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Observing electron rearrangement in the simplest chemical reaction AGNIESZKA JARON-BECKER, JILA and Dept. of Physics, University of Colorado, Boulder, CO, 80309, WEN LI, Department of Chemistry, Wayne State University, Detroit, MI, 48202, MARGARET MURNANE, HENRY KAPTEYN, ANDREAS BECKER, JILA and Dept. of Physics, University of Colorado, Boulder, CO, 80309 — We present the theory that analyzes the experiment in which an intense ultrashort laser pulse ionizes a dissociating bromine molecule, allowing for the real-time observation of an electron rearrangement during the break-up of a chemical bond. Our results for alignment dependent ionization yields as a function of time during the dissociation as well as the kinetic energy release of the ions agree well with the experimental data. Angular dependent ionization yields strongly depend on the nature of the orbital that has been ionized. This allows us to identify how the changes in the experimental results correspond to the competition of contributions from several dynamically changing valence orbitals. The angular dependent ionization yields also serve as sensitive test for defining the moment of the break-up of the molecular bond. We find that the system remains molecular-like for a much longer time than expected and the electrons do not localize onto the individual atoms until the fragments are quite far apart, in a region where the potential energy curve for the dissociation is essentially flat, and where there is negligible wave function overlap for the two atoms.

Agnieszka Jaron-Becker
JILA and Dept. of Physics, University of Colorado, Boulder, CO, 80309

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