MorphCT Results - PAHs

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1 Mobility Results

ID	Simulation Name	Density ($g\,cm^{-3}$)	Anisotropy (Arb. U.)	Anisotropy (Shape)	Mobility ($cm^2\,V^{-1}\,s^{-1}$)
1	PE_MultiStack_Eclipsed	1.06	0.9456	Thin Tube	5.87×10^{0}
2	PE_SingleStack_Eclipsed	1.06	0.2016	Fat Tube	4.73×10^{-2}
3	PE_SingleStack_Ordered	1.06	0.0844	Oblate Spheroid	5.09×10^{-2}
4	PT_MultiStack_Eclipsed	1.01	0.1245	Oblate Spheroid	2.48×10^{-1}
5	PT_MultiStack_Ordered	1.01	0.1313	Oblate Spheroid	1.65×10^{-3}
6	PT_SingleStack_Eclipsed	1.01	0.7264	Thin Tube	1.15×10^{0}
7	PT_SingleStack_Ordered	1.01	0.2536	Oblate Spheroid	2.04×10^{-1}

Table 1: The results from MorphCT for the various PAH morphologies.

Representative Values From Literature:

- PE Mobility: 2E-1 (one paper reports 5E2)
- PT Mobility: 8E-1

Comments:

- The mobilities reported here vary significantly, but generally have good experimental agreeement
- As expected, the eclipsed systems **1**, **2** and **6** generally have higher anisotropies than their comparable ordered systems. This is due to a higher degree of order along the stack, which makes it easier for carriers to travel along the stack, resulting in more anisotropic transport.
- However, this trend is only the case for the single-stack systems, where the columns pack off the simulation volume axes. This means, due to periodic boundary conditions, that the simulation volume actually only contains a single stack as carriers can 'hop to adjacent stacks' by simply continuing along the current one.
- The discrepancy between the off-axis single-stack systems (**2**, **3**, **6**) and the along-axis multiple-stack systems (**1**, **4**, **5**) is visible in the comparisons of the perylothiophene systems.

- Anisotropy is significantly lower in the eclipsed case (**4** compared to **6**) when multiple stacks are present, compared to a single stack. This could partially be a result of the slight herringbone structure observed in the multiple-stack systems increasing the transfer integrals to neighbouring stacks, permitting more parity between transport along- and between-stacks.
- Mobility is also lessened by at least an order of magnitude. This again could result from the herringbone structure which forces neighbouring molecules within a stack slightly further apart to accomodate the alternating orientations of molecules between stacks.

- The perylene systems **1** and **2** do not exhibit the above behaviour - the mobility trend is reversed (the single-stack mobility in **2** is two orders of magnitude slower than the multi-stack mobility of **1**). This reinforces the idea that the difference between the single- and multi-stack cases is a factor of the herringbone-like packing observed in perylothiophene, as the perylene systems do not exhibit the same herringbone-like structure. What is the reason for the two order of magnitude discrepancy in the mobility then, if neither system exhibits herringbone packing?

