Multi-configuration Dirac–Hartree–Fock (MCDHF) calculations for Zn-like sequence from $Z = 48$ to 54*

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The 4s4p excitation energies and the $4s^2$–4s4p E1 transitions for zinc-like ions from $Z = 48$ to 54 are calculated by the multi-configuration Dirac–Hartree–Fock (MCDHF) method in this paper. The results for fine-structure energy levels, wavelengths and lifetimes between $Z = 48$ (Cd) and $Z = 54$ (Xe) are presented and compared with other theoretical and experimental results. The calculated values including core-valence correlation are found to be very similar to other theoretical and experimental values. We believe that our calculated values can guide experimentalists in identifying the fine-structure levels in their future work.

Keywords: core valence correction, multi-configuration Dirac–Hartree–Fock, energy level, wavelength

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1. Introduction

Spectroscopy of highly stripped ions is important for plasma diagnostics in controlled fusion research and provides important tests of relativistic atomic structure calculations. Ions of the zinc isoelectronic sequence have two valence electrons outside a closed $n = 3$ core and provide a model for studying effects of strong correlation on closely spaced levels in heavy atoms. For the excitation energies of the 4s4p $^3P_{0,1,2}$ and $^1P_1$ states from the $4s^2{}^1S_0$ ground state of Zn-like ions, there exist many experimental and theoretical studies.

For low- to mid-Z ions (for $Z \approx 30$ to 54,) empirical data can be found from Ref. [1] for $Z = 34$ and 35, from Ref. [2] for $Z = 36$, from Ref. [3] for Z from 37 to 42, from Ref. [4] for Z from 37 to 50 and from the NIST database[5] for Z from 30 to 37, 42, and 54. Among the more accurate calculations in this Z range, the multi-configuration Dirac–Fock (MCDF) results of Liu *et al.*[6] for Z from 30 to 47 accord with experimental results within 0.1 eV–0.2 eV.

For mid- to high-Z ions (for Z from 50 to 92), experimental results were obtained from the spectra of laser-produced plasmas,[7−10] tokamak discharges,[11−13] and the Livermore electron beam ion trap.[14−17] While calculations were based on the MCDF method,[9,18−19] the Hebrew University-Lawrence Livermore Atomic code (HULLAC),[20] the semi-relativistic Cowan code,[21] the multi-configuration relativistic random-phase approximation (MCRRPA),[22] the relativistic multi-reference Mϕller–Plesset (MR–MP) perturbation theory,[23] the second-order relativistic many-body perturbation theory (RMBPT),[24] and relativistic configuration-interaction approach[25] were also used to calculate the energies of the zinc isoelectronic sequence. The multi-configuration Dirac–Hatree–Fock (MCDHF) method has been used in our previous work.[26]

Much work has been well done for providing more accurate theoretical results comparable to experimental results. But for the range Z from 48 to 54, the fine structure still needs to be investigated. Our calculations are motivated by the need for accurate fine structure data in a variety of scientific applications, which can be used to improve the understanding of the origin of these effects, explain the existing results and provide further predictions.

On the basis of our previous work,[27,28] in this paper, besides the well-known problems arising from the necessity of considering some of the core electrons within the atom and the effects of electron correla-

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tion, the relativistic effect also needs to be taken into account for obtaining the accurate calculations. The calculation methods used are based on the MCDHF[29] method, as represented by the GRASP2K codes created by Grant *et al.*[30] and further developed by Jönsson *et al.*[31] The GRASP92 codes were modified and extended by Parpia *et al.*[32] As will be shown in the present work, the MCDHF method, which has been applied successfully to a number of atomic systems and spectroscopic properties, is used to investigate the convergence of fine-structure, transition rates, wavelengths and line strengths in zinc-like ions ($48 \leq Z \leq 54$). The variational wave-functions and the reliability of the calculated expectation values are verified from the analysis of the convergence patterns and from the comparison with the available theoretical and experimental data.

2. Model and method

2.1. Theory

The extended optimal level (EOL) version of the MCDF method is used to calculate the transitions. The theoretical basis of our present computational approach has been widely discussed elsewhere.[33−36] Hence we only repeat the essential features here.

