Relativistic configuration-interaction calculations of the n=3-3 transition energies in highly charged tungsten ions

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Relativistic configuration-interaction calculations of the $n = 3 - 3$ transition energies in highly-charged tungsten ions

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Abstract

A large-scale relativistic configuration-interaction (CI) calculation of the $n = 3 - 3$ transition energies for Ne- to Ar-like tungsten is carried out. The calculation is based on the relativistic no-pair Hamiltonian and uses finite B-spline orbitals in a cavity as basis functions. Quantum electrodynamic and mass polarization corrections are also included. Results are compared with other theories and with experiment, and are generally found to be more reliable than previous theoretical predictions.

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I. INTRODUCTION

Tungsten is of interest in fusion research as it is a promising material in future magnetic confinement fusion reactors such as the ITER due to its desirable properties with low hydrogen retention, high melting point and high thermal conductivity. However, since tungsten is a high-Z element, even with 10 - 20 KeV reactor temperature, line emission in the x-ray and vacuum ultraviolet (VUV) regions are major concerns in realizing the magnetically confined fusion reactors. To understand its influence as a plasma impurity, reliable transition energy data are needed for many ionic stages of tungsten which show up in relevant emission spectra.

There are not many experimental and theoretical studies in the literature for the $n = 3 - 3$ transition energies of highly-charged tungsten ions. Early calculations of the sodium isoelectronic sequence are mostly based on the Dirac-Fock (DF) [1–3] or model potential [4] methods with a relatively crude accuracy of a few eV. High-precision relativistic many-body perturbation theory (RMBPT) calculations of the correlation energies for selected Na-like ions were carried out by Johnson et $al.$ [5], but quantum electrodynamic (QED) corrections, which are important for high-Z ions, were not included. Kim et $al.$ [6] later used these RMBPT results to provide accurate relativistic correlation corrections to their DF energies for Na-like ions with $14 \leq Z \leq 92$, and calculated the QED corrections with the ad hoc Welton method [7]. Reliable QED corrections from ab $initio$ calculations were first given by Blundell [8] who added them to the RMBPT energies [5] to give accurate transition energies for a few Na-like ions, though tungsten was not included. Theoretical $n = 3 - 3$ resonance line energies for Mg-like ions include results from the multiconfiguration Dirac-Fock (MCDF) calculations by Cheng and Johnson [9] and Zou and Froese-Fischer [10], the relativistic random-phase approximation calculations by Shorer et $al.$ [11], the relativistic perturbation calculations with model potentials by Ivanova et $al.$ [12], and the relativistic configuration-interaction (RCI) calculations for low- to mid-Z ions by Chen and Cheng [13]. For the aluminum isoelectronic sequence, transition energies and radiative rates have been calculated with the MCDF method by Huang [14] and the RMBPT method by Safronova et $al.$ [15]. In other Al-like calculations [16–18], either tungsten is not included or results are presented in graphical forms only. Finally, there is a recent RMBPT study of the wavelengths and transition rates in several highly-charged tungsten ions, including Mg- and

Al-like tungsten, by Safronova and Safronova [19].

On the experimental front, there are a few measurements of the $n = 3 - 3$ wavelengths of highly-charged tungsten ions. Ralchenko *et al.* measured EUV spectra from Ca-like W^{54+} to Na-like W^{63+} [20], and magnetic-dipole lines among the $3d^n$ levels of Co-like W^{47+} to K-like W^{55+} [21], at the National Institute of Standards and Technology (NIST) electron beam ion trap (EBIT) facility. Gillaspy *et al.* [22] measured the $3s - 3p$ D-line doublets in highly-charged Na-like ions as well as the wavelengths of several $3s - 3p_{3/2}$ and $3p_{1/2} - 3d_{3/2}$ lines in Si-, Al-, and Mg-like ions, including tungsten ions, at the same facility, though the experimental uncertainties reach half an eV for the $j = 1/2 - 3/2$ transitions. Recently, Clementson and Beiersdorfer [23] carried out more accurate wavelength measurements for a few $3s_{1/2} - 3p_{3/2}$ and $3p_{1/2} - 3d_{3/2}$ lines in K-like W^{55+} through Ne-like W^{64+} ions at the Lawrence Livermore National Laboratory EBIT facility. The experiment relies on the calculations of the Flexible Atomic Code (FAC) [24] for line identifications. The FAC is a relativistic configuration-interaction code with Dirac-Hartree-Slater basis functions. It uses the long-wavelength approximation for the Breit energy and obtains screened QED corrections from the hydrogenic values [25, 26] by simple Z-scalings. Clementson and Beiersdorfer also calculated the transition energies with the GRASP code [27] which is based on the MCDF method, with similar QED corrections as those from the FAC.

