MorphCT Results - Voronoi Neighbour Analysis

Matthew Jones

October 12, 2017

1 Jobs run using the new Voronoi cell neighbourlist calculation

NOTE, In order to test the full pipeline after the recent changes to MorphCT, these jobs have been re-fine-grained (using the same MD parameters) so are somewhat different morphologies to previously. I didn't think this would make much of a difference, but it seems like it might. We need to perform a sensitivity analysis by comparing these results to the previously fine-grained morphologies but using the new neighbourlist calculation, to see how sensitive our results are to the fine-graining process.. Unfortunately, I have had some issues running the previous morphologies through the new Voronoi cell neighbourlist calculation, so these are delayed but should hopefully be completed by the end of the week.

ID	**Simulation Name**	**Density** ($g\,cm^{-3}$)	**Anisotropy** (Arb. U.)	**Anisotropy** (Shape)	**Mobility** ($cm^2\,V^{-1}\,s^{-1}$)	**Intra-** %
1	p1-L15-f0.0-P0.1-T1.5-e0.5	1.676	0.0676	—	1.17×10^{1}	12.53%
2	p1-L15-f0.0-P0.1-T1.75-e0.5	1.061	0.0065	Spherical	3.48×10^{-1}	17.59%
3	p1-L15-f0.0-P0.1-T2.0-e0.5	0.892	0.0026	Spherical	4.46×10^{-1}	17.58%
4	p1-L15-f0.0-P0.1-T2.25-e0.5	0.787	0.0044	Spherical	5.52×10^{-1}	17.83%
5	p1-L15-f0.0-P0.1-T2.5-e0.5	0.685	0.0041	Spherical	4.03×10^{-1}	18.00%
6	0001_withImages	1.061	0.0059	Spherical	2.65×10^{-1}	17.46%
7	0005_withImages	1.336	0.0077	Spherical	4.68×10^{-2}	13.34%
8	0010_withImages	1.345	0.0063	Spherical	7.50×10^{-1}	13.73%
9	0020_withImages	1.428	0.0137	Spherical	1.22×10^{0}	13.23%
10	0040_withImages	1.450	0.0077	Spherical	7.92×10^{-2}	13.78%
11	0100_withImages	1.510	0.0228	Spherical	4.33×10^{0}	12.89%
12	0200_withImages	1.554	0.0721	Ellipsoid	4.94×10^{0}	12.74%
13	0300_withImages	1.593	0.1041	Disk	6.44×10^{0}	12.61%
14	0500_withImages	1.638	0.1186	Disk	9.26×10^{0}	12.55%
15	1000_withImages	1.662	0.0957	Disk	9.11×10^{0}	12.49%

Table 1: The results from the new data given a snapshot of the pristine P3HT morphology at a given snapshot corresponding to simulation time, τ.

