Modeling Photoactive Organic Materials

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Photoresponsive molecular materials provide synthetic tunability to control the charge transport for transistor, solar harvesting, or singlet fission applications. Photoexcitation often results in nuclear rearrangement to stabilize the new excited electronic configuration. In solution this rearrangement leads to slight vibrational cooling, in the solid state the confinement of the molecules can alter the excited state decay mechanism. In particular thermal dissipation in solid state molecular materials contributes to dynamic disorder that effects charge carrier properties. In particular, molecular materials move charges in some directions much more efficiently than others due to the packing of the molecules. Noncovalent interactions between the molecular components mean that dynamic disorder in these materials can have a large impact on the electronic properties of these materials at room temperature. This work explores how packing and vibrations in organic crystals affect charge transport. In particular, including zero-point energy corrections even in perfect single crystal organics show a detrimental effect of both inter- and intra-molecular vibrations on the mobility of charge carriers.