Charge Transport in Imperfect Organic Field Effect Transistors: Effects of Explicit Defects and Electrostatics

Table S1. Electronic structure parameters for nickel(II) and copper(II) phthalocyanine molecules considered in this work, including orbital energies and reorganization energy for hole transfer.

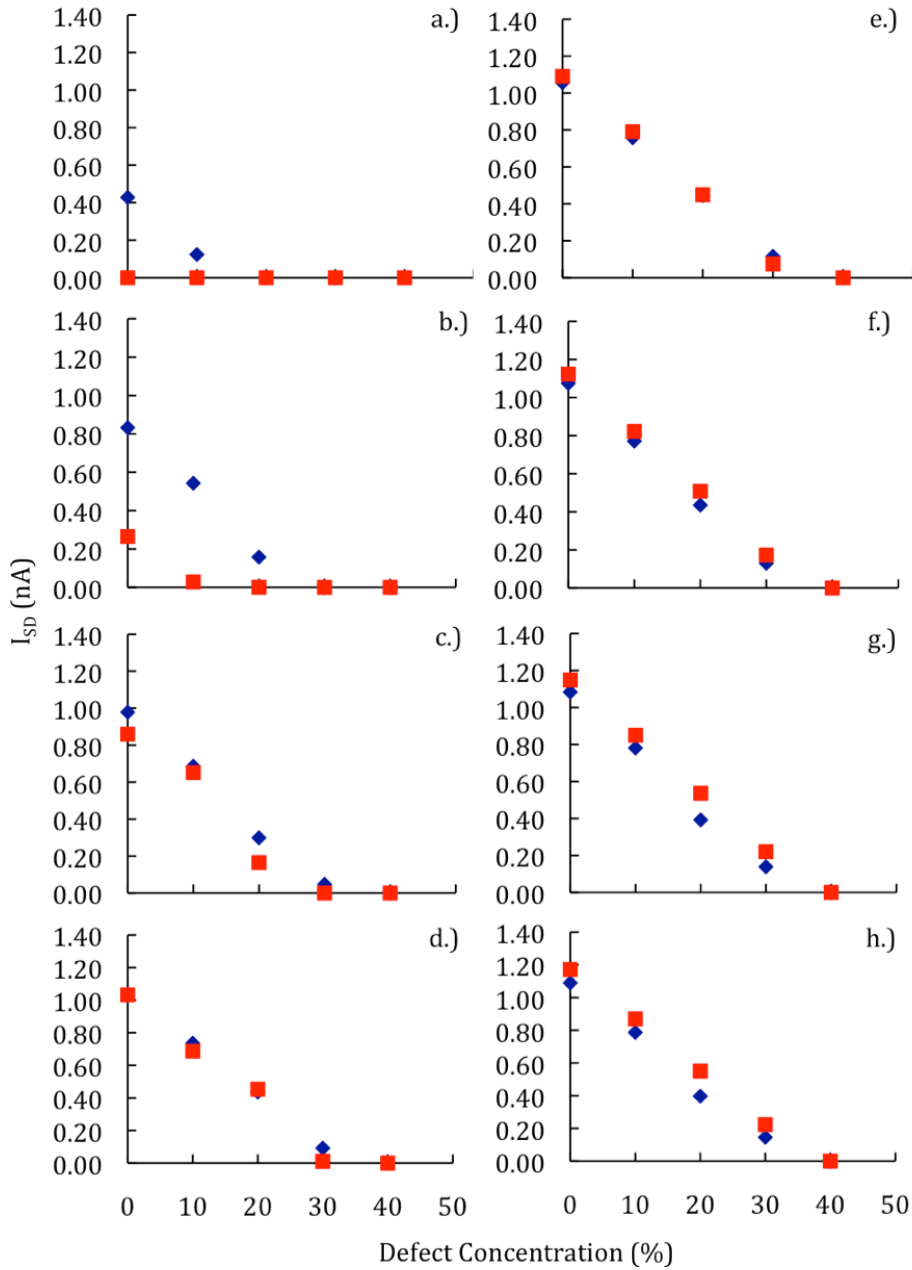| Compound	HOMO Energy (eV)	LUMO Energy (eV)	Reorganization Energy (eV)
phthalocyanine ligand	-5.37	-3.23	0.329
Nickel (II) phthalocyanine	-5.34	-3.09	0.208
Copper (II) phthalocyanone	-5.36	-3.10	0.274

Figure S1: I_{SD} vs. trap concentration snapshots. Snapshots are shown after the following numbers of steps (iterations), a.) 100,000, b.) 250,000, c.) 500,000, d.) 750,000, e.) 1,000,000, f.) 1,250,000, g.) 1,500,000, h.) 1,750,000. Blue diamonds represent calculations that include Coulomb interactions and red squares represent calculations that do not include Coulomb interactions.
