

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Exciton transfer rate between two neutral *trans*-polyacetylene chains QING LU, Boston University, Mechanical Engineering Department, MING-HAI LI, XI LIN, Boston University, Mechanical Engineering Department — We use the perturbation theory to compute the exciton transfer rate between two neutral *trans*-polyacetylene chains described by the Su-Schrieffer-Heeger (SSH) Hamiltonian. Considering the highly polarizable nature of *trans*-polyacetylene, we compute Coulomb interactions directly without the point dipole approximation as introduced in the conventional Forster approach. We find a much softer chain separation dependence of the energy transfer rate between two *trans*-polyacetylene chains, scaling as $1/r^n$ where $n \sim 4$ which is different from the well-known $n=6$ in the Forster formula or $n=5$ in the Hamaker formula for one-dimensional pairwise interactions. At a typical separating distance of 3.5 \AA , the $\pi - \pi$ interaction density is 0.21 eV/ \AA and the exciton transfer time is 72.6 ps . We are extending our calculations for poly-(*p*-phenylenevinylene) (PPV) and the complex porphyrin assembly using our recently developed adapted SSH Hamiltonian.

Qing Lu
Boston University, Mechanical Engineering Department

Date submitted: 20 Nov 2009

Electronic form version 1.4