While FAC and GRASP are invaluable for line identifications, neither of them are high-precision calculations. In the past, we have carried out accurate RCI calculations with *ab initio* QED corrections for a few $3s - 3p_{3/2}$ transition energies of Na-, Mg-, Al- and Si-like uranium and results are in excellent agreement with measurements [28]. We shall use similar methods to calculate the $n = 3 - 3$ transition energies of some of the measured x-ray lines in highly-charged tungsten ions to show that high-precision relativistic correlation methods such as the RCI are important for accurate transition energy calculations and that Breit and QED corrections, which are significant for these high-Z ions, must also be evaluated reliably. In the following two sections, we shall first give a brief description of the present RCI calculations. Results will then be presented and discussed in Section IV, and comparisons will be made with with other theories and with experiment. A summary will be given in the last section.

II.   THEORETICAL METHOD

The details of our RCI method have been given before [29]. We shall only outline the essential points here. The calculation is based on the N-electron *no-pair* Hamiltonian [30, 31]

$$H_{\text{no-pair}} = \sum_{i=1}^{N} h_i + \Lambda_{++} (H_{\text{C}} + H_{\text{B}}) \Lambda_{++} \tag{1}$$

where h_i is the one-electron Dirac Hamiltonian, H_{C} and H_{B} are the Coulomb and frequency-dependent Breit interactions, respectively, and Λ_{++} is the positive-energy projection operator for excluding the negative-energy states and preventing the appearance of electron-positron pairs in higher-order perturbation calculations which leads to the continuum dissolution problem [32] that plagues the relativistic many-electron Dirac Hamiltonian. The eigenfunction $\Psi(J^\pi M)$ of an atomic state with angular momentum (J, M) and parity π is expressed as a linear combination of the many-electron configuration-state functions $\phi(\gamma_i JM)$ such that

$$\Psi(J^\pi M) = \sum_i c_i \phi(\gamma_i JM) \tag{2}$$

where γ_i are sets of quantum numbers representing different electronic configurations with the same parity π, and c_i are configuration mixing coefficients. Variation of the energy functional $\langle \Psi | H | \Psi \rangle$ with respect to c_i, subjected to the wavefunction normalization condition $\langle \Psi | \Psi \rangle = 1$, leads to the CI equation

$$\sum_j (H_{ij} - \lambda \delta_{ij}) c_j = 0. \tag{3}$$

where $H_{ij} = \langle \phi_i | H | \phi_j \rangle$ are the CI matrix elements. We use one-electron B-spline basis functions for a Dirac electron moving in a model potential and confining to a finite cavity [33] to construct many-electron configuration-state functions. B-spline orbitals form finite, complete basis sets representing the bound and continuum states. They also cleanly separated into positive- and negative-energy states so that the no-pair requirement can easily be implemented by using only positive-energy B-spline orbitals. In this work, B-spline basis sets are calculated in Dirac-Kohn-Sham (DKS) potentials with cavity radii of 2.2 a.u., though results are not sensitive to these choices. The numbers of B-spline orbitals generated for each of the angular symmetries s, $p_{1/2}$, $p_{3/2}$, ... are $n = 35$ for the Na- and some of the Mg-like lines and $n = 30$ for the others. We only use the first 20 or so B-spline orbitals

in the calculations which has been found to be quite sufficient in giving results stable to the last digits quoted here which is about 0.01 eV, as remaining orbitals are very high in energies and do not contribute much to the calculations. Resulting CI expansions reach 350,000 configurations, and Davidson's method [34, 35] is used to solve the large-scale CI matrix equation for the lowest-few eigenstates.

