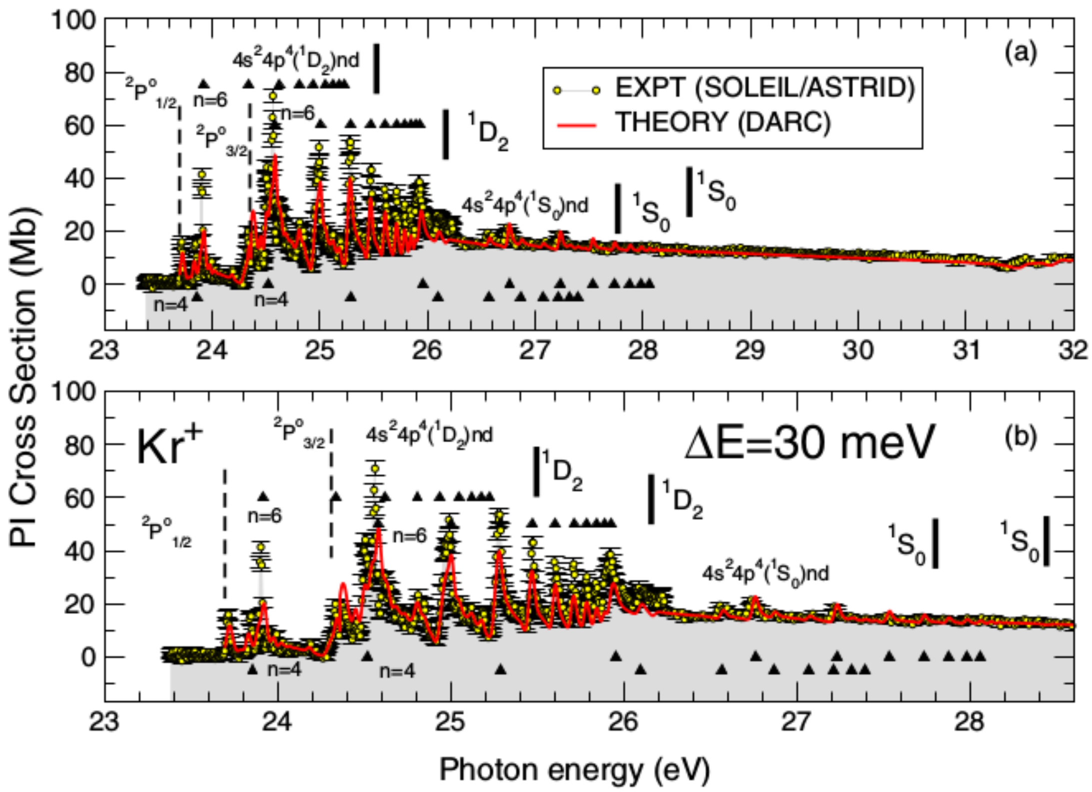
Dirac R-matrix photoionization calculations in Support of Astrophysical Spectral Diagnostics : Dr C P Ballance and Dr C Ramsbottom

A newly developed relativistic photoionisation R-matrix code that harnesses the capabilities of Europe's supercomputer network has been developed that focuses on calculating spectra from the middle of the periodic table (Trans-Fe elements) for astrophysical needs.

Selenium and krypton are the two most widely detected trans-iron elements in PNe (Photoionized Nebulae) and other nebulae, owing to their relatively strong near-infrared fine-structure transitions [Kr III] 2.199 and [Se IV] 2.287 m first identified by Dinerstein (2001). Se and Kr abundances were derived in over 80 PNe from observations of these K-band transitions, providing the first large-scale investigation of s-process enrichments in PNe. From a fundamental perspective, we are always comparing with the latest experimental measurements throughout the world, when they become available, as the figure below illustrates. As experimental resolution improves, currently at the $10meV$ level, it spurs theoretical development to match this accuracy, McLaughlin and Ballance 2012 .



As stated in Sterling al 2015, the "abundance determinations of Se and Krand indeed all n-capture elementsin astrophysical nebulae are plagued by uncertainties. The most important of these uncertainties stems from the absence of reliable atomic data. However, atomic data needed to reliably correct for the abundances of unobserved ionization stages are unknown. Such "ionization correction factors," or ICFs, are most reliably derived via numerical simulations of astrophysical nebulae (Stasiska 1978; Kingsburgh Barlow 1994; Kwitter Henry 2001; Rodrguez Rubin 2005; Delgado-Inglada et al. 2014 (see references with Sterling paper). However, the simulations are only as accurate as the underlying atomic physics that they include. Specifically, ionization equilibrium solutions in photoionized nebulae rely on accurate photoionization (PI) cross sections and rate coefficients for radiative recombination (RR), dielectronic recombination (DR), and charge transfer (CT). Until recently, these data were unknown for nearly all n-capture-element ions. " The R-matrix collisional group, with the exception of charge transfer has expertise in calculating these remaining processes and has the potential to contribute significantly to the identification and modelling of these elements.

0.1 Plan of work

0.2 Background

It would be beneficial if the prospective student has had an entry-level quantum mechanical course. There is the intent that the student would develope, calculate and employ the calculated fundamental atomic data with numerical simulations. Therefore, an interest in solving problems from first principles, an interest in programming on large scale parallel computer architectures with the end focus of applying these results to the interpretation of astrophysical observation is a must. However, more important is an interest in the topic as these skill-sets can be acquired during the project.

0.3 Aims and future benefits of the project

- There is opportunity calculate the missing atomic and collisional data, for yet unidentified lines of Trans-Fe elements
- There is a strong computational aspect, therefore an interest in computational modelling, and in particular utilizing powerful parallel supercomputers is required.
- The student has the unique opportunity to be a valuable bridge between the atomic structure and collsional calculations (CTAMOP) and the astrophysical requirements of ARC
- Beyond academia, numerical programming and experience with high performance computing are valauble marketable skills.

0.4 Useful background references

- B M McLaughlin and C P Ballance, J. Phys. B: At. Mol. Opt. Phys. 45 (2012) 095202
- N Sterling *et al* ArXiv:1505.01162v1 [astro-ph.SR] 5 May 2015