Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

On The Geometric Nature of "Singlet Fission" in Certain Crystalline Conjugated Polymers NOAH RAHMAN, Department of Chemistry, University of California - Santa Barbara — In recent years, the coherent fission of low-lying singlet electronic excitations in conjugated polymers has attracted interest as a possible way to exceed the Shockley-Queisser limit in organic photovoltaics. Femtosecond spectroscopic and fluorescence measurements of such singlets and the resulting triplets in crystalline anthracene, tetracene and naphthalene reveal curious phenomena associated with certain vibrational modes, such as ultrafast propagation on a timescale inconsistent with conventional intersystem crossing, long-lived electronic coherence, and triplet magnetic anisotropy whose structure is consistent across all three materials. This conflicts with NRG and quantum chemical simulations, which posit isotropic triplets. I explain this by a dynamical Rashba spin-orbit interaction that decays as R^{-6}. This arises from a geometric SU(2) gauge potential generated by a nuclear-motion-induced parametric near-degeneracy of the molecular electronic states. The anisotropy is shown to follow from the work of Affleck and Oshikawa on spin one-half Heisenberg chains. Possible directions for future work are discussed, especially with regard to adiabatic pumping and topological insulators.

Noah Rahman
Department of Chemistry, University of California - Santa Barbara

Date submitted: 21 Dec 2012 Electronic form version 1.4