GEC13-2013-000439

Abstract for an Invited Paper
for the GEC13 Meeting of
the American Physical Society

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

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The study of electron impact single ionization of atoms and molecules has provided valuable information about fundamental collisions. The most detailed information is obtained from triple differential cross sections (TDCS) in which the energy and momentum of all three final state particles are determined. These cross sections are much more difficult for theory since the detailed kinematics of the experiment become important. There are many theoretical approximations for ionization of molecules. One of the successful methods is the distorted wave (DW) approximation. One of the strengths of the DW approximation is that it can be applied for any energy and any size molecule. One of the approximations that has been made to significantly reduce the required computer time is the OAMO (orientation averaged molecular orbital) approximation. Surprisingly, the M3DW-OAMO approximation yields reasonably good agreement with experiment for ionization of H_2 by both low and intermediate energy incident electrons. On the other hand, the M3DW-OAMO results for ionization of CH_4 [1,2] and NH_3 [3] did not agree very well with experiment. Consequently, we decided to check the validity of the OAMO approximation by performing a proper average over orientations and we found much better agreement with experimental data. In this talk we will show the current status of agreement between experiment and theory for low and intermediate energy single ionization of small, medium, and large molecules.

[1] Nixon et al 2012 J.Chem. Phys. 136 094302
[2] Xu et al 2012 J. Chem. Phys. 137 024301
[3] Nixon et al 2013 J. Chem. Phys. 138 174304

[1]This work is supported by the US National Science Foundation under Grant. No. PHY - 1068237. Computational work was performed with Institutional resources made available through Los Alamos National Laboratory.