PAMOP Consortium at HLRS

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Introduction

The PAMOP (PetaScale Atomic, Molecular and Optical Physics) group is in international collaboration which develops and implements collisional theory on high perfomance supercomputing architectures. Atomic and molecular structure with the subsequent collsional calculations are fundamental to numerous areas but we shall focus on their application within magnetically confined fusion plasmas and the interpretation of astrophysical spectra.

Methods and Interests

We all collectively employ the Schroedinger (Dirac) equations either by solving a coupled-set of equations, or in the case of Prof Pindzolsa's work by solving the time-dependent Schroedinger equation directly on a multi-demensional lattice. This overlaps with the work of Dr Babb, which focuses on atom-ion ion collisions relevant for astrophysics.

The majority of the light particle collisions whether they are photons or electrons is carried out within an R-matrix framework. In simple terms, it divides configuration space into two regions. The boundary is set by the most diffuse atomic or molecular orbital used in the close-coupling expastion. From the nucleus to this boundary the full many-bodied problem is solved, whereas beyond this region the problem reduces to an electron moving in the multipole expansion of the target, with the R-matrix acting as an interface between the two regions.

Our colleagues at Auburn University, span both the theoretical and experimental worlds. They maintain several magnetically confined plasma devices, used to test the impurity influx evident within large tokamak devices such as ITER, Cadarache, France. Together with the electron-impact excitation and ionisation rates from the R-matrix method , they are able to confirm Molydenum and Tungsten spectrum observed in those devices. Their collsional radiative codes employing a wide variety of Maxwellain averaged rates are able to predict in the short term the density and temeprature of the plasma from the walls inwards. The long term goal would be using these rates to predict erosion, impurity influx and the redeposition of wall materials.

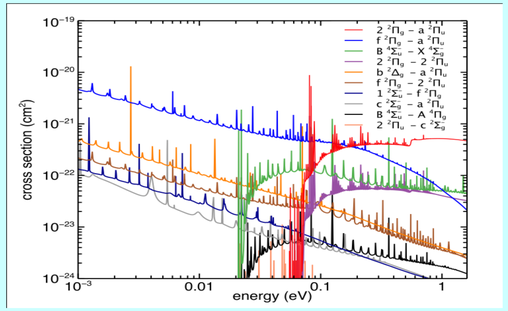
With the advent of neutron-star merger detection, heavy atomic elements are not only of interest to fusion , as spectral lines for Au and Pt (Z=79,78) which are close to tungsten (Z=74)

Heavy-particle Collisions[1]

Formation of the dicarbon cation C_2^+ by the radiative association process in collisions of a carbon atom and a carbon ion,

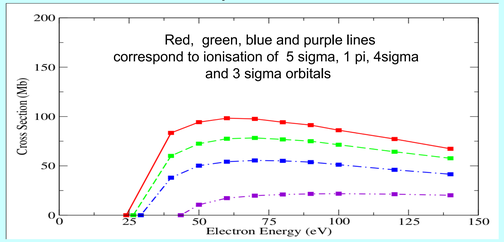
$$C(^3P) + C^+(^2Po) \rightarrow C_2^+ + h\nu \quad (1)$$

An example of dicarbon cation astrochemistry, as it is one of the species participating in hydrocarbon chemistry, for example, in interstellar clouds and photon-dominated regions.



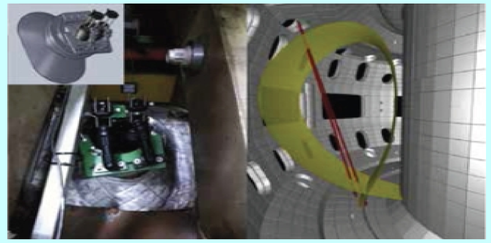
Electron-molecule Collisions[2]

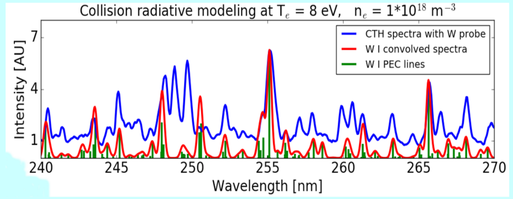
The CN molecule is of considerable astrophysical importance. Carbon and nitrogen are produced during the evolution of low and high mass stars, so the presence of CN can be used as a probe of star formation history.



Magnetically-confined Fusion[3]

Schematic of the installation of Auburn spectrometers at General Atomics DIIID device with the red lines illustrating the line of sight through the plasma to tungsten tiles on the floor. The subsequent spectral plot further illustrates the predictive capablity of theory, to suggest interesting wavelength regions, especially if multiple Ion stages of Tungsten are evident.





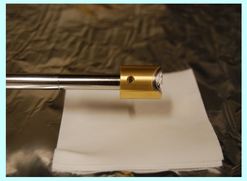
This predictive capability is undepinned by large scale R-matrix calculations for the electron-impact excitation and ionisation of W.

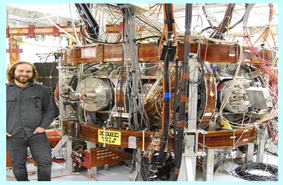
Code Development and Future Directions

There have been two major developments over the last year to the R-matrix codes. The first has been in terms of interfacing time-idependent code with the RMT (R-matrix with time-dependence) variants. This has allowed the semi-relativistic codes to now Involve laser interactions. In fact, the inclusion of spin-orbit splitting combined with laser pulses with arbitrary polarization have enabled some fundamnental manipulation of electrons within an atom

Secondly, the R-matrix method, nearly always rquires the formation and diagonalisation of several symmetric Hamiltonian matrices for which every eigenvalue an eigenvector is required. The diagonalisation code has now been modified to include mpi_ibcasts within the code. This now allows for the overlap of computation with the distribution of the Hamiltonian matrices, which has an ever increaseing benefit when matrices exceed 50 by 50 K. This code will employed for the remaining ion statges of Tungsten for both excitation and ionization.

With neutron star merger work and magnetically-confined fusion work converging on heavy elements from Z=74-79 we will be focusing on identifying strong transitions within the visible wavelength.This aligns with the proposed work of our Auburn University colleagues. Initially structure calculations to identify strong transtions before moving to electron-impact excitation





The gold probe tip (left) and the Compact Toroidal Hybrid Experiment (CTH) (right) at Auburn University

References

[1] Radiative Association of Atomic and Ionic Carbon
James F. Babb, R. T. Smyth and B. M. McLaughlin
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[2] Electron Ionization of the CN^+ Molecule
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[3] Dirac R-matrix calculations for the electron-impact excitation of neutral tungsten providing noninvasive diagnostics for magnetic confinement fusion
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