

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ultrafast Spectroscopy Reveals Frenkel-CT Mixed Excitonic States in Copper Phthalocyanine ROBERT YOUNTS, TERRY MCAFEE, BHOJ GAUTAM, DANIEL DOUGHERTY, HARALD ADE, KENAN GUNDOGDU, North Carolina State University — In organic semiconducting systems, intermolecular charge transport and energy diffusion take place along the π - π stacking direction, which is beneficial for opto-electronic devices. Therefore it is essential to study electronic state structure in the π - π stacking direction in organic solids. We studied a model quasi-one-dimensional molecular crystal copper phthalocyanine, which has strong intermolecular coupling along the π - π stack. In this work, we used polarization resolved transient absorption spectroscopy and identified the coupling of low-lying singlet Frenkel (intramolecular) excitons with CT (intermolecular) excitons. Our study shows an evolution between localized and delocalized excitations which can be utilized to tune charge transport properties in molecular crystals. These studies provide fundamental understanding of electronic state structures, which will be essential for tailoring electronic properties of desired applications.

Robert Younts
North Carolina State Univ

Date submitted: 06 Nov 2015

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