Excitons and Exciton Confinement in Organic Heterojunctions

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Excitons play a central role in photogeneration in organic detectors and solar cells. The efficiency of the exciton dissociation process is directly related to molecular structure of the donor and acceptor molecules and the film morphology. In our work, we have focused on understanding the microscopic nature of these interactions in both fullerene and non-fullerene based junctions. We have developed quantum mechanical models coupled with molecular dynamics simulations to understand the role that morphology plays on the energy of the charge transfer state – i.e. the intermediate between exciton and free polaron – and ultimately its ability to generate free charge at a low expense of energy. We find that quantum confinement of the exciton by crystalline domains in dilute donor-acceptor blends can result in substantial energy shifts in the state, thereby impacting its binding energy.[1, 2] Further, we have developed models that quantitatively relate the energy loss in non-fullerene acceptors to the molecular structure itself. Ultimately, this understanding of exciton and CT state energetics has led to very high efficiency (>15%) organic solar cells, with prospects of reaching 20% in the not distant future.[3] The models, experiments and implications of these findings will be discussed in my presentation. Finally, if there remains time, I will discuss confinement effects in novel quantum well structures comprising a combination of organic and inorganic semiconductors, including 2D solids.[4]

[1] X. Liu, K. Ding, A. Panda, and S. R. Forrest, "Charge transfer states in dilute donor-acceptor blend organic heterojunctions," *ACS Nano,* vol. 10, p. 7619, 2016.

[2] K. Ding, X. Liu, and S. R. Forrest, "Charge Transfer and Collection in Dilute Organic Donor-Acceptor Heterojunction Blends," *Nano letters,* 2018.

[3] X. Che, Y. Li, Y. Qu, and S. R. Forrest, "High Fabrication Yield Organic Tandem Photovoltaics Combining Vacuum- and Solution-Processed Subcells with 15% Efficiency," *Nature Energy,* vol. 3, p. 422, 2018.

[4] A. Panda, C. K. Renshaw, A. Oskooi, K. Lee, and S. R. Forrest, "Excited State and Charge Dynamics of Hybrid Organic/Inorganic Heterojunctions. II. Experiment," *Phys. Rev. B,* vol. 90, p. 045303, 2014.