Adapting Lattice swelling model to Förster exciton diffusion theory:

Chromophore density C in units of chromophores/nm^3 = Nchrom/VNP

Using a 10 nm particle, and the respective numbers of chromophores per 10 nm particle determined from latspace.m

Nchrom, PFBT = 320 chromophores per NP

Nchrom, MEHPPV = 770 chromophores per NP

VNP, sphere = (4/3)\*pi\*r^3 = 524 nm3

CPFBT = 0.61 chromophores/nm^3

CMEHPPV = 1.47 chromophores/nm^3

We can determine chromophore spacing x from C by

x = C-1/3 = (VNP/Nchrom)1/3, which is the cube root of the volume per chromophore, yielding

~0.9 nm for MEH-PPV, and ~1.2 nm for PFBT

Diffusion constant from Bardeen ARPC/Förster theory

, where from Bardeen ARPC

When plugged in for LD we get



Plugging in what we know from the chromophore density information and assuming R0 = 4 nm, this gives LD ranging from ~160 nm to ~220 nm for PFBT, and LD ranging from ~300 nm to ~400 nm for MEH-PPV. (Bardeen mentions that LD is grossly overestimated using this method for small chromophore separations).

Regardless, given that the per time step energy transfer probability for a random walk is:

, that we originally describe using to give 

We can plug in Förster’s verion of D and see what happens:

,

And we can use the relation of C1/3 = 1/x, giving

,

Which yields pet >> 1 for time steps of 1-10 ps, using the minimum value of .

Alternate solution:

Given the swelling factor *f* :



And that , we can restate *f* as

, which still gives

**, for the chromophore spacing increase (larger number in numerator).

Then, using the fact that according to Förster theory, the diffusion constant D is proportional to C4/3, we can adjust the FRET probability by raising the swelling factor to the power 4/3, which yields:

, which is similar to what we did according to the Silbey paper, and doesn’t use the more complicated definition of D from Förster theory.

The larger chromophore spacing still ends up in the denominator to reduce pet as the particle swells, we just use k = 4 instead of 2 (which was still in their range of values for the power of k).