Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Photoionization and scattering amplitudes for polyatomic molecules using the overset grid complex Kohn variational method[1]
LOREN GREENMAN, University of California, Davis and Lawrence Berkeley National Laboratory, ROBERT R. LUCCHESE, Texas A&M University and Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory — Recent attosecond dynamics experiments [Calegari, et. al., Science 346, 336 (2014)] and coincidence experiments that measure molecular frame photoionization angular distributions [McCurdy, et. al., Phys. Rev. A 95, 011401(R) (2017)] can be explained using photoionization amplitudes calculated by the complex Kohn variational method (along with time-dependent perturbation theory), although such methods with channel coupling and exchange have so far been limited to small molecules. We have recently overcome this limitation, in large part by using overset grids. These are composed of multiple atom-centered subgrids in addition to a central master grid, with switching functions that partition wavefunctions between grids. We present here the extension of the overset grid complex Kohn variational method to photoionization and to multichannel electron scattering, along with results for the photoionization of SF6 and electron scattering in the RNA base uracil.

[1]Army Research Office, MURI W911NF-14-1-0383

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Date submitted: 06 Apr 2017 Electronic form version 1.4