Explanations:

**Reorg energy:**

Dimer consistently lower reorg energy for all functionalisations why?

Katherine, Closed ring?

Functional Groups?

**Transfer Integral:**

Base 2 Js poor compared to Base 1, poor overlap due to bulky Net group restricting pi overlap

Dimer vs monomer? Base 3 vs. Base 4?

Katherine, Closed ring?

Functional Groups?

**Mobility:**

Dimer vs. Monomer:

Dimer better mobility, from Jochen:

1. The phenalenyl parent structures form a spiro structure that arranges the phenalenyl components in neat stacks, where the distance and formation of pi-dimers (or not!) is crucial for the conductivity. I forgot the exact paper that this was published in, but it’s probably one of Haddon’s JACS papers from 2008/2010 (he had several on these structures). I’ve also attached a good review that will probably have a discussion of the phenomena. Design and Applications  
   of Single-Component Radical Conductors Dafei Yuan,1,2,3 Wuyue Liu,1,2,3 and Xiaozhang Zhu1,2,\*
2. The mixed valence (i.e. one cation, one radical) has been proposed to increase the conductivity by having a half-filled valence band. I’ve attached a 2022 paper where the authors use a different type of spiro-boronate structure. **Partially Oxidized Purely Organic Zwitterionic Neutral Radical Conductor: Multi-step Phase Transitions and Crossover Caused by Intra- and Intermolecular Electronic Interactions**

Katherine, Closed ring?

Functional Groups?