Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Modeling energy transport in π-conjugated dendrimers containing triple bonds PAK KAU LIM, YONGWOO SHIN, XI LIN, Department of Mechanical Engineering and Division of Materials Science and Engineering, Boston University — An accurate, transferrable, and computational efficient adapted Su-Schrieffer-Heeger model Hamiltonian is developed to describe triple bonds in linear and fractal-dimensional π-conjugated systems. Chemical accuracy in the computed optical gaps is found for the cases of poly-(thiophene-ethynylene) and ploy-phenylacetylene of arbitrary lengths, with all errors less than 3% as compared to existing UV-visible adsorption spectra. The computed exciton migration processes in the phenylacetylene dendrimers indicates that such conjugated Bethe tree structures are efficient energy transduction funnels.

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Date submitted: 26 Nov 2011 Electronic form version 1.4