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Interfacial disorder drives charge separation in molecular semiconductors

ADAM WILLARD, MIT

One of the fundamental microscopic processes in photocurrent generation is the dissociation of neutral photo-excitations (i.e., Frenkel excitons) into free charge carriers (i.e., electrons and holes). This process requires the physical separation of oppositely charged electrons and holes, which are held to together by an attractive electrostatic binding energy. In traditional inorganic-based photovoltaic (PV) materials, this binding energy is generally small and easily overcome, however, in organic-based PVs (OPVs) the exciton binding energy can significantly exceed thermal energies. The inability of bound charges to overcome this large binding energy has been implicated as a primary source of efficiency loss in OPVs. Here I present results from our recent efforts to explore the role of static molecular disorder in mediating this process. Using a simple lattice model of exciton dynamics we demonstrate that random spatial variations in the energetic landscape can mitigate the attractive Coulomb interaction between electrons and holes. We show that this effect manifests as a reduction in the free energy barrier for exciton dissociation that grows more pronounced with increasing disorder. By considering the competition between this thermodynamic effect and the disorder-induced slowing of dissociation kinetics we demonstrate that exciton dissociation yields are expected to depend non-monotonically on the degree of static disorder.