Attosecond electron dynamics in molecular systems: probing of electron density and molecular orbitals by sudden photoionization

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Ultrafast UV excitation can prepare nonstationary electronic states that are a coherent superposition. In molecules it is of interest to probe such states both before the onset of nuclear motion and in the very early stages of the unfolding of chemistry. A suitable probe can be a sudden XUV ionization of the coherent excited electronic states. We discuss the ultrafast electron dynamics for the LiH and ABCU (C10H19N) molecules computed at the many electron level solving the time-dependent Schrödinger equation. Specifically we generate molecular frame photoelectron angular distributions (MFPAD) resulting from the sudden XUV ionization. We are able to relate the angular patterns of the MFPAD to the spatial localization of the electronic states that participate in the coherent superposition of states that is ionized and the corresponding Dyson molecular orbitals.