GEC20-2020-000297

Abstract for an Invited Paper
for the GEC20 Meeting of
the American Physical Society

Electronic excitation cross sections in low energy electron scattering from polyatomic molecules[1]

JIMENA GORFINKIEL, The Open University

State-of-the-art software, based on the use of the R-matrix method and designed to model the interaction of low energy electrons and positrons with polyatomic molecules as well as photoionization, can be used to determine quantitatively accurate electron excitation cross sections for small and mid-size molecules below the ionization threshold. In my talk, I will describe how recent developments of UKRmol+ software suite (CPC **249** (2020) 107092, https://www.ukamor.com/#/software) have enabled highly accurate studies for small targets, the study of bigger targets than ever before and the investigation of the effect of the environment by means of small molecular clusters. I will show examples of the use of the UKRmol+ suite to study scattering from BeH_2 (PRA **101** (2020) 052709), pyrimidine (JCP **144** (2016) 024302) for which agreement with electron energy loss spectroscopy results is excellent, and other targets. I will also discuss other processes that can be investigated with the same approach.

[1]The work has been supported by EPSRC under grants EP/P022146/1, EP/R029342/1 and EP/G055599/1