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Mapping Ultrafast Dynamics of Excited LiH Molecules by Two Color UV-UV Pump-Probe Schemes[1] R. Y. BELLO, C. W. MCCURDY, U. C. Davis and Lawrence Berkeley National Lab., R. R. LUCCHESE, Lawrence Berkeley National Lab. — Attosecond and femtosecond pump-probe schemes provide a sensitive tool for understanding the coupled electronic and nuclear dynamics in molecules. In this context, we report a theoretical investigation of single ionization of the LiH molecule using a two-color UV-UV sequence. Our approach is based on the accurate solution of the time-dependent Schrödinger equation in its full dimensionality, using the eigenstates of the Hamiltonian as the basis set with ionization amplitudes from the Schwinger method. This scheme allows for a detailed analysis of the correlated electron-nuclear dynamics of the system. While total ionization yields (dissociative and non-dissociative) provide information about the amplitudes and phases that build up the molecular wave-packet in the neutral states, molecular frame photoelectron angular distributions (differential in both electronic and nuclear energies) exhibit the changing character of those states, i.e., from ionic to covalent. In addition, the time dependent mean momentum of the wave-packet on neutral states is mapped onto the kinetic energy release of the atomic fragments produced by the probe ionization pulse.

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