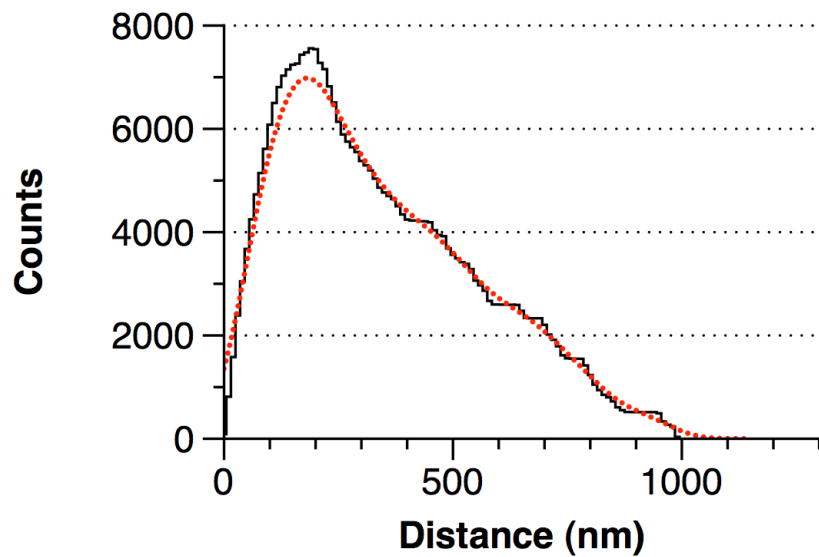
Figure S2. Distribution of distances between an arbitrary site and a charged defect (for 1% defect sites) across the entire film. Note that the distances follow a Poisson distribution, with more long-range interactions than small.
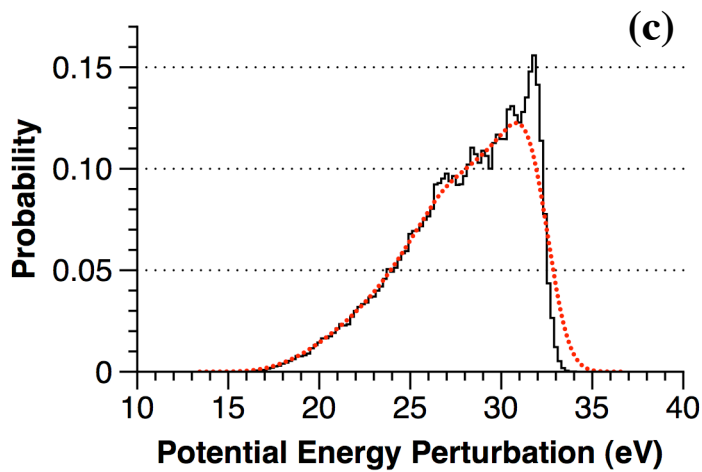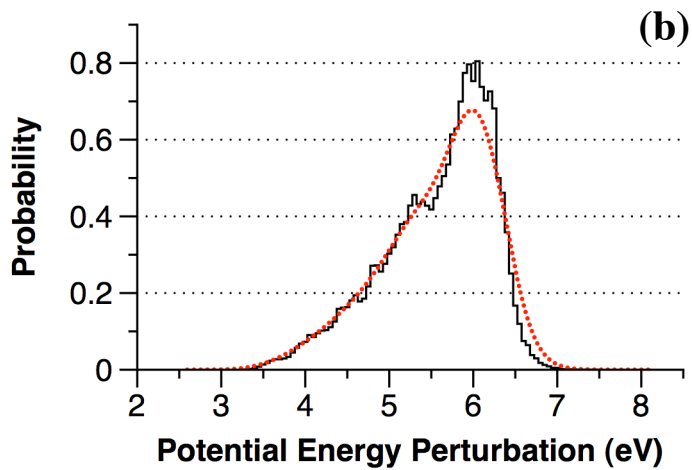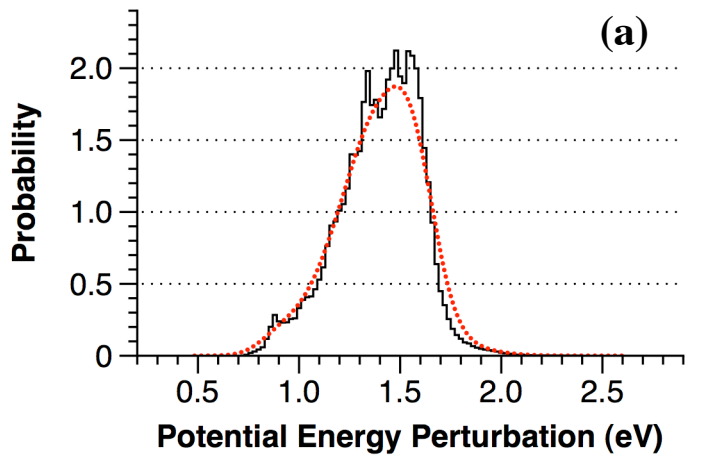
