Abstract Submitted
for the DAMOP18 Meeting of
The American Physical Society

Photoionization cross sections for polyatomic molecules with the overset grid implementation of the complex Kohn variational method LOREN GREENMAN, Kansas State University, ROBERT LUCCHESE, Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory — With the recent implementation of the complex Kohn variational method on an overset grid [Phys. Rev. A 96, 052706 (2017)], we have extended the capabilities of variational scattering methods to complex molecules and exact treatments of the exchange interaction. This opens the door to accurate descriptions of correlated electron scattering processes, with implications for processes like the dissociative electron attachment to uracil. Here, we present an extension of this technique to the calculation of electron-ion scattering and photoionization cross sections. This is accomplished by matching to Coulomb functions on a boundary.

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Date submitted: 26 Jan 2018 Electronic form version 1.4