Photoionization calculations in molecules using an overset grid implementation[1] CARLOS MARANTE, Lawrence Berkeley National Lab. , LOREN GREENMAN, Kansas State University, ROBERT L. LUCCHESE, Lawrence Berkeley National Lab., C. WILLIAM MCCURDY, U. C. Davis and Lawrence Berkekey National Lab., THOMAS N. RESCIGNO, Lawrence Berkeley National Lab. — The ultrafast electronic processes in molecules demand, theoretically, the challenging representation of the correlated short-range structure and the asymptotic highly oscillatory behavior of an electron in the continuum at the same time. We solve these requirements using an overset grid implementation, that consist of a central grid and multipole atom-center subgrids, allowing a simultaneous spherical expansions of the wave function about the multiple centers, which together with the Complex Kohn variational method, has proven to be effective in electron-neutral scattering problems, in which applying repeatedly the free particle Green function and potential $\hat{G}_0^+\hat{V}$ onto the channel Bessel function, leads to a Padé approximant to the T-matrix. We have extended this formalism to photoionization problems by imposing a fixed spherical boundary matches to Coulomb boundary conditions in the outer region as well as adding a pseudo-potential to enforce orthogonality to the occupied orbitals of the target. We show the performance of the method by computing the valence photoionization cross sections of N_2, CF_4, SF_6 and their electron angular distributions.

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