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Structure-Property Correlations and Effect on Dynamics in intramolecular Singlet Fission[1] MOSHE CHESLER, SUMIT MAZUMDAR, University of Arizona — Utilizing singlet fission (SF) in organic photovoltaics is a promising direction for overcoming fundamental efficiency limits in single-junction solar cells and thus may lead to development of more highly efficient next generation renewable energy technology. Attention in this area has recently shifted from intermolecular SF (xSF) between chromophores in a solid to intramolecular SF (iSF) between those in a dimer for which linked acene chains have presented as strong candidates for potential use in SF-based solar cells. We have performed high-order configuration interaction (CI) calculations on several candidate systems and found that the photophysics of such systems is highly dependent on various factors such as linkage between the chromophores and relative difference in chromophore size. While this sensitivity to structural changes makes developing a comprehensive theory and reliable set of design strategies for SF materials difficult, analyzing the electronic structure of the low-lying eigenstates of the SF process together with the ground state absorption spectrum for various molecules can provide a qualitative prediction for the dynamics of relevant systems and may ultimately help guide future materials characterization and design.

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