1.1 3D Carrier Network

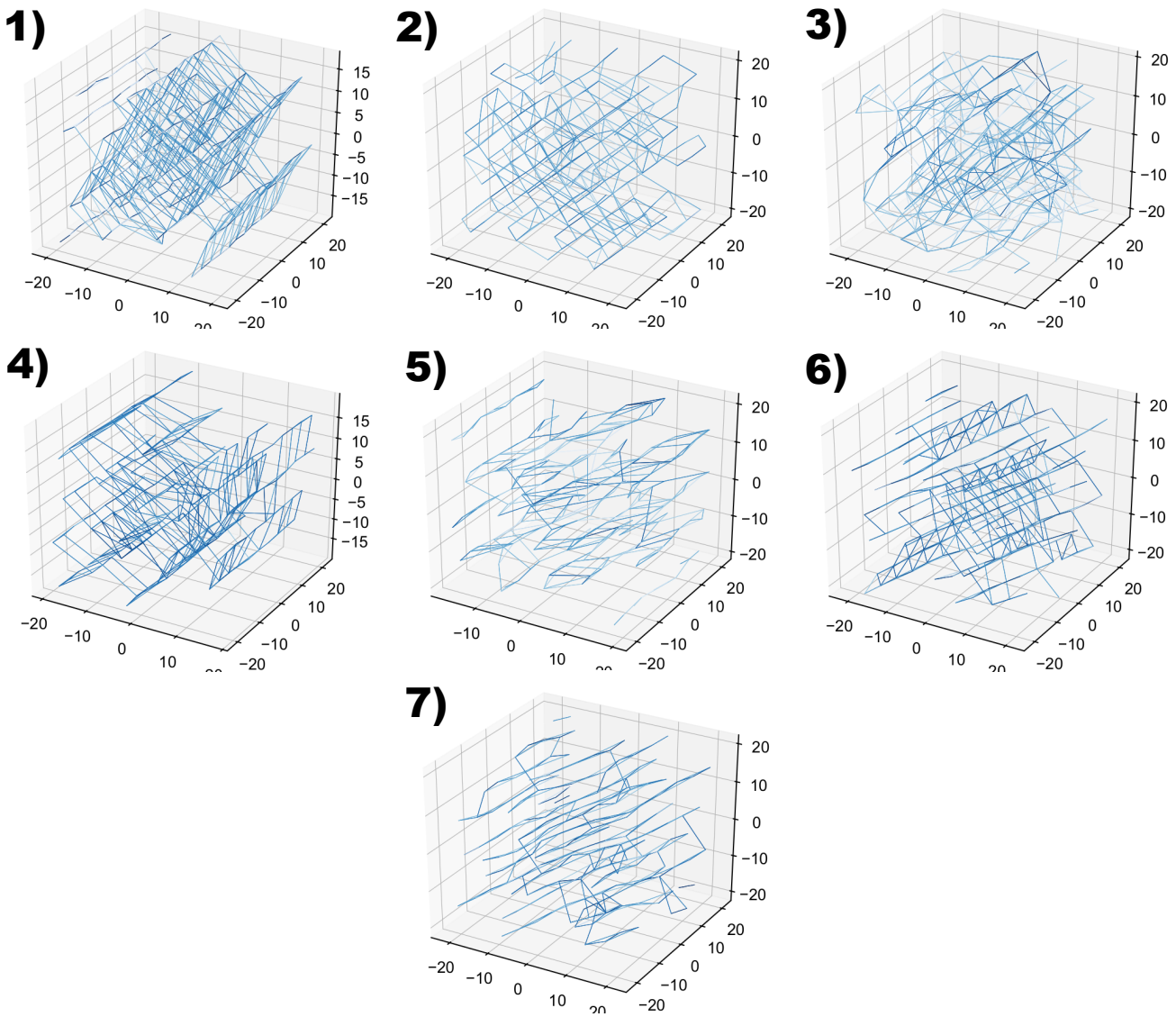

Figure 1: The 3D heatmap of charge transport routes within the morphologies **1** - **7**. Dark routes describe commonly accessed hops between pairs of chromophores, whereas pale routes are less widely used in the KMC simulations. Each node therefore represents the location of a single chromophore. The intensity value for the route is currently taken to be `I = np.log10(freq) / np.log10(max_freq)`.

