Abstract Submitted
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Complex-Kohn Approach to Molecular Ionization by High-Energy Electrons: Application to H_2, H_2O and CH_4[1] CHIH-YUAN LIN, LBNL, C.W. MCCURDY, LBNL and UC Davis, T.N. RESCIGNO, LBNL — The complex Kohn variational method, which has been extensively applied to low-energy molecule scattering, is extended to treat molecular ionization by fast electrons under the assumption that the incident and scattered electrons can be described by plane-waves. In contrast to other perturbative approches, the interaction between the slow ejected electron and the residual molecular ion is treated by a close-coupling method and for that we employ the complex Kohn variational method. The formulation reduces to the computation of the continuum generalized oscillation strength, which amounts to a generalization of the molecular photoionization problem to which the Kohn method has been successfully applied. The essential point is that the use of a correct electron-ion scattering wave function as the final state for the ejected electron enables us to treat high-energy electron impact ionization of molecules at the same level of sophistication achieved for atomic targets. We will present fully differential cross sections for ionization of water and methane, as well as for excitation/ionization of H_2, along with comparisons to available experimental data.

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