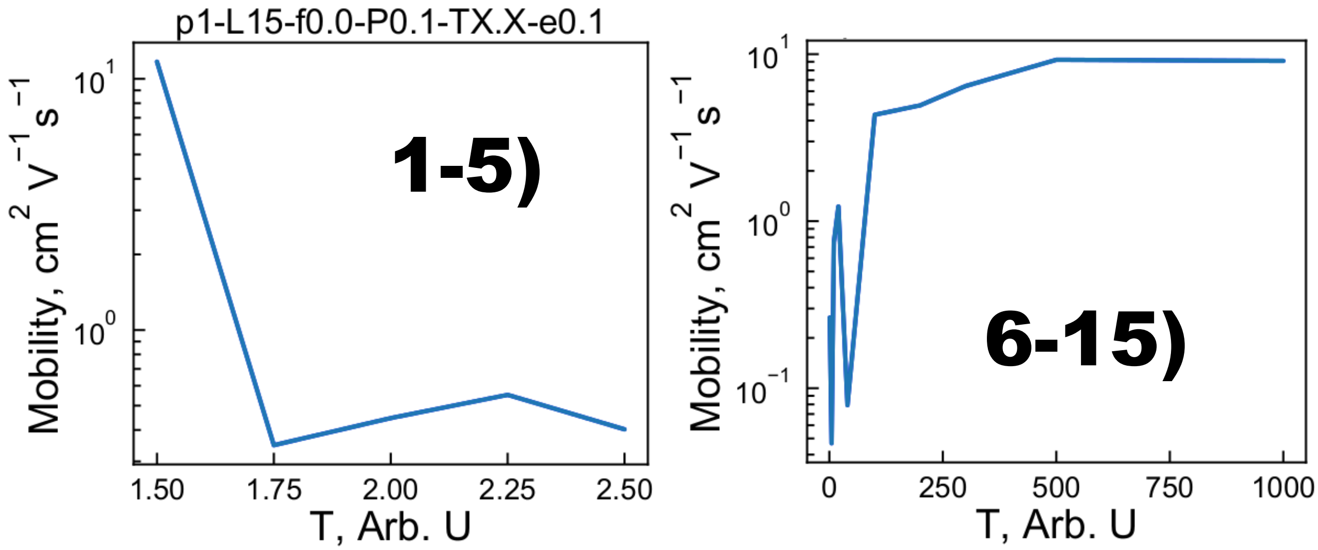

Figure 1: The mobility trend observed as a function of increasing dimensionless evolution time

Representative Values From Literature:

