Abstract for an Invited Paper
for the GEC08 Meeting of
The American Physical Society

Electron- and Photon-Induced Fragmentation Dynamics in Simple Atoms and Molecules[1]

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Advanced imaging techniques such as COLTRIMS, coupled with high-resolution electron- and new X-ray photon sources, have triggered a new class of kinematically complete experiments that probe the details of electron- and nuclear dynamics in simple atoms and small molecules. The interpretation of these experiments presents a formidable challenge for contemporary theory, often involving fully differential cross section and excited-state reaction dynamics calculations that require precise, non-perturbative quantum mechanical methodology. I will illustrate this topic with several examples in which state-of-the-art *ab initio* theory can shed light on experiments which probe electron and/or nuclear fragmentation dynamics in simple systems. The examples will include sequential and non-sequential two-photon double ionization of helium, diffraction effects in high-energy photo-double ionization of H_2, core-hole localization in molecular nitrogen, inner-valence shell fragmentation of carbon monoxide and electron-induced three-body breakup of water.

[1]Work performed under the auspices of the USDOE and supported by the OBES Division of Chemical Sciences.