Our theoretical energies also include contributions from the nuclear recoil and quantum electrodynamic (QED) corrections. Recoil corrections for the $n = 3 - 3$ transitions are small and consist of the normal mass shifts and specific mass shifts. The former are implicitly included by the use of the finite-mass Rydberg constant in converting energies from atomic units to eV, while the later are approximately given by the mass polarization (MP) corrections which are calculated as expectation values of the operator $H_{\mathrm{MP}} = \frac{1}{M} \sum_{i<j} \mathbf{p_i} \cdot \mathbf{p_j}$, where M is the nuclear mass, using RCI eigenfunctions. As for the QED corrections, we start by evaluating the one-electron self-energy and vacuum polarization corrections. Leading vacuum polarization corrections are calculated as expectation values of the Uehling potential. Wickmann-Kroll corrections [36], like the self-energies [37], are computed non-perturbatively to all orders of $Z\alpha$. To account for screening and relaxation corrections, one-loop QED energies are calculated in DKS potentials specific to the valence configurations of the initial and final states. Corrections from two-loop Lamb shifts are also included. They are small at around 0.01 eV and are order-of-magnitude estimates only. The sums of the one-electron QED corrections, weighted by the effective occupation numbers from the RCI calculations, give the many-electron QED energies.

III.   CI EXPANSIONS

In this work, we study mostly the $3s - 3p_{3/2}$ and $3p_{1/2} - 3d_{3/2}$ x-ray lines measured in [23], along with a few $3s - 3p_{1/2}$ lines measured in [20]. As the sizes of the CI expansions increase very quickly with the number of $n = 3$ valence electrons, we limit our calculations to Ne- to Si-like lines, along with one Ar-like line. The fifteen $n = 3 - 3$ transition lines considered here are listed in Table I. For the eleven lines that are measured in [23], we use the same line labels there consisting of an isoelectronic identifier followed by an integer (Na-1, Mg-2, etc.). For the other four lines measured in [20], we use similar line labels, but with the trailing integer replaced by a Greek alphabet as in Na-α, Mg-β, Al-γ and Al-δ. For each of these

lines, we start by defining reference configurations for the upper and lower states consisting of core and valence electrons. Single and double excitations of at least one valence electron and up to one core electron from these reference configurations are then included in the CI expansions to account for valence-valence (VV) and core-valence (CV) correlations. In the case of Na-like ions, core-core (CC) correlations with the excitations of two core electrons are also included. Descriptions of the CI expansions are given in the following. For brevity, the $1s^2$ core is omitted if it is not explicitly involved in the excitations. Also, B-spline basis sets consist of 30 orbitals for each angular symmetries unless otherwise specified.

1) For the Ne-1 line of W^{64+}, the reference states are $2s^2 2p_{1/2}^2 2p_{3/2}^3 3\bar{l} + 2s^2 2p_{1/2} 2p_{3/2}^4 3\bar{l}$, with the F-like $2s^2 2p^5$ core and $3\bar{l} = 3s, 3p$ valence electrons. The CI expansions from valence excitations and CV correlations between the $n = 2$ and $n = 3$ shells include the configurations $2s^2 2p^5 nl$, $2s^2 2p^4 nln'l'$ and $2s2p^5 nln'l'$. One- and two-electron excitations are limited to $n, n' \leq 20$ and $l, l' \leq 3$.

