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Boosting charge separation in organic photovoltaics: unveiling dipole moment variations in excited non-fullerene acceptor layers

Mid-infrared transient absorption spectroscopy (MIR-TA) is quite useful to investigate the intramolecular and intermolecular charge-transfer and charge-dissociation. Using MIR-TA, we revealed that charge-transfer and charge-dissociation can occur even in a neat film of non-fullerene acceptor ITIC without donors. In neat ITIC layers, the intermolecular charge-transfer immediately proceeds after photoirradiation to form weakly-bound excitons, which are further dissociated into free electrons and holes. Theoretical calculations indicate that this pathway is triggered by the large dipole moment change on the excited state generated at the lower symmetric V-type molecular stacking of ITIC.