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

1.1 3D Carrier Network

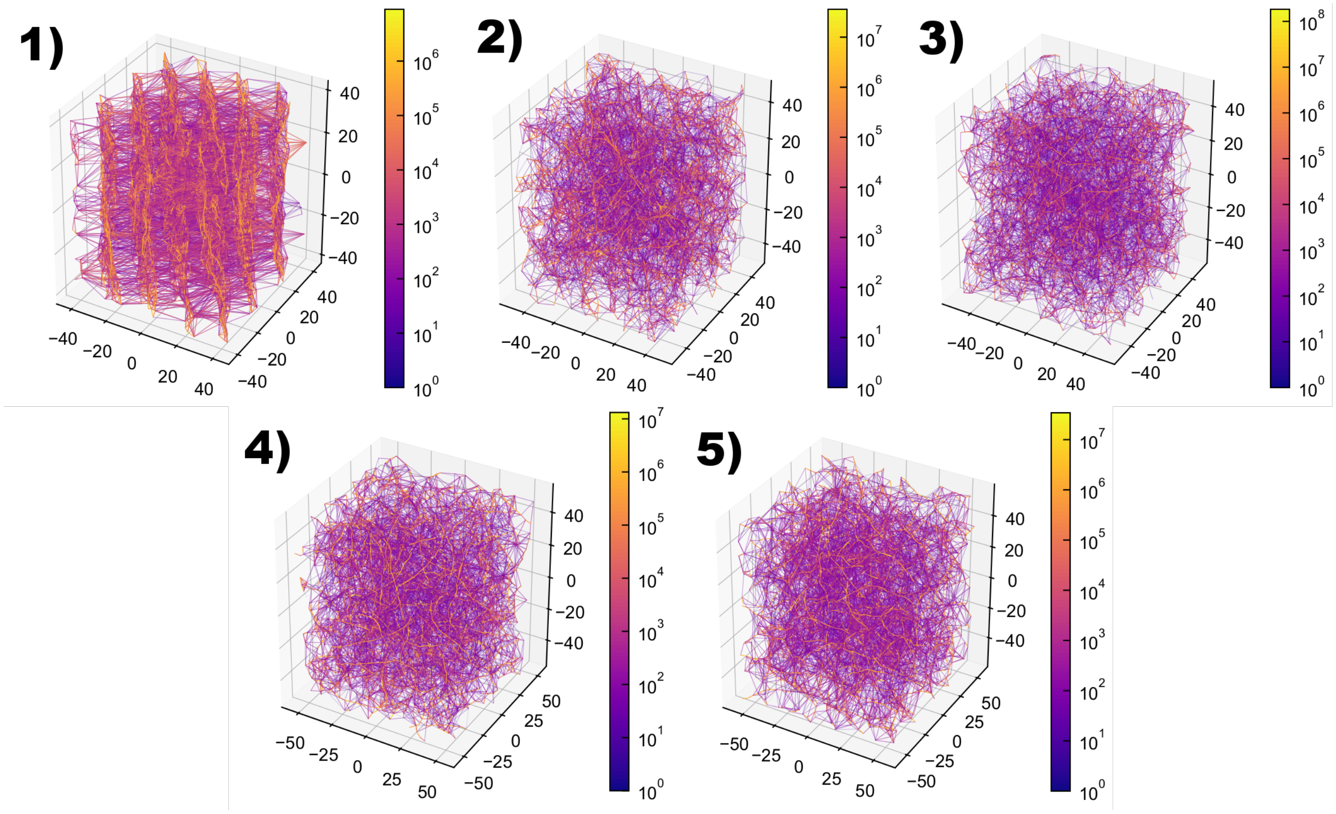

Figure 2: The 3D heatmap of charge transport routes within the morphologies **1 - 5**. More yellow routes describe commonly accessed hops between pairs of chromophores, whereas more purple routes are less widely used in the KMC simulations. Each node therefore represents the location of a single chromophore. The intensity value for the route is currently taken to be `I = np.log10(freq) / np.log10(max_freq)`.