2) For the Na-1 and Na-α lines of W^{63+}, the reference states are $1s^2 2s^2 2p^6 3\bar{l}$ with the Ne-like core and $3\bar{l} = 3s, 3p$ valence electrons, and B-spline basis sets consist of 35 orbitals for each angular symmetries. The basic CI expansions from valence excitations and CV correlations arising from single- and double-excitations of the $1s$, $2s$, $2p$ core and $3\bar{l}$ valence electrons include the configurations $1s^2 2s^2 2p^6 nl$, $1s^2 2s^2 2p^5 nln'l'$, $1s^2 2s2p^6 nln'l'$ and $1s2s^2 2p^6 nln'l'$, with $n, n' \leq 23$ and $l, l' \leq 5$. We also includes CC correlations from the $n = 2$ subshells with the configurations $1s^2 2s^2 2p^4 3\bar{l}nln'l'$, $1s^2 2s2p^5 3\bar{l}nln'l'$ and $1s^2 2p^6 3\bar{l}nln'l'$, with $n, n' \leq 23$, and $l, l' \leq 3$. The reduced basis sets are adequate for the small CC corrections and help keep the sizes of these large-scale CI calculations manageable.

3) For the Mg-2 and Mg-β lines of W^{62+}, the reference states are the Ne-like core plus $3s^2 + 3p^2$ for the lower state and $3s3p + 3p3d$ for the upper state. With $3\bar{l} = 3s, 3p$ and $3s, 3p, 3d$ for the lower and upper states, respectively, the CI expansions include VV correlations ($2s^2 2p^6 nln'l'$) and CV correlations from the $n = 2$ core and $n = 3$ valence shells ($2s^2 2p^5 3\bar{l}nln'l'$, $2s2p^6 3\bar{l}nln'l'$) with $n, n' \leq 22$ out of 35 B-spline orbitals and $l, l' \leq 5$. For the Mg-1 line, the upper reference state is $3s3d + 3p^2$ and the CI expansions also include VV and CV correlations from the $n = 2$ core and $n = 3$ valence shells, though with smaller basis sets of $n, n' \leq 19$ out of 30 B-spline orbitals. No CC correlation is included for these Mg-like lines.

4) For the six Al-like lines of W^{61+}, the core is again the Ne-like ground state, while the

three valence electrons are from the $3s, 3p$ shells, except for the upper states of Al-1 which are from the $3s, 3d$ shells. The basic CI expansions include VV and CV correlations from the $n = 2$ core and the $n = 3$ valence shells with $n \leq 20$ and $l \leq 5$, except for Al-3 and Al-4 where $n \leq 18$ and $l \leq 3$.

5) For the Si-1 and Si-2 lines of W^{60+}, the reference states consist of the Ne-like core with four valence electrons from the $3\bar{l} = 3s, 3p$ subshells for the lower states and $3\bar{l} = 3s, 3p, 3d$ and $3s, 3p$ subshells for the upper states of Si-1 and Si-2, respectively. We consider VV correlations only with the excitations of up to two valence electrons to $3\bar{l}\,3\bar{l}'nln'l'$ states, with $n, n' \leq 20$ and $l, l' \leq 5$.

6) For the Ar-1 line of W^{56+}, the core is the Ne-like ground state and valence shells are $3s, 3p$ for the lower state and $3s, 3p, 3d$ for the upper state. CI expansions again include VV correlations only with $n \leq 18$ and $l \leq 5$.

IV. RESULTS AND DISCUSSION

In Table II, contributions to the transition energies of the fifteen $n = 3 - 3$ tungsten lines are shown. They include Coulomb and frequency-dependent Breit energies from the present RCI calculations, along with the mass polarization and QED corrections which are also calculated here. The eleven lines with labels ending in an integer (Na-1, Mg-2, etc.) have energies ranging from $500 - 640$ eV. They are from $3s_{1/2} - 3p_{3/2}$ and $3p_{1/2} - 3d_{3/2}$ transitions which, in the high-Z jj-coupling limit, are very close in energy. The remaining four lines with labels ending in a Greek alphabet (Na-α, Mg-β, Al-γ, Al-δ) are from the $3s_{1/2} - 3p_{1/2}$ transitions with lower energies of $150 - 200$ eV.

