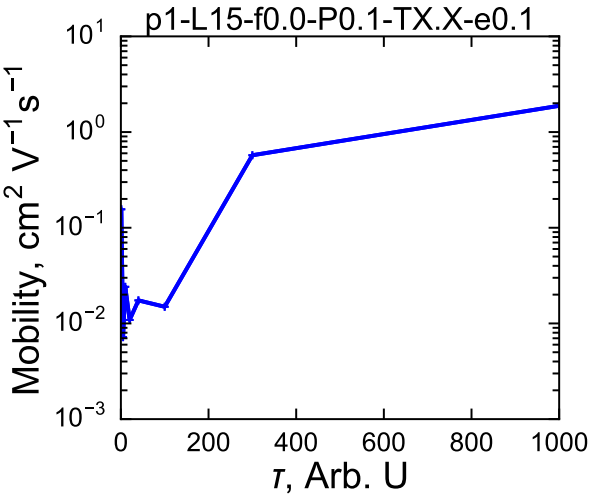

Figure 1: The mobility trend observed as a function of increasing dimensionless evolution time

1.1 3D Carrier Network

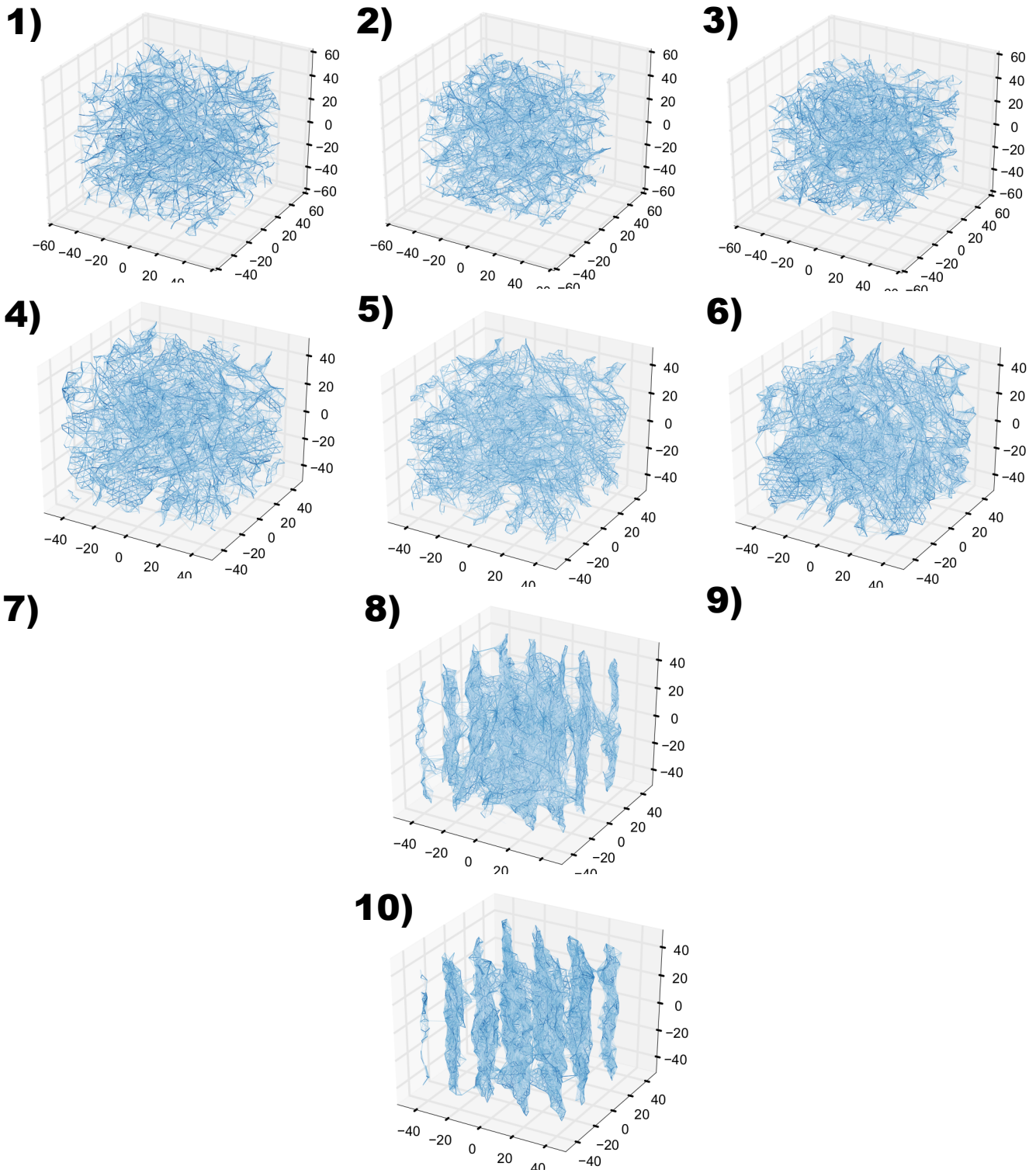

Figure 2: The 3D heatmap of charge transport routes within the morphologies **1** - **10**. Dark routes describe commonly accessed hops between pairs of chromophores, whereas pale routes are less widely used in the KMC simulations. Each node therefore represents the location of a single chromophore. The intensity value for the route is currently taken to be `I = np.log10(freq) / np.log10(max_freq)`.