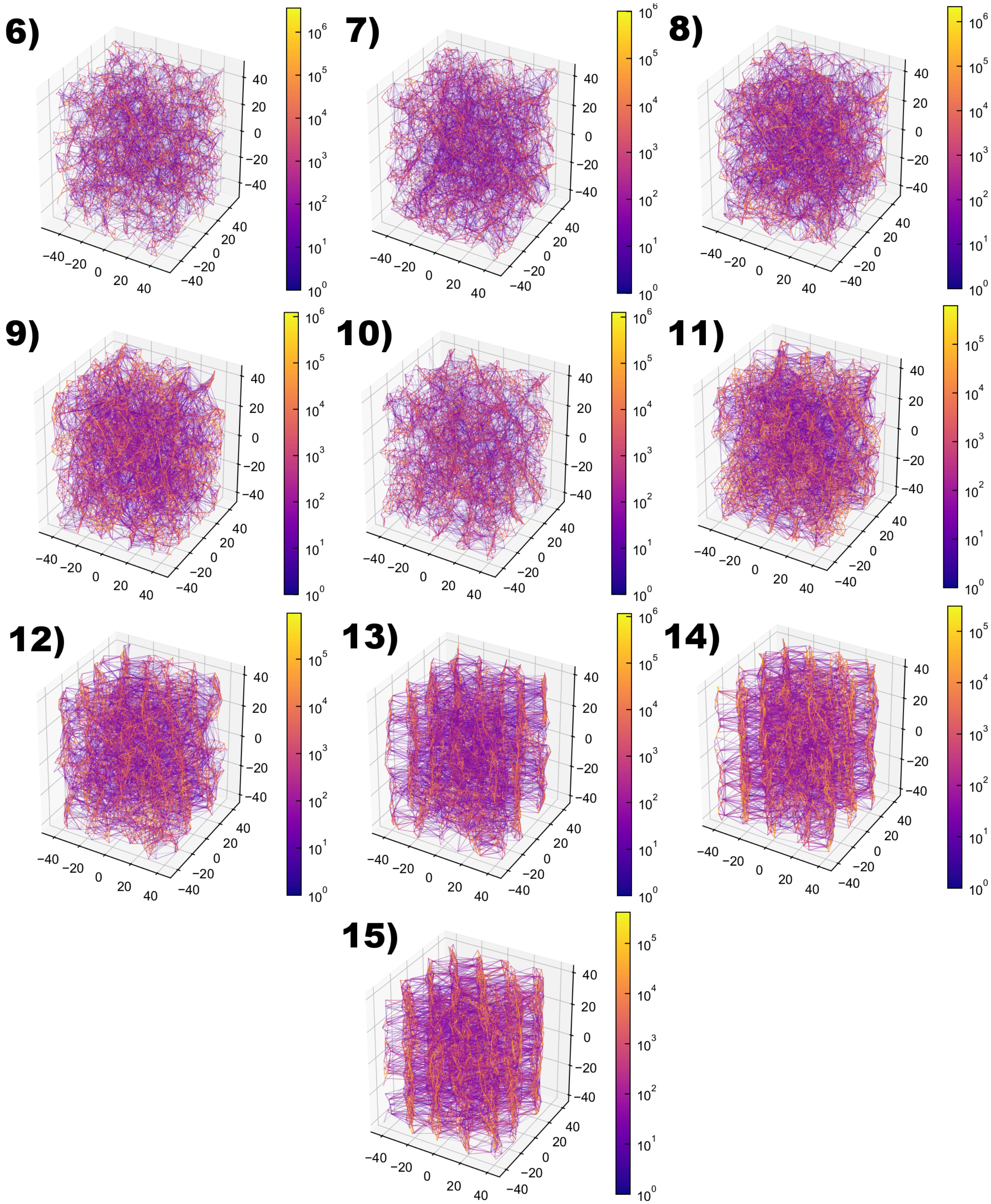

Figure 3: The 3D heatmap of charge transport routes within the morphologies **6 - 15**. More yellow routes describe commonly accessed hops between pairs of chromophores, whereas more purple routes are less widely used in the KMC simulations. Each node therefore represents the location of a single chromophore. The intensity value for the route is currently taken to be `I = np.log10(freq) / np.log10(max_freq)`.