Transition energies are dominated by the Coulomb energies, with large corrections from the Breit and QED corrections for these high-Z ions. While the Breit energies depend on the details of the electronic configurations and vary in magnitude from 0.27 to 8.67 eV, most of the QED corrections are about -4.5 eV in size as they are dominate by the QED energy of the $3s$ electron in $3s - 3p$ transitions. Exceptions are the Mg-1, Al-1, Si-1 and Ar-1 lines which are $3p_{1/2} - 3d_{3/2}$ transitions and QED corrections are substantially smaller at -0.88, -1.17, -1.06 and -0.37 eV, respectively. In all cases, mass polarization corrections are very small at about -0.01 eV and are quite negligible.

We note that to keep the sizes of the CI expansions computationally manageable, most

of the RCI results only included VV and CV correlations from single and double excitations from the reference states, and some with VV correlations only. For the Na-like tungsten ions, however, CC correlations from the $1s$, $2s$ and $2p$ subshells are also included. They amount to -0.03 and 0.02 eV corrections to the Coulomb energies for the Na-1 and Na-α lines, respectively. Furthermore, with the choices of the reference states here, we found that it is important to include triple excitations in our RCI calculations of the Al-1 and Al-3 lines. Specifically, for the $3s^23d$ $J=3/2$ upper state in Al-1, we include the configurations $2s^22p^63pnln'l'$, $2s^22p^53s3pnln'l'$ and $2s2p^63s3pnln'l'$. For the $3s3p_{1/2}[1]3p_{3/2}$ $J=3/2$ upper state in Al-3, we include the configurations $2s^22p^53s^2nln'l'$, $2s^22p^53s3dnln'l'$, $2s2p^63s^2nln'l'$ and $2s2p^63s3dnln'l'$. For these two lines, corrections from triple excitations reduce the transition energies by 1.89 and 0.84 eV, respectively. In general, the accuracies of our RCI energies are limited by the extensiveness of the CI expansions and theoretical uncertainties are assigned to the Coulomb energies in Table II accordingly. The accuracies of the QED energies, on the other hand, are not as sensitive to correlation effects and their uncertainties are estimates based on the approximated treatment of screening and relaxation corrections.

In Table III, the $n = 3 - 3$ transition energies for tungsten ions are compared between theories and experiments. For simplicity, we do not show the measured results of Gillaspy *et al.* [22] here because for the $3s - 3p_{1/2}$ Na-α line, it is essentially the same as the other NIST measurement by Ralchenko *et al.* [20], and for the $3s - 3p_{3/2}$ Na-1, Mg-2 and $3p_{1/2} - 3d_{3/2}$ Al-1, Si-1 lines, their uncertainties, at around 0.5 eV, are much higher than those of Clementson and Beiersdorfer [23], which are around 0.1 eV. Theoretical energies relative to the experimental energies shown in Table III are plotted in Fig. 1. It can be seen that the present RCI results are more accurate than those of FAC and GRASP. For the Na-1 and Na-α lines, our RCI energies are in excellent agreement with the RMBPT results of Sapirstein and Cheng [38], both are in good agreement with experiment and have the same QED corrections from *ab initio* calculations outlined earlier. For the $3p_{1/2} - 3d_{3/2}$ Mg-1 line and the $3s - 3p_{1/2}$ Mg-β, Al-γ and Al-δ lines, our RCI energies are also in good agreement with the RMBPT results of Safronova and Safronova [19], though with larger discrepancies up to 0.2 eV which are likely due to differences in QED corrections: While our QED energies are directly calculated, those in [19] are either scaled from the Na-like QED results of Blundell [8], or from Mohr's hydrogenic results [25, 26] with *ad hoc* screening corrections. For the $3s - 3p_{3/2}$ Mg-2 line, however, the RMBPT result of [19] is higher than our RCI energy,

