# Atomic- structure properties and electron impact excitation of impurity ions

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In the research coordination meeting, I will present our progress on the computational implementation of the relativistic distorted wave theory (RDW) for calculating excitation rate coefficients within the Jena Atomic Calculator (JAC) toolbox. To address the need for large-scale calculations involving complex shells and heavy atoms and ions, we incorporated parallel programming to expedite the computation of cross sections, collision strengths, effective collision strengths and rate coefficients which are crucial for modelling various laboratory and astrophysical plasmas. Enhancements to input parameter flexibility have made the JAC more user-friendly, enabling efficient electron-impact excitation (EIE) calculations for all atoms and ions, including impurity ions relevant to our project.

Further, our detailed results will be presented on the atomic-structure properties and electron impact excitation of impurity ions. In particular, we focused on highly charged Ar-like $Kr^{18+}$ and S-like $Xe^{38+}$. For Kr XIX, we focused on the lowest 128 fine-structure levels originating from the $3s^23p^6$, $3s^23p^53d$, $3s3p^63d$ and $3s^23p^43d^2$ configurations. In case of S-like $Xe^{38+}$, the lowest 75 levels that belong to $2s^22p^63s^23p^4$, $2s^22p^63s3p^5$, $2s^22p^63s^23p^23d^2$, $2s^22p^63s3p^43d$ and $2s^22p^6\ 3s^23p^33d$ configurations were considered. We reported energy levels, lifetimes, wavelengths, weighted oscillator strengths, and transition probabilities for multipole transition types (E1, E2, M1, and M2). To achieve this, we employed the GRASP2018 code, which implements the fully relativistic multiconfigurational Dirac–Hartree–Fock method (MCDHF) and accounts for Breit interaction and quantum electrodynamic effects. We performed another set of calculations using the many-body perturbation theory implemented in the flexible atomic code (FAC). By comparing the results obtained from GRASP2018 and FAC, we established the accuracy and consistency of our calculations. Furthermore, using the RDW theory, we studied electron impact excitation of all transitions to upper levels from the ground and metastable levels and reported EIE cross sections as a function of incident electron energies. To enhance the practical utility of our findings, we also provided analytical fittings of these cross sections and excitation rate coefficients for their applications in plasma modelling. Our work contributes to the atomic properties and excitation cross sections of Ar-like $Kr^{18+}$ and S-like $Xe^{38+}$, addressing a marked gap in the available atomic data.

Additionally, we developed detailed collisional radiative (CR) models to diagnose low-temperature Kr plasma. Energies and transition parameters for $Kr^{+}$ and $Kr^{2+}$ were calculated using the MCDHF method. Results were compared with NIST and previously reported values to ensure accuracy. Bound state functions derived from these calculations were used to

compute EIE cross sections for transitions from the five lowest levels over an electron energy range from the threshold to 300 eV, using the RDW approximation. The reliability of the CR model was confirmed through comparisons with experimental measurements.