1.2 Anisotropies

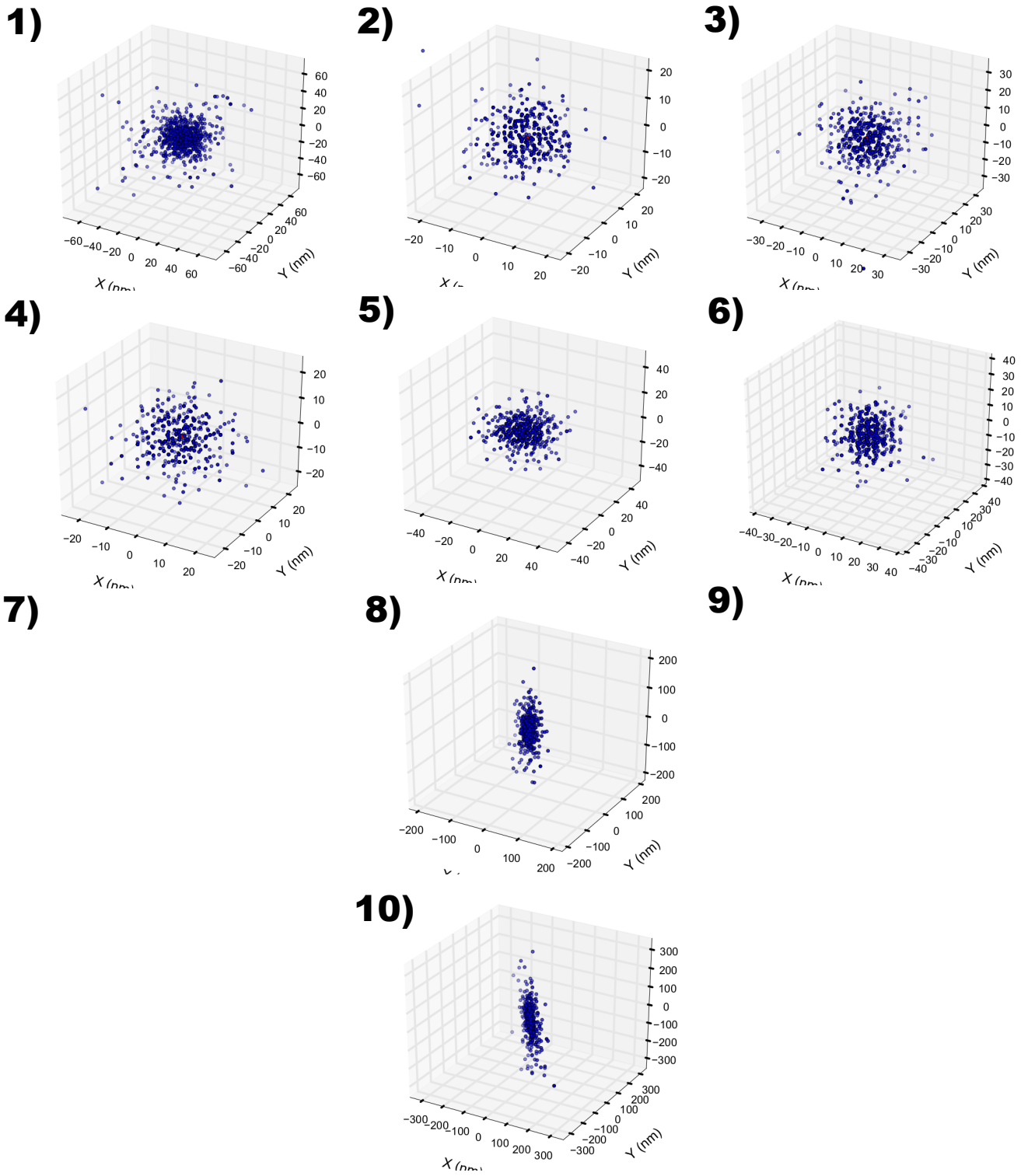

Figure 3: The periodic anistropies of the carrier transport within the morphologies **1** - **10**.