which is in good agreement with experiment, by 0.63 eV and this is probably not due solely to the discrepancy in QED corrections. Indeed, for the $4s^2\,{}^1S_0 - 4s4p\,{}^1P_1$ transition in Zn-like ions, which is the same as Mg-2 but with $n = 4$ instead of $n = 3$ valence electrons, it has been show in [29] that the RMBPT energies of Blundell *et al.* [39] also deviate from the RCI energies of the present authors [29], which agree very well with experiment along the entire Zn isoelectronic sequence, by up to 0.5 eV at high Z, and that these discrepancies are largely removed in the revised RMBPT calculations of Blundell [40] who updated the QED corrections and, more importantly, the Breit energies with frequent-dependent, retarded calculations. It is thus possible that the Breit corrections also play an important role in the large discrepancy of the Mg-2 line energies between RMBPT and RCI here. In general, differences between RCI and experiment go up with the numbers of $n = 3$ valence electrons, as it is increasingly more difficult to include all dominant configurations in the CI expansions. For the Al-1, Al-3 and Al-4 lines, the discrepancies are likely due to inadequate treatment of triple excitations. For the Si-1, Si-2 and Ar-1 lines, they probably come from the lack of CV correlations as we are limited by the sizes of the RCI calculations to VV correlations only.

V.   SUMMARY

We have calculated a few $n = 3 - 3$ transition energies for highly-charged Ne- to Ar-like tungsten using a large-scale RCI method. QED corrections including screening and relaxation effects are also included. Our results are generally in very good agreement with experiments and show the importance of reliable treatments of Breit and QED corrections for these high-Z ions. At present, theoretical accuracies are limited by the sizes of CI expansions which also affected the open-shell systems that can be treated. Nevertheless, these computational constrains can be overcome with more efficient and compact basis sets as well as faster and more capable computers. Tungsten is of great interests in fusion reactor designs and it is desiable to have more precision measurements of the $n = 3 - 3$ as well as $n = 2 - 2$ transitions in highly-charged tungsten ions.

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TABLE I: Spectral lines studied in this work. The Ne-1 line has a $1s^2 2s^2 2p^5$ $J^\pi = 3/2^-$ F-like core. Other lines have a $1s^2 2s^2 2p^6$ $J^\pi = 0^+$ Ne-like core. Upper and lower state identifications are given by core + the respective valence configurations.

Ion	Line	Lower state	J^π_{lower}	Upper state	J^π_{upper}
W^{64+}	Ne-1	$3s$	1^-	$3p_{3/2}$	0^+
W^{63+}	Na-1	$3s$	$1/2^+$	$3p_{3/2}$	$3/2^-$
	Na-α	$3s$	$1/2^+$	$3p_{1/2}$	$1/2^-$
W^{62+}	Mg-1	$3s3p_{1/2}$	1^-	$3s3d_{3/2}$	2^+
	Mg-2	$3s^2$	0^+	$3s3p_{3/2}$	1^-
	Mg-β	$3s^2$	0^+	$3s3p_{1/2}$	1^-
W^{61+}	Al-1	$3s^2 3p_{1/2}$	$1/2^-$	$3s^2 3d_{3/2}$	$3/2^+$
	Al-2	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[1]3p_{3/2}$	$1/2^+$
	Al-3	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[1]3p_{3/2}$	$3/2^+$
	Al-4	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p_{1/2}[0]3p_{3/2}$	$3/2^+$
	Al-γ	$3s^2 3p_{1/2}$	$1/2^-$	$3s3p^2_{1/2}$	$1/2^+$
	Al-δ	$3s3p^2_{1/2}$	$1/2^+$	$3s^2 3p_{3/2}$	$3/2^-$
W^{60+}	Si-1	$3s^2 3p^2_{1/2}$	0^+	$3s^2 3p_{1/2}3d_{3/2}$	1^-
	Si-2	$3s^2 3p^2_{1/2}$	0^+	$3s3p^2_{1/2}3p_{3/2}$	1^-
W^{56+}	Ar-1	$3s^2 3p^6$	0^+	$3s^2 3p_{1/2}3p^4_{3/2}3d_{3/2}$	1^-

TABLE II: Contributions (eV) from Coulomb, Breit, MP, and QED to the $n = 3 - 3$ transition energies for tungsten ions. Numbers in parentheses are error estimates.

