Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Real-time visualization of excited-state dynamics in molecular chains[1] YONGHUI LI, CARSTEN ULLRICH — Time-dependent density-functional theory allows one to calculate excitation energies and the associated transition densities in principle exactly. The transition density matrix (TDM) provides additional information on electron-hole localization and coherence of a specific excitation. We have extended the TDM concept into the real-time domain in order to visualize the excited-state dynamics in conjugated molecules. Our computational scheme is based on solving the time-dependent Kohn-Sham equations with the OCTOPUS code and then calculating the time-dependent Kohn-Sham TDM using a spatial partitioning scheme. The method is applied to show in real time how locally created electron-hole pairs spread out over neighboring conjugated molecular chains. The coupling mechanism, electron-hole coherence, and the possibility of charge separation are discussed.

[1]This work is supported by NSF Grants DMR-0553485 and DMR-1005651

Yonghui Li

Date submitted: 18 Nov 2010 Electronic form version 1.4