Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Time-dependent transition densities[1] YONGHUI LI, CARSTEN A. ULLRICH, University of Missouri — To visualize and interpret the induced charges and electron-hole coherences of electronic excitations in molecules, a real-space density matrix analysis is a useful computational tool. We extend this technique into the nonlinear, real-time domain and define the time-dependent transition densities in the context of time-dependent density-functional theory. This opens up the possibility of a real-time monitoring of the optical excitation dynamics in molecules, providing a visualization tool for processes such as exciton migration or charge-transfer excitations. The method will be illustrated for simple one-dimensional model systems.

[1]Supported by Research Corporation and NSF DMR-0553485

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Date submitted: 20 Nov 2008 Electronic form version 1.4