Line	Coulomb	Breit	MP	QED	Total
Ne-1	590.68(5)	1.71	-0.01	-4.50(5)	587.88(7)
Na-1	538.01(3)	-0.50	-0.01	-4.41(4)	533.09(5)
Na-α	160.24(3)	4.13	-0.01	-4.85(4)	159.51(5)
Mg-1	586.17(8)	-5.13	-0.01	-0.88(4)	580.15(9)
Mg-2	550.13(5)	-0.52	-0.01	-4.34(5)	545.27(7)
Mg-β	156.00(5)	3.81	-0.01	-4.75(5)	155.05(7)
Al-1	602.39(30)	-4.65	0.00	-1.17(4)	596.57(30)
Al-2	554.60(10)	-0.27	-0.01	-4.32(5)	550.00(11)
Al-3	544.96(30)	-1.68	-0.01	-3.62(4)	539.65(30)
Al-4	505.19(30)	-0.31	-0.01	-4.27(5)	500.60(30)
Al-γ	167.95(10)	4.24	-0.01	-4.73(5)	167.45(11)
Al-δ	199.66(10)	-8.67	-0.01	5.11(5)	196.09(11)
Si-1	618.22(40)	-4.65	-0.01	-1.06(4)	612.47(40)
Si-2	549.12(40)	-1.35	0.00	-3.61(4)	544.16(40)
Ar-1	636.67(50)	-5.41	0.00	-0.37(4)	630.89(50)

TABLE III: Comparison between theory and experiment for the $n = 3 - 3$ transition energies of tungsten ions. Numbers in parentheses are theoretical and experimental uncertainties.

Line	RCI[a]	FAC[b]	GRASP[b]	RMBPT[c]	Expt[b]
Ne-1	587.88(7)	591.27	591.10		588.02(17)
Na-1	533.09(5)	533.56	533.38	533.08[d]	533.20(11)
Na-α	159.51(5)	159.74[e]		159.50[d]	159.59(4)[e]
Mg-1	580.15(9)	580.45	573.42	580.03	580.12(16)
Mg-2	545.27(7)	546.16	544.87	545.90	545.35(10)
Mg-β	155.05(7)	155.17[e]		155.25	155.15(4)[e]
Al-1	596.57(30)	598.35	600.79		597.34(12)
Al-2	550.00(11)	550.89	552.76		549.99(10)
Al-3	539.65(30)	540.24	542.48		539.98(14)
Al-4	500.60(30)	500.54	499.65		500.3(2)
Al-γ	167.45(11)	167.65[e]		167.37	167.46(5)[e]
Al-δ	196.09(11)	196.03[e]		195.97	196.24(9)[e]
Si-1	612.47(40)	612.90	613.78		611.66(15)
Si-2	544.16(40)	544.60	544.65		543.96(12)
Ar-1	630.89(50)	631.41	632.35		630.03(22)

[a]This work.
[b]Clememtson and Beiersdorfer [23] unless otherwise specified.
[c]Safronova and Safronova [19] unless otherwise specified.
[d]Sapirstein and Cheng, [38].
[e]Ralchenko *et al.* [20].

FIG. 1: (Color online) Theoretical energies relative to the experimental energies. Solid circles are the present RCI results. Open squares and crosses are RMBPT results of [38] and [19], respectively. Solid triangles and open inverted triangles are FAC and GRASP results, respectively. Horizontal error bars are experimental uncertainties.