

Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

Time-dependent transition density matrix for visualizing charge-transfer excitations in photoexcited organic donor-acceptor systems¹

YONGHUI LI, CARSTEN ULLRICH, University of Missouri — The time-dependent transition density matrix (TDM) is a useful tool to visualize and interpret the induced charges and electron-hole coherences of excitonic processes in large molecules. Combined with time-dependent density functional theory on a real-space grid (as implemented in the octopus code), the TDM is a computationally viable visualization tool for optical excitation processes in molecules. It provides real-time maps of particles and holes which gives information on excitations, in particular those that have charge-transfer character, that cannot be obtained from the density alone. Some illustration of the TDM and comparison with standard density difference plots will be shown for photoexcited organic donor-acceptor molecules.

¹This work is supported by NSF Grant DMR-1005651

Yonghui Li
University of Missouri

Date submitted: 28 Sep 2013

Electronic form version 1.4