1.3 MSDs

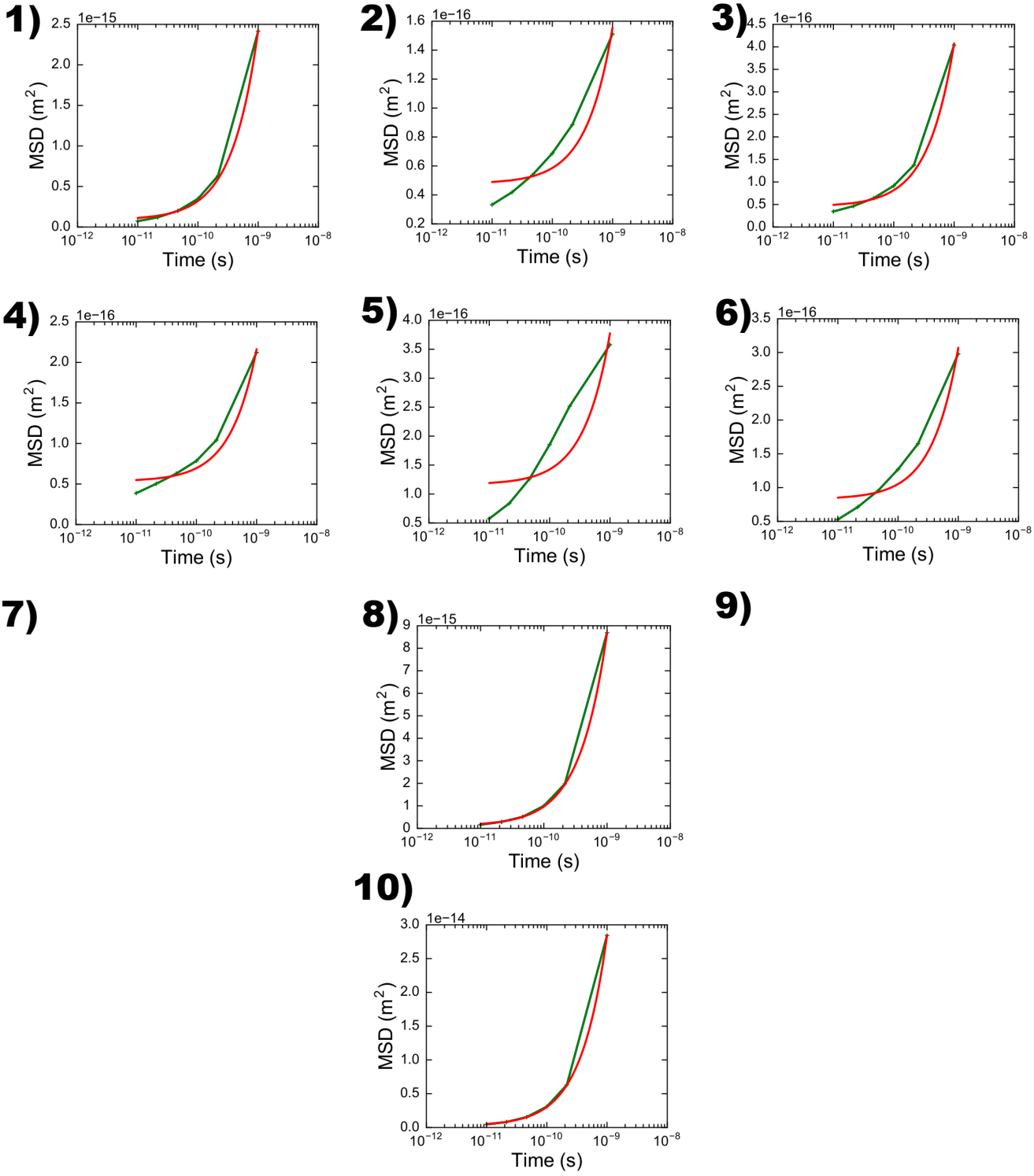

Figure 4: The semi-log-x mean squared displacement curves of the carriers within the morphologies **1** - **10**.

