Electron-molecule collision calculations for plasma physics applications

Jonathan Tennyson [1]

[1]*University College London, U.K.*

Plasma models require data on electron-driven processes for a wide variety of species. Cool plasma such as those that occur naturally in the Earth\'s ionosphere and the interstellar medium, or those harnessed for a wide variety of technological processes, are largely molecular in composition. These molecular plasmas include many transient species whose behaviour when colliding with electrons is poorly known and hard to characterise experimentally. My group at UCL performs electron collision calculations using the fully quantum mechanical R-matrix method. These calculations have been used to study problems ranging from electron-impact rotational excitation of interstellar molecular ions, excitation and dissociation of molecules found at the edge fusion plasmas, processes important for spacecraft re-entry physics and collisions important for models of technological plasmas. My talk will feature illustrative examples including:

1. The electron chemistry of NF_3, NF_2 and NF mixtures which are important in remote plasma sources which are being developed for isotropic etching and thin deposition in microelectronic fabrication;

2, Development of a radiative-collisional model for BeH/BeD/BeT, a species whose emission spectra is being actively monitored in fusion plasmas;

3. Electron impact vibrational excitation and dissociation of atmospheric molecules.

The role of databases, and in particular QDB (Tennyson et al, 2017), for accessing key datasets for modelling will be discussed.

Tennyson, J et al, 2017, Plasma Sources Sci. Tech. 26, 055014; www.quantemol.com/qdb