Large-Scale Relativistic Calculations for Atomic Structure and Electron Impact Excitation of Impurity Ions

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As a part of the coordinated research project (CRP) on "Atomic Data for Injected Impurities in Fusion Plasmas", we revisited the status of atomic-structure parameters for Na-like Ar^{7+}, Kr^{25+} and Xe^{43+} ions. It is found that, for Ar^{7+}, fine structure energies and radiative parameters of a few higher levels, viz., $7f,\ 7g,\ 7i,\ 8p,\ 8f,\ 8g,\ 8i$ are absent from the literature. For Kr^{25+}, these parameters are available for $n = 3-6$, $l = s,\ p,\ d,\ f$ levels only. The situation is even worse for Xe^{43+}. Although its level energies are available up to $n = 3-6$, $l = s,\ p,\ d,\ f$, transition probabilities have been published for only a few transitions among the low-lying states. Therefore, we carried out relativistic calculations for energies, E1 transition parameters and lifetimes for the lowest 71 levels of Na-like Ar^{7+}, Kr^{25+} and Xe^{43+} ions. The configurations of our interest include $1s^22s^22p^6nl$, where $n = 3-9$ and $l = 0-6$. The present study adds new results for $n = 7$, 8, 9 levels of Kr^{25+} and Xe^{43+} and remarkably improves the amount of atomic data for these ions. We used the fully relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) method integrated in the latest version of the general-purpose relativistic atomic structure package (GRASP2018). Due to lack of existing data for $n \geq 7$ and further, to examine the reliability of our results, we have performed separate calculations using the many-body perturbation theory (MBPT) inbuilt in the flexible atomic code (FAC). A good agreement is achieved by comparing the two results and also with the available previous results. Moreover, we estimated the uncertainties in the computed lifetimes and transition parameters and assigned their accuracy class as per the NIST nomenclature. Further, using the accurate wavefunctions for these three ions, we are currently studying electron impact excitation from the ground state to their excited states using relativistic distorted wave (RDW) approximation. Our RDW code takes into account the relativistic correction to the Coulomb potential, i.e., the Breit interaction in the $T-$ matrix evaluation. We aim to determine the effective collision strengths from the calculated cross sections by assuming the Maxwellian distribution of electrons' energy. The work is currently under progress.

We also performed MCDHF calculations for excitation energies, transition parameters and lifetimes for 255 levels with $n < 5$ configurations of B-like Xe^{49+}. In this work, we estimated the uncertainties in the lifetimes and line strengths. Most transitions have line strength with $A+$ to B accuracy class. Additionally, new results for 130 levels are provided in this work. Further, we identified that very limited atomic-structure parameters are available for Ar-like Kr^{18+}. We are in the process of performing MCDHF and MBPT calculations for the lowest 150 fine-structure levels belonging to the $3s^23p^6, 3s^23p^53d, 3s3p^63d, 3s^23p^43d^2, 3s3p^53d^2$ configurations. We have got some preliminary results for energy levels, lifetimes, wavelengths, and line strengths for electric and magnetic dipole (E1,M1) and quadrupole (E2,M2) transitions. Detailed analysis to determine the statistical uncertainties is to be followed after completing the whole set of calculations.