

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The Time-Dependent Particle-Hole Map¹ CARSTEN ULLRICH,
University of Missouri, YONGHUI LI, Vanderbilt University — The particle-hole map (PHM) is proposed as a new visualization tool to analyze electronic excitations in molecules in the time- or frequency domain, to be used in conjunction with TDDFT or other ab initio methods. The purpose of the PHM is to give detailed insight into electronic excitation processes which is not obtainable from local visualization methods such as transition densities, density differences, or natural transition orbitals. The PHM provides information on the origins, destinations, and coherences of charge fluctuations during an excitation process. In contrast with the transition density matrix, the PHM has a statistical interpretation involving joint probabilities of individual states and their transitions, and it is easier to read and interpret. We discuss and illustrate the properties of the PHM and give several examples and applications to excitations in one-dimensional model systems and in organic donor-acceptor systems.

¹Work supported by NSF grant DMR-1408904

Carsten Ullrich
University of Missouri

Date submitted: 01 Nov 2015

Electronic form version 1.4