Figure S3. Distributions of site energy shifts for (a) 0.25%, (b) 1%, and (c) 5% charged defects, reflecting a reciprocal Poisson distribution and a large low-energy tail.
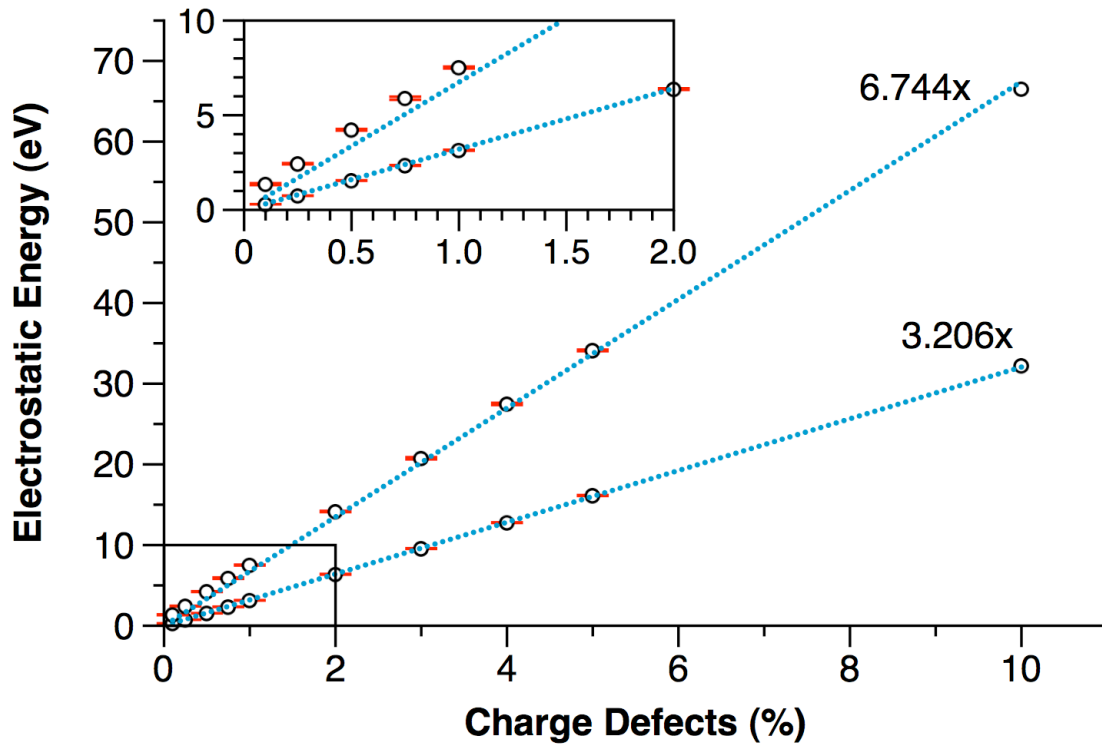
Figure S4. Scaling of site energy shifts for charged defects, indicating the minimum and maximum energy shift for each concentration. Horizontal lines reflect error bars.