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Molecular Disorder: Two Case Studies

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ABSTRACT

Disorder is ubiquitous in condensed-phase systems, and its existence may be favored or disfavored depending on the applications. In this talk, I will discuss two cases where molecular disorder plays important roles. In the first case, proton disorder in ice gives rise to the lack of cross peaks in the OH-stretch two-dimensional infrared spectra for ice, which are anticipated to exist due to the substantial resonant vibrational energy transfer in ice. In the second case, our simulation benchmarked against experiment suggests that a moderate amount of energetic disorder in organic donor-acceptor blends may facilitate the dissociation of the inter-facial charge-transfer exciton, potentially leading to a higher charge-generation efficiency.

BIO:

Liang Shi received his Ph.D. in Theoretical Chemistry with Prof. James Skinner at the University of Wisconsin, Madison in 2014. He did his postdoctoral work at MIT under the direction of Prof. Adam Willard. In 2016, he joined the Chemistry and Chemical Biology program at UC Merced, and his research focuses on developing and applying multi-scale modeling methods to understand the structure, dynamics, and spectroscopy of condensed-phase molecular systems, such as novel optoelectronic materials.