Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Reliable Prediction of Charge Transfer Excitations in Molecular Complexes LEEOR KRONIK, Weizmann Institute of Science, Israel, TAMAR STEIN, ROI BAER, Hebrew University of Jerusalem, Israel — We show how charge transfer excitations at molecular complexes can be calculated quantitatively using time-dependent density functional theory (DFT). Predictive power is obtained from range -separated hybrid functionals using non-empirical tuning of the range-splitting parameter. Excellent performance of this approach is obtained for a series of complexes composed of various aromatic donors and the tetracyanoethylene (TCNE) acceptor, paving the way to systematic non-empirical quantitative studies of charge-transfer excitations in real systems.

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Date submitted: 19 Nov 2008 Electronic form version 1.4