Training in data calculations for environmental applications: Databases on atomic and molecular reactions: Quantemol EC

Scientific field: Quantum physics, engineering sciences, numerical calculations,

Key words: quantum mechanics, databases, R-matrix, electron-molecules collisions, plasma and engineering applications, software, cross sections, rate coefficients, electron-induced processes,

Collaborations: Pr. V. Kokoouline at *University of Central Florida, Orlando, USA.*

Salary: 600 €/month

Period: from January 2023 for 6 months

Subject

Cross sections for collisions involving electron-molecules are of fundamental importance in a plethora of research fields ranging from engineering to plasmas. For instance, cross sections are used in low temperature plasma modelling in order to improve the plasma-based processes for material treatment, atmospheric depollution or etching and doping. In this context, the software *Quantemol N* has been designed and developed at the University of College London (UCL) by Prof. Tennyson to provide full accessibility to the highly sophisticated UK molecular R-matrix codes, used to model electron polyatomic molecule interactions.

One of the most important processes taking place in low temperature plasma is the vibrational (de-)excitation (VE) and dissociative recombination (DR) of molecules by electron impact. Despite important efforts, still now little information is available on VE and DR of large polyatomic molecules (H_2O, CO_2, NO_2, N_2O, SO_2, HCO^+, CH_3^+, etc.). In this context, we developed at Centralesupélec theoretical approaches based on a combination of the normal mode approximation for vibrational states of the target molecule and the UK R-matrix to evaluate the scattering matrix for vibrational transitions, both employed to compute cross sections. An implementation of the developed methods is on the way in collaboration with Dr. Maria Tudorovskaya from Quantemol team at UCL and Prof. Kokoouline from University of Centrale Florida (UCF). See https://www.youtube.com/watch?v=BAB1Ka1xxY4.

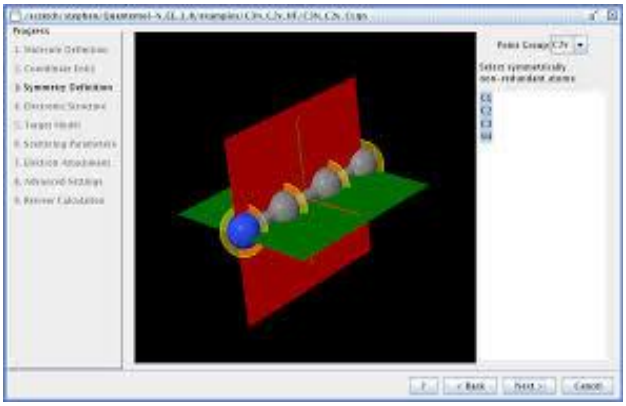

Figure 1: Screenshot of the Quantemol N interface (https://www.quantemol.com/)

The objective of this proposed project is to perform series of tests of the implemented codes throughout the updated version of *Quantemol EC*. These tests will be carried out in close collaboration with UCL and UCF. The candidates would take part of an exciting project aiming to produce and enrich databases on atomic and molecular reactions needed in various applications. This work leads to the publication of peer-reviewed articles. An exchange and long term stay in both institutions could be planned during and/or at the end the project.

Tools

Quantemol Software (see Figure 1) and PYTHON/FORTRAN codes dealing with the R-matrix formalism, the theory of electron-molecule collisions and the structure calculations (Molpro/Gaussian software). QM standard textbooks. **Once again, it is not mandatary that the candidate has to master the above tools. The project could be adapted according to his/her motivation, interest and skills.**

Collaboration with the University of Central Florida and/or University College London with a possibility of stay is planned for this project.

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