1.2 Anisotropies

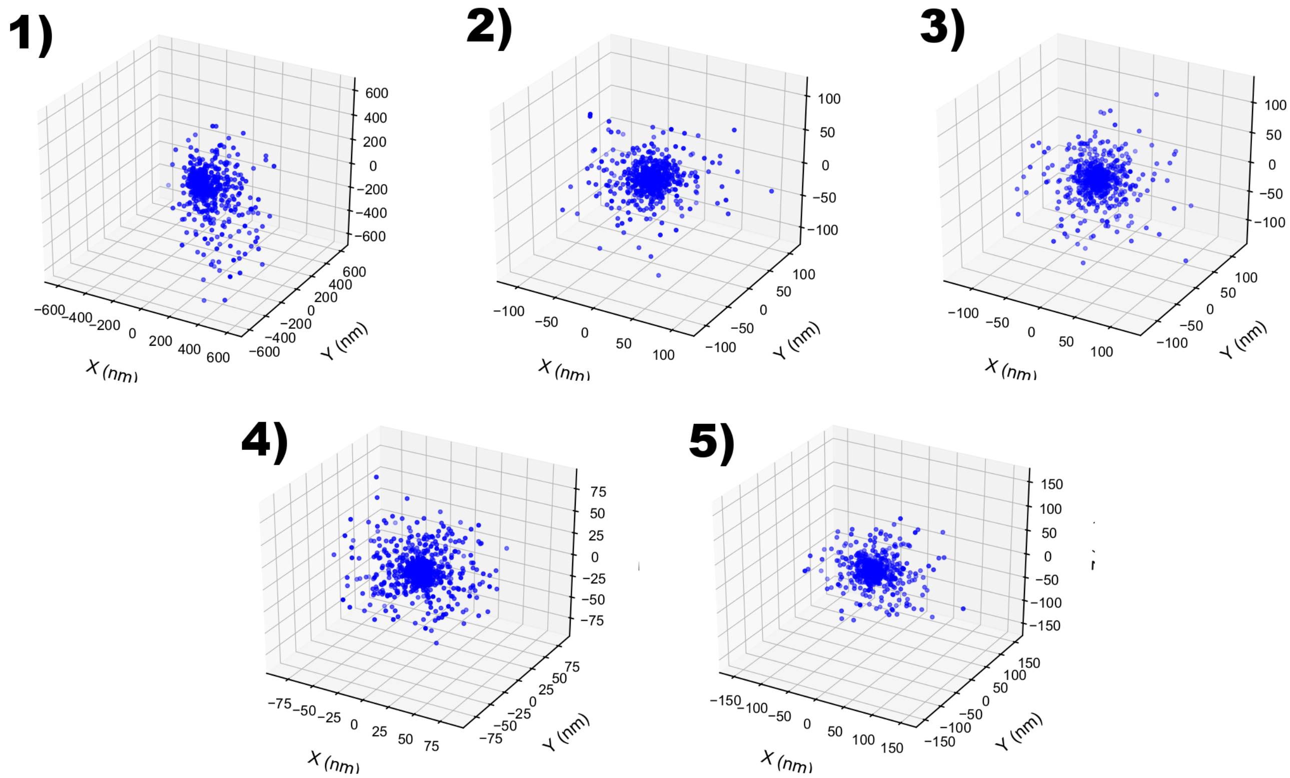

Figure 4: The periodic anisotropies of the carrier transport within the morphologies **1 - 5**.

