Theoretical determination of Zinc Kα spectra using Multiconfigurational Dirac-Hartree-Fock Calculations

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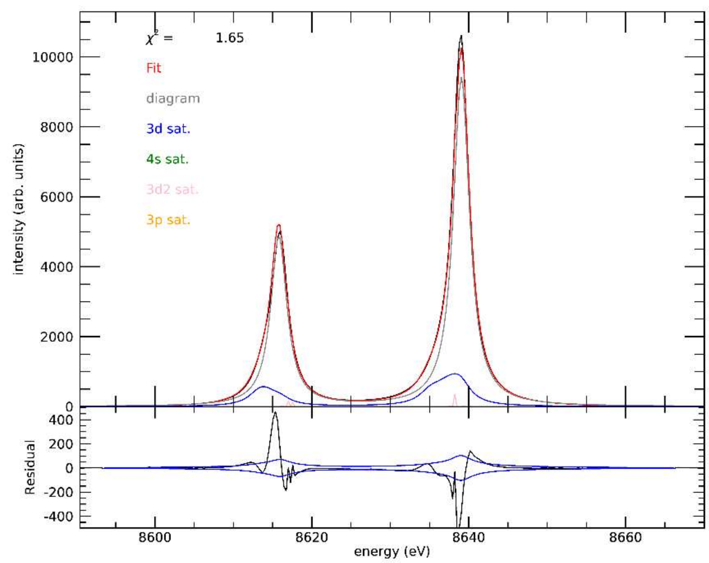
The Kα spectrum is widely employed in X-ray spectroscopy for elemental analysis, industry, fundamental atomic physics, and tests of quantum electrodynamics. Despite the prevalent use, several discrepancies exist between theoretical calculation and empirical data. The 3d transition metals, $Z \in \{21,30\}$, have been of interest for several decades due to their open d orbital. Zinc should represent a baseline for these studies due to its full 3d orbital. Surprisingly, few experimental and theoretical studies exist.

A Kα transition is the radiative decay of an excited atom where a 1s vacancy is filled by a 2p electron. Kα spectra have well-documented asymmetries, widely hypothesised to be the result of shake events. Typically termed 'shake-offs', these occur when the preliminary ionisation process removes other electrons in addition to the 1s core thereby changing the potential. Consequently, satellite transitions are observed.



This work uses multiconfiguration Dirac-Hartree-Fock (MCDHF) calculations to obtain *ab initio* transition eigenenergies and relative intensities of zinc Kα diagram and satellite spectra from the 3p, 3d, $3d^2$ and the 4s shake-off events. This is the first time this has been attempted for this system.

In fitting these results to data from Ito et al. [1] we may test the current standard of atomic physics and relativistic quantum mechanics. We obtain a very promising goodness-of-fit measure $\chi^2_{reduced} \leq 2$. These results follow recent work by Dean et al. [2] and Nguyen et al. [3] in scandium and copper. The diagram spectrum of zinc requires fewer spin state configurations than other 3d transition metal systems. Although the MCDHF calculations are simpler in principle, we find that approach to convergence, especially for the satellite transitions, are of equal difficulty. Therefore, the success with $\chi^2_{reduced}$ emphasises the importance of satellite spectra in the data. The importance of Kα spectra to several fields in science and industry and especially for zinc applications suggests that work in understanding experimental and theoretical discrepancies is valuable.

[1] Y. Ito et al. *J. Quant. Spec. Rad. Transf.* (2015) **151**

[2] J. W. Dean et al. *J. Phys. B* (2022) **55** (7) 075002.

[3] T. V. B. Nguyen et al. *Phys. Lett. A* (2022) **426** 127900