1.2 MSDs

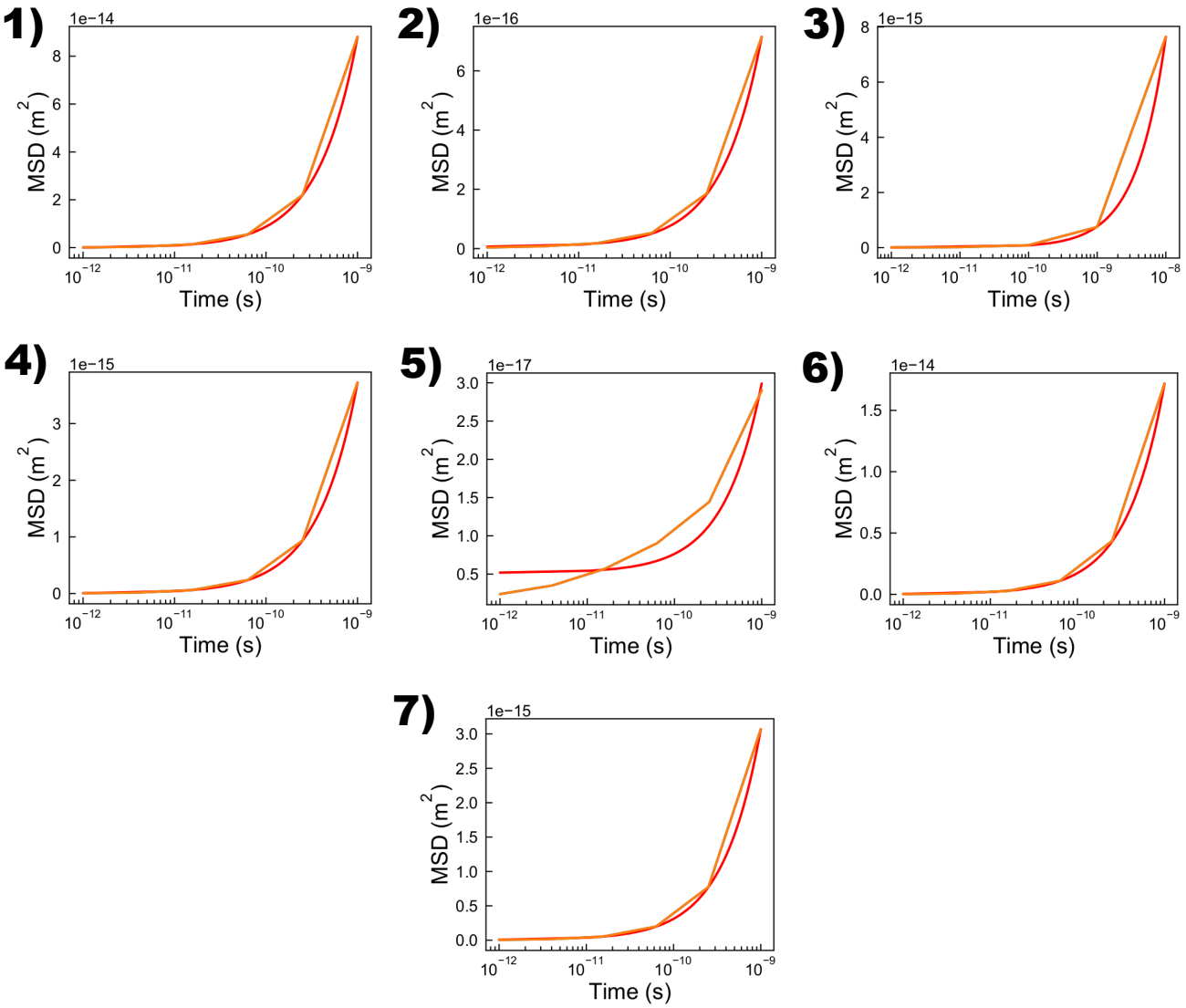

Figure 2: The semi-log-x mean squared displacement curves of the carriers within the morphologies **1** - **7**.

- These are among the best fits we've ever had with MorphCT.
- The 'odd one out' here is **5**, which exhibits slight saturation leading to a poorer fit.
- Fitting parameters have r values of ¿ 99.999%, except for **5** which has r = 97.29%