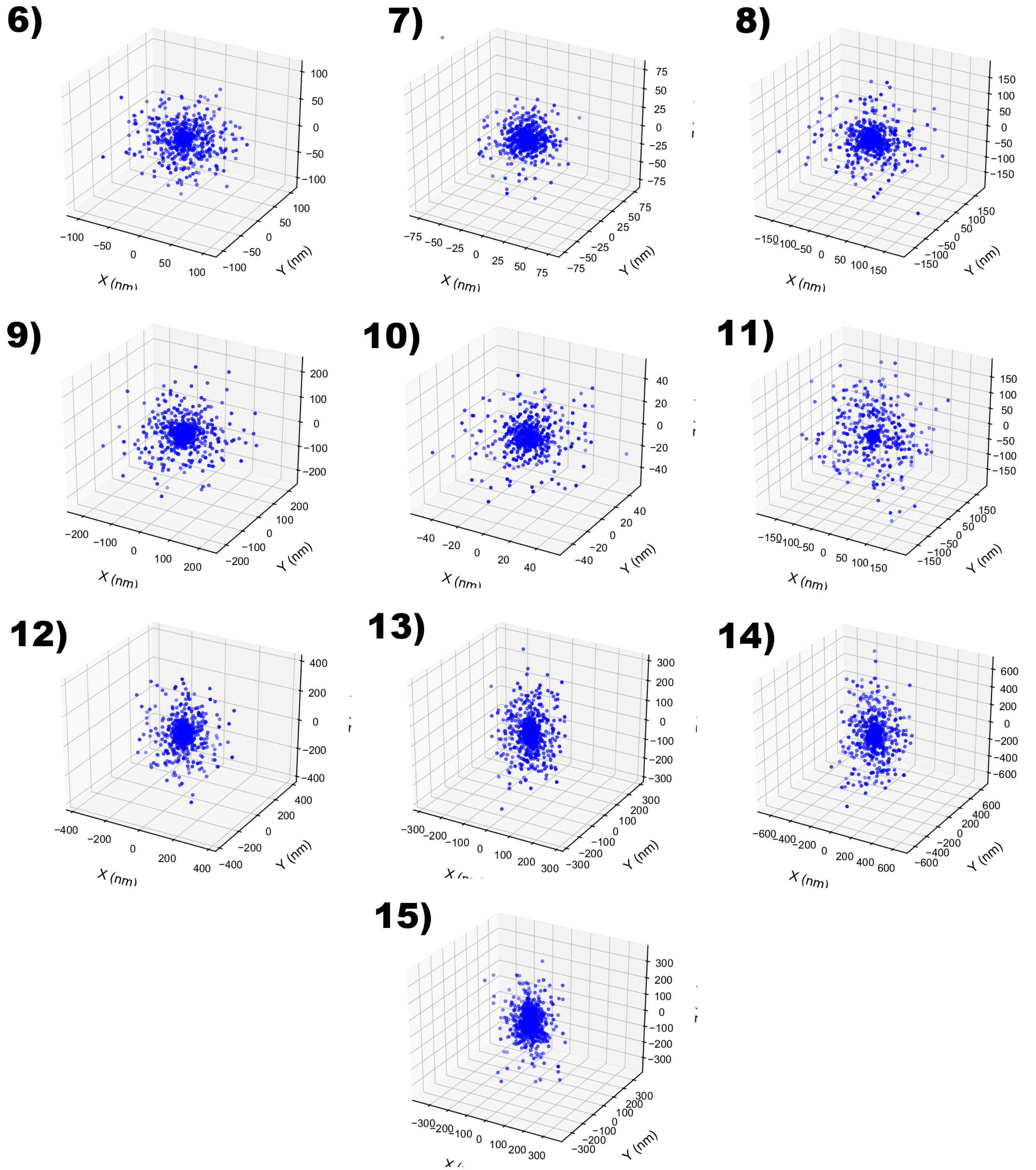

Figure 5: The periodic anisotropies of the carrier transport within the morphologies **6 - 15**.

1.3 MSDs

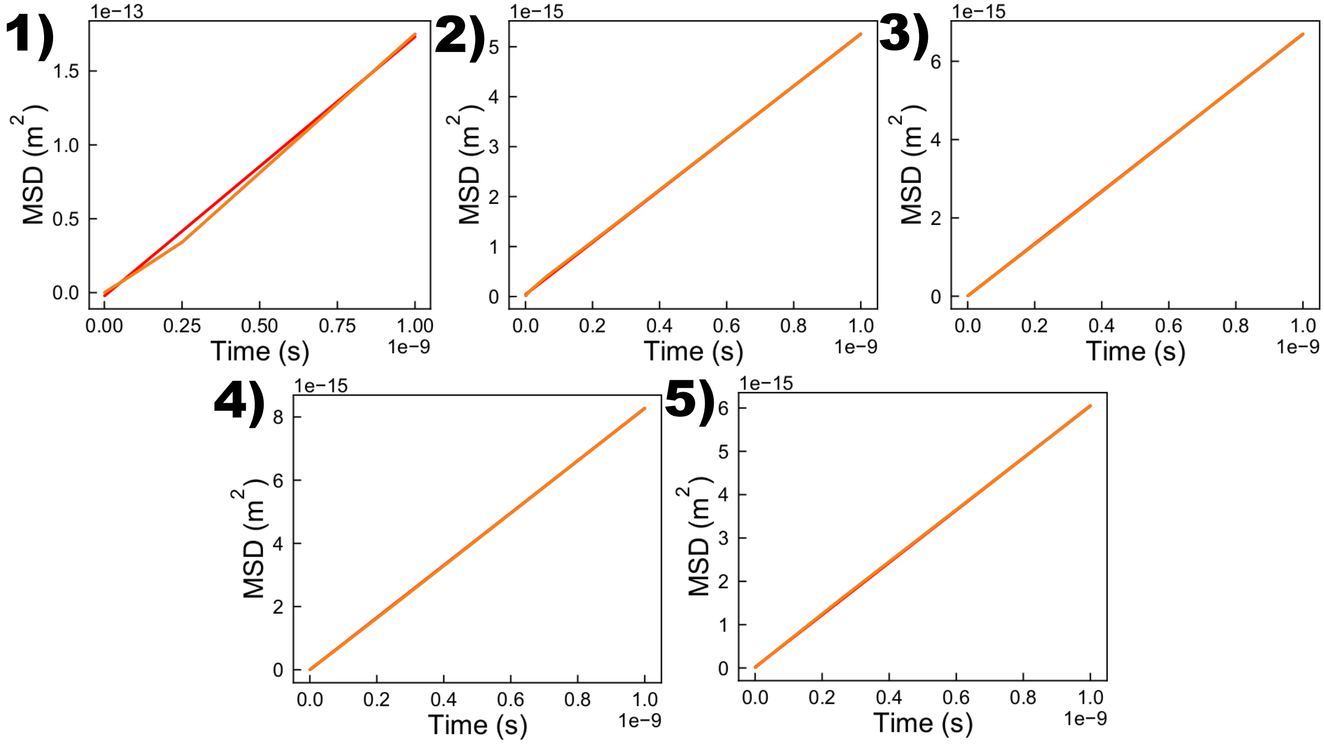

Figure 6: The linear mean squared displacement curves of the carriers within the morphologies **1 - 5**.