1.4 Hopping Rate Distributions

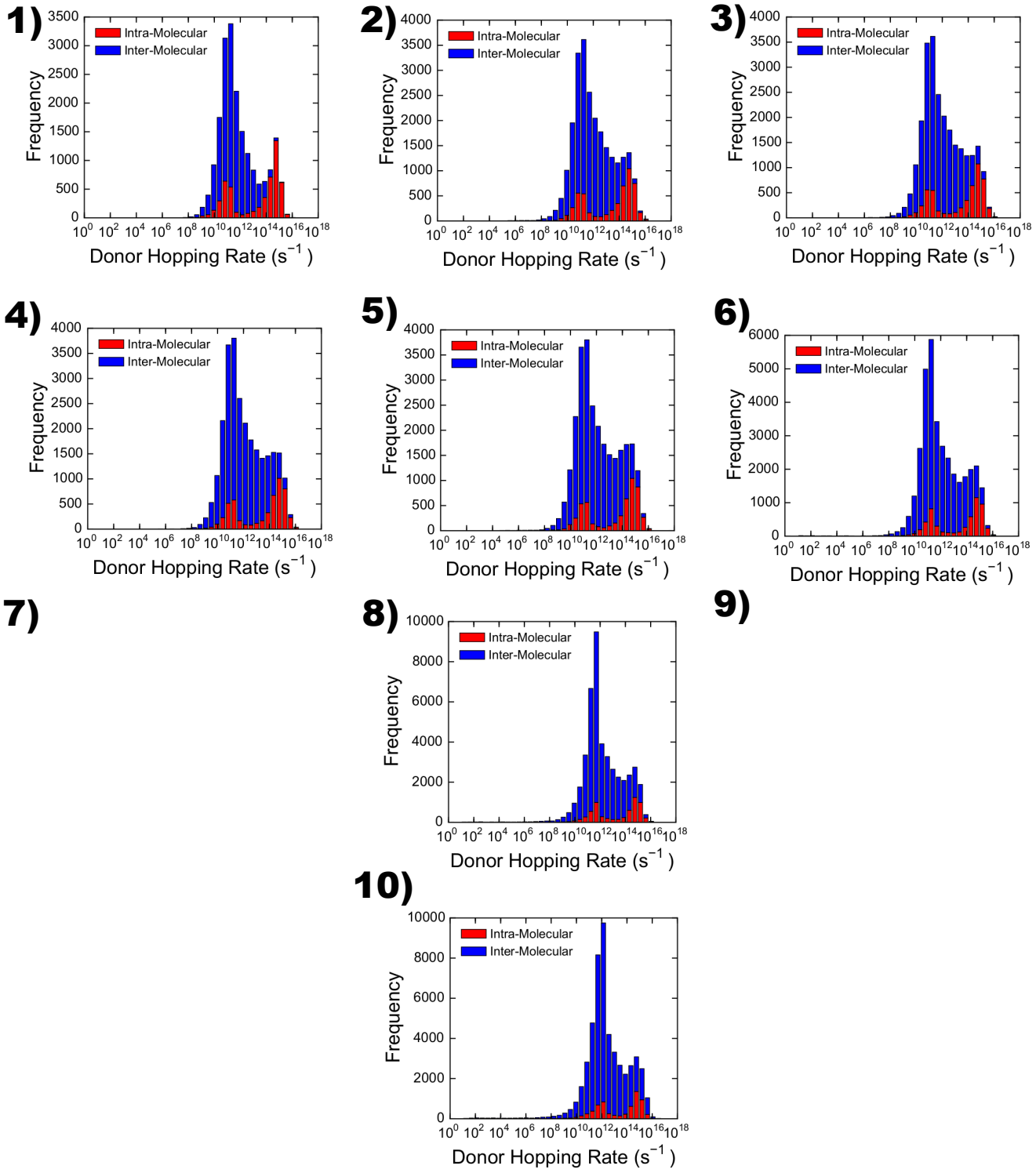

Figure 5: The stacked hopping-rate distributions for intra- and inter-molecular hops executed by carriers within the morphologies **1** - **10**.

References

[1] Gregory M. Newbloom, Katie M. Weigandt, and Danilo C. Pozzo. Structure and property development of poly(3-hexylthiophene) organogels probed with combined rheology, conductivity and small angle neutron scattering. *Soft Matter*, 8(34):8854, 2012.

[2] Amy M. Ballantyne, Lichun Chen, Justin Dane, Thomas Hammant, Felix M Braun, Martin Heeney, Warren Duffy, Iain McCulloch, Donal D C Bradley, and Jenny Nelson. The Effect of Poly(3-hexylthiophene) Molecular Weight on Charge Transport and the Performance of Polymer:Fullerene Solar Cells. *Advanced Functional Materials*, 18(16):2373–2380, aug 2008.

[3] Ralf Mauer, Marcel Kastler, and Frédéric Laquai. The Impact of Polymer Regioregularity on Charge Transport and Efficiency of P3HT:PCBM Photovoltaic Devices. *Advanced Functional Materials*, 20(13):2085–2092, may 2010.

[4] Shyam S. Pandey, Wataru Takashima, Shuichi Nagamatsu, Takeshi Endo, Masahiro Rikukawa, and Keiichi Kaneto. Regioregularity vs Regiorandomness: Effect on Photocarrier Transport in Poly(3-hexylthiophene). *Japanese Journal of Applied Physics*, 39(Part 2, No. 2A):L94–L97, feb 2000.

[5] Youngkyoo Kim, Steffan Cook, Sachetan M. Tuladhar, Stelios A. Choulis, Jenny Nelson, James R. Durrant, Donal D. C. Bradley, Mark Giles, Iain McCulloch, Chang-Sik Ha, and Moonhor Ree. A Strong Regioregularity Effect in Self-Organizing Conjugated Polymer Films and High-Efficiency Polythiophene:Fullerene Solar Cells. *Nature Materials*, 5(3):197–203, mar 2006.