GEC15-2015-000056

Abstract for an Invited Paper
for the GEC15 Meeting of
the American Physical Society

Accuracy of Theoretical Calculations for Electron-Impact Ionization of atoms and Molecules[1]

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In the last two decades, there have been several close-coupling approaches developed which can accurately calculate the triply differential cross sections for electron impact ionization of effective one and two electron atoms. The agreement between experiment and theory is not particularly good for more complicated atoms and molecules. Very recently, a B-spline R-matrix with pseudostates (BSRPS) approach was used to investigate low energy electron impact ionization of neon and very good agreement with experiment was found. The perturbative 3-body distorted wave (3DW) approach which includes the exact final state electron-electron interaction (post collision interaction - PCI) gave comparably good agreement with experiment. For ionization of molecules, there have been numerous studies of high-energy electron impact. These studies are called EMS (Electron Momentum Spectroscopy) and they were very valuable in determining the accuracy of molecular wavefunctions since the measured cross sections were proportional to the momentum space molecular wavefunction. More recently, lower energy collisions have started to be measured and these cross sections are much more difficult for theory since the detailed kinematics of the experiment become important. So far, the only close coupling calculation reported for ionization of molecules is the time-dependent close-coupling calculation (TDCC) which has been developed for ionization of H2 and it yields relative good agreement with experiment. Again the molecular 3-body distorted wave (M3DW) gave equally good agreement with experiment. For polyatomic molecules, the only theory available is the M3DW. In this talk, I will show the current status of agreement between experiment and theory for low and intermediate energy single ionization of atoms and molecules.

[1]Work supported by the NSF and XSEDE.