1.4 Hopping Rate Distributions

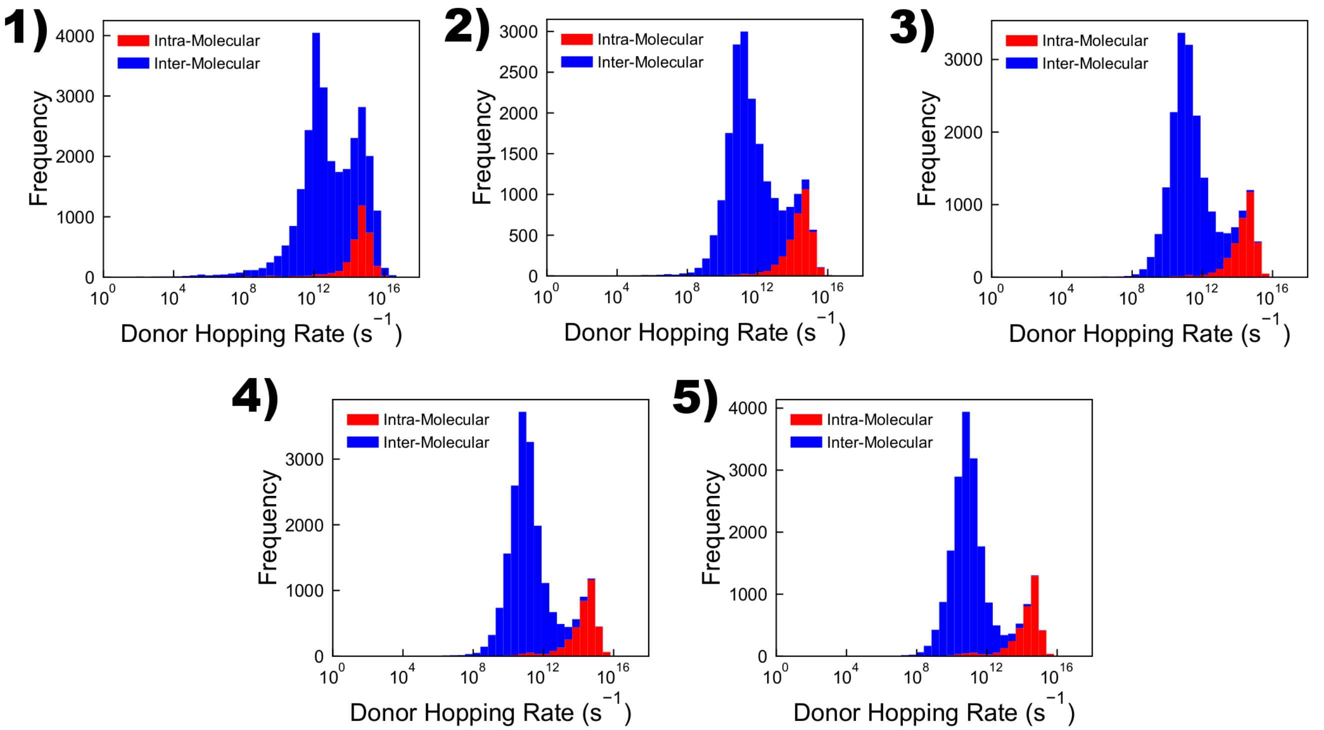

Figure 7: The stacked hopping-rate distributions for intra- and inter-molecular hops executed by carriers within the morphologies **1 - 5**.

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.