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High accuracy theoretical calculation of wavelengths and transition probabilities in Se- through Ga-like ions of tungsten

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ABSTRACT

The *Ab initio* multiconfiguration Dirac-Hartree-Fock (MCDHF) calculations of atomic parameters have been carried out with high accuracy for four highly charged tungsten ions from Se-like W^{40+} to Ga-like W^{43+}. The second-order relativistic many-body perturbation theory (MBPT) was used to confirm the accuracy of the MCDHF calculations. Excitation energies, wavelengths and transition rates of E1, M1, E2, M2, E3 and lifetimes are presented. The core-valence electron correlation effects arising from deep subshells 3*d* and 3*p*, have been taken into account along with relativistic effects. The calculated wavelengths are in good agreement with available experimental results.

1. Introduction

A surge of interest in tungsten followed after this metal was suggested as the best wall material to be used in the International Tokamak Experimental Reactor (ITER) project [1], as well as in other future magnetic fusion energy devices [2–5]. Many experimental and theoretical studies have been carried out, see the reviews in Ref. [6–12]. and references therein.

On the experimental side, a few EUV spectral lines were measured in N-shell tungsten ions with the $(1s^22s^22p^63s^23p^63d^{10})4s^24p^k$ $(k = 1, \ldots, 6)$ ground configurations. These observations were made at the ASDEX Upgrade tokamak and at various electron beam ion trap (EBIT) facilities in the past twenty years [13–18].

On the theoretical side, Fournier et al. [8] performed calculations for the $4s^24p^k$ tungsten ions $(k = 1, \ldots, 6)$ with the fully relativistic parametric potential RELAC program [19,20], and reported transition properties for electric dipole (E1), magnetic dipole (M1), electric quadrupole (E2), and magnetic quadrupole (M2) transitions. However, they included limited electron correlation effects and ignored Quantum Electro-Dynamical (QED) corrections in the calculations. Kramida et al. [9] gave compiled experimental data on observed wavelengths, from which the corresponding energy levels were derived. And for some of the levels, no connections to the ground state could be derived from ovserved transitions, and parametric calculations with the Cowan Code [21] had been used to derive approximate positions of these levels. All of these data were collected in the Atomic Spectra Database (ASD) of the National Institute of Standards and Technology (NIST) [22]. Quinet [23] calculated energy levels, wavelengths, and forbidden M1 and E2 transition rates for the states of the ground configurations with an open 4*p* shell for tungsten ions using the fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) approach implemented in the dGRASP code [24]. However, only the valence-valence (VV) electron correlation effects were considered.

Recently, Gaigalas et al. [25], Froese Fischer [26] and Hu et al. [27] performed MCDHF calculations with the GRASP2K package [28], targeting at W^{38+} $(4s^24p^6)$, W^{39+} $(4s^24p^5)$, and W^{43+} $(4s^24p)$

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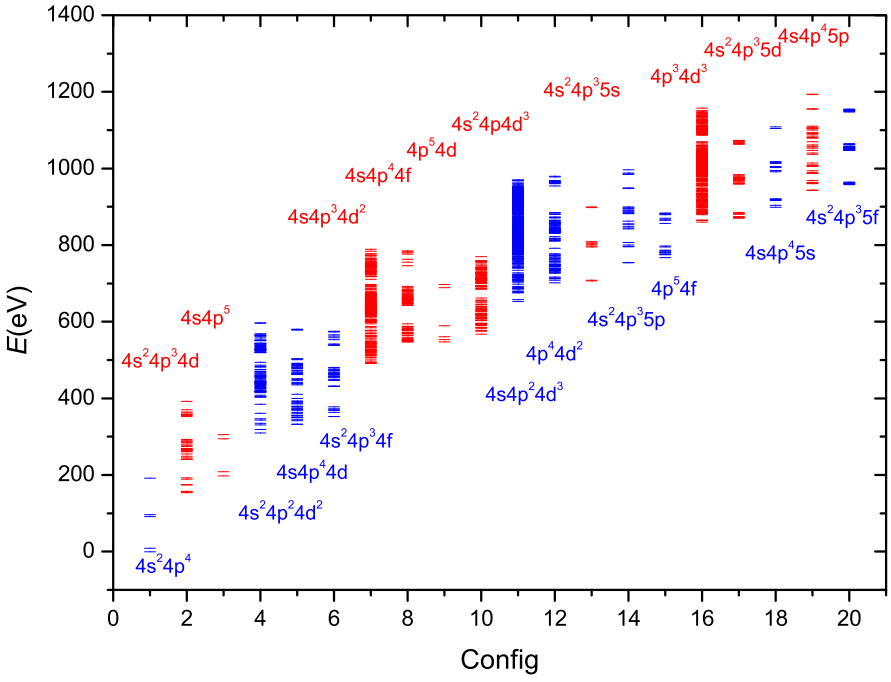

