

Bonds in Motion: the time-dependent electron localization function — T. BURNUS, M. A. L. MARQUES, AND E. K. U. GROSS — Physics Department, Freie Universität Berlin, Germany. As early as during our undergraduate studies we are confronted with the concept of a chemical bond. The idea is simple and elegant: electron pairs shared between neighbouring atoms provide the necessary attraction to bind the molecule. Unfortunately, the one-electron molecular orbitals that stem from a DFT or Hartree–Fock calculation are generally quite delocalized over several atoms and have little to do with our intuitive picture of a bond. There are, however, quantities that bring into evidence the subtle nature of covalent bonding. One such quantity is the electron localization function (ELF). In this communication we present a generalization of the ELF to the time-dependent domain. In time-dependent systems, the ELF contains an additional term coming from the electron current (or from a different perspective from the phases of the wave functions). By depicting the time-depend ELF over time, we are able to follow the evolution of bonds during chemical reactions. First results showing the time-dependent ELF for the interaction of small molecules with laser fields are presented in form of a movie.