1.3 Hopping Rate Distributions

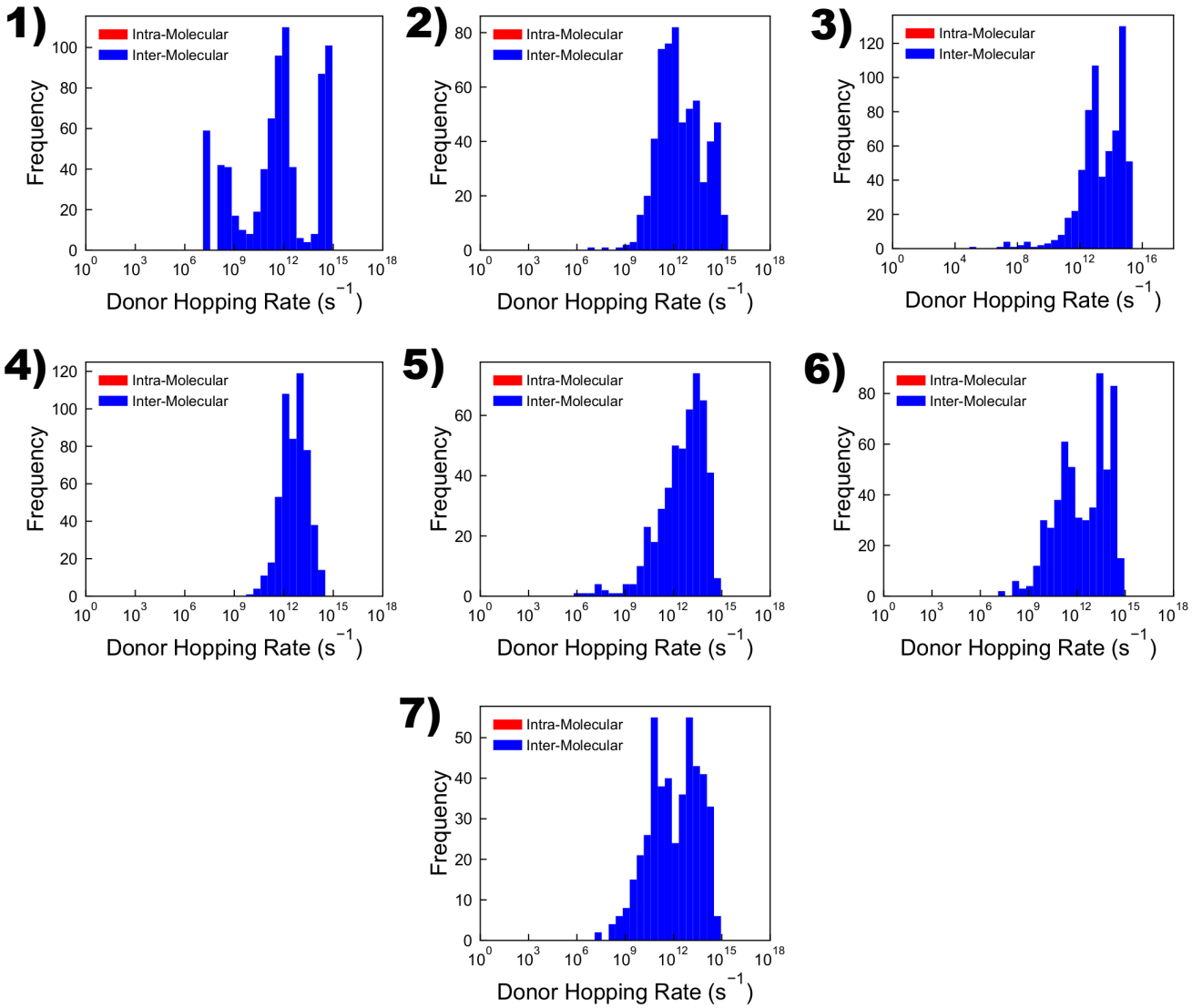

Figure 3: The hopping-rate distributions for hops executed by carriers within the morphologies **1** - **7**. It would require some pretty clever ad-hoc code, but it would be really nice to split this into intra- and inter-stack hops!

- The hopping rate distributions vary quite a lot! Some are single-mode, others bimodal, and one is tri-modal.
- I will make more comments here after I've made the code mentioned above where we compare intra- to inter-stack hops

2 Outstanding Questions

- TBA