Fig. 1. The sketch of transition energies (in eV) in various configurations of W^{40+}. The levels of even and odd parities are printed in blue (-) and red(-) colors, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

ions. These calculations included VV electron correlation [25] or the 3*d* core-valence (CV) electron correlation effects [26,27] at the most. Wang et al. [29,30] focused on the other relatively more complex structures, *i.e*, $4p^3$, and $4p^4$, but only the VV electron correlation effects were considered. In our recent work on W^{38+} ($4s^24p^6$) [31] and W^{39+} ($4s^24p^5$) [32], we found that the core-valence correlation effects from the deeper 3*p* subshell are also important for accurate energy and transition data calculations.

This work is an extension and continuation of our recent efforts [31–37] to supply complete highly accurate atomic data for M- and N-shell ions . In particular, the present work fills the gap in accurate atomic data for the ions from Se-like W^{40+} to Ga-like W^{43+}, which will help in analyses of future experimental spectra and improve the assessment of blending for diagnostic lines of interest.

2. Calculation and methodology

Using the relativistic configuration interaction (RCI) method implemented in the Flexible Atomic Code (FAC) [38], preliminary calculations were performed to determine the multi-reference (MR) configurations and the scope of the results for our MCDHF calculations. As an example, a schematic diagram of excitation energies for different configurations of W^{40+} is shown in Fig. 1. The configurations $4s^24p^4$, $4s^24p^34d$, and $4s4p^5$ are the lowest ones. Therefore, the MR configurations for the W^{40+}, W^{41+}, and W^{42+} ions, which have similar diagrams of excitation energies, are $4s^24p^k$, $4s^24p^{k-1}4d$, and $4s4p^{k+1}$ with $k = 4, 3$, and 2, respectively. For Ga-like W^{43+} ion, due to its simpler energy structure, it was possible to include the $4s^24f$, $4s4p4d$ and $4p^3$ configurations in the MR set, in addition to the $4s^24p$, $4s^24d$ and $4s4p^2$. The resulting energy and transition data for these configurations in each ion are provided in the present work.

Using the MCDHF method implemented in the GRASP2K program suite [28], exciation energies, and E1, M1, E2, M2, and E3 transition properties for W^{40+} through W^{43+} ions are provided for all of the levels belonging to the MR configurations mentioned above. To confirm the accuracy of the results, we also perform an independent second-order relativistic many-body perturbation theory (MBPT) calculation [39,40] using the FAC code.

Table 1
The average relative change $\delta\bar{E}_{n,n-1}$ of transition energies from the present MCDHF-CV_{3p} calculations with increasing configuration set AS_n ($n = 0, \ldots, 4$) for the ions from Se-like W^{40+} to Ga-like W^{43+}.

Seq.	Ion	$\delta\bar{E}_{1,0}$	$\delta\bar{E}_{2,1}$	$\delta\bar{E}_{3,2}$	$\delta\bar{E}_{4,3}$
Ga-like	W^{43+}	−0.419	0.020	−0.021	−0.001
Ge-like	W^{42+}	−0.104	−0.061	−0.043	−0.010
As-like	W^{41+}	−0.137	−0.113	−0.047	−0.015
Se-like	W^{40+}	−0.231	−0.135	−0.066	−0.024

The above two state-of-the-art methods both start from the Dirac-Coulomb (DC) Hamiltonian, then corrections to the instantaneous electron-electron interaction are introduced in both approaches through the frequency-independent Breit interaction [41,42], and the self-energy and vacuum polarization [43,44] in first order QED corrections are also taken into account.

The MCDHF method is superior, because in this method the correlation effects can be increased systematically by means of the active set (AS) [45,46] of orbitals, which are in turn used to generate configuration state functions (CSFs) [46], adopting the restricted active space (RAS) [47]. Then the atomic eigenstates, also known as the atomic state functions (ASFs) could be obtained in terms of a linear combination of CSFs. Hence, the convergence of the atomic properties of interests can be monitored until an effectively complete basis set of CSFs has been found. Then, the Breit interaction and the dominant QED contributions (BQ effects) are added in a final perturbative relativistic configuration interaction (RCI) calculation performed without re-optimisation of the orbitals. Once well-converged and effectively complete ASFs have been obtained, radiative transition properties can also be determined.

We start the MCDHF calculation without any virtual excitations from the MR set mentioned before, which is usually referred to as the Dirac-Hartree-Fock (DHF) calculation. Here we use the notation AS_0 to denote the active set for this first step. Subsequently, we limit our calculation to single and double (SD) virtual excitations from the multi-reference configurations, since it has been shown that the contribution from triple and quadruple excitations is small