In the MCDHF method, the atom is represented by an atomic state function (ASF), which is a linear combination of configuration state functions (CSFs)

$$\Psi_i(J^p) = \sum_{\alpha=i}^{n_{\rm csf}} C_{i\alpha}\varphi(\Gamma_\alpha J^p), \tag{1}$$

where $C_{i\alpha}$ is the mixing coefficient for state i and $n_{\rm csf}$ is the number of CSFs included in the evaluation of ASFs. The ASFs thus constructed are used for solving the Dirac–Hartree–Fock equation and the Dirac–Coulomb Hamiltonian is

$$\hat{H}^{\rm DC} = \sum_{i=1}^{N} \hat{H}_{\rm D}(i) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} |\hat{r}_i - \hat{r}_j\,|^{-1}, \tag{2}$$

where the first term on the right-hand side, in JJ coupling, is the one-body contribution for an electron due to the kinetic energy and its interaction with the nucleus. The two-body Coulomb interactions between the electrons comprise the second term. In the relativistic self-consistent field procedure both the radial parts of the Dirac orbitals and the expansion coefficients $C_{i\alpha}$ are optimized to self-consistency. The contributions from Breit interaction, vacuum polarization, self-energy and finite nuclear mass corrections are not included in Eq. (2) and are generally added as a first-order perturbation correction after self-consistency has been obtained. The transverse Breit interaction

$$B_{ij} = -\frac{1}{2r_{ij}}\left[\alpha_i\cdot\alpha_j + \frac{(\alpha_i\cdot r_{ij})(\alpha_j\cdot r_{ij})}{r_{ij}^2}\right] \tag{3}$$

is included in subsequent configuration interaction (CI) calculations.

2.2. Calculation procedure

In this work, we include different correlations into the calculation in a systematic approach. The correlation energy is defined as the energy difference between the exact solution to the Dirac equation and the Dirac–Fock (DF) solution. The contribution from different types of correlation can then be defined as the energy difference between the solution including the particular correlation under investigation and the DF solution. To classify the correlations, the atomic electrons can be divided into two parts: valence electrons and core electrons. As a result, the correlation between the valence electrons is defined as valence correlation (VV) and the correlation between the valence electrons and the core electrons is defined as core–valence correlation (CV). The remaining correlation is core–core correlation (CC), which describes the correlation between the core electrons.

In the MCDHF approach, the correlation is represented by different constraints on the generation of the CSFs included in Eq. (1). If we include only the VV, the core electrons are kept fixed in all the CSFs generated. To include CV, we allow one of the core electrons to be excited to generate the CSFs. Finally, the CC correlation can be taken into account by allowing more than one core electron to be excited.

For Zn-like ions, the ground and first excited configurations are $4s^2$ and 4s4p respectively. In the first step, the active set (AS) is

$$\text{AS1} = \{4\text{s}, 4\text{p}, 4\text{d}, 4\text{f}\}. \tag{4}$$

Then, we increase the active set in the following way:

$$\text{AS2} = \text{AS1} + \{5\text{s}, 5\text{p}, 5\text{d}, 5\text{f}, 5\text{g}\}, \tag{5}$$

$$\text{AS3} = \text{AS2} + \{6\text{s}, 6\text{p}, 6\text{d}, 6\text{f}, 6\text{g}\}, \tag{6}$$

$$\text{AS4} = \text{AS3} + \{7\text{s}, 7\text{p}, 7\text{d}, 7\text{f}, 7\text{g}\}, \tag{7}$$

$$\text{AS5} = \text{AS4} + \{8\text{s}, 8\text{p}, 8\text{d}, 8\text{f}, 8\text{g}\}. \tag{8}$$

In the VV, CV and CC used different active sets, each of which is discussed here clearly.

Here, in our valance–valence (V–V) method, we set $1s^22s^22p^63s^23p^63d^{10}$ as our core electrons in the calculation. Then we increase the principal quantum number n and optimize the orbitals AS1, AS2, AS3, AS4, and AS5.

In the C–V model, the core is $1s^22s^22p^63s^23p^63d^9$ and then we optimize the layer by n. We generate the CSFs in the form of $1s^22s^22p^63s^23p^63d^9$ASn, $n = 1, 2, 3, 4$.

For the C–C model, wavefunctions are generated by $1s^22s^22p^63s^23p^63d^8$ASn, $n = 1, 2, 3$.

3. Results and discussion

While considering the convergence and the accuracy of our calculation and comparing the three interactions (i.e. VV, CV, and CC), we monitor the VV and CV forms of the MCDHF excitation energies for Cd^{18+}–Xe^{24+} for orbital sets of increasing size, denoted by n. We should point out that the the deviation of the CC results from the experimental results are very large and the CC results are not given here. The remaining results are listed in Table 1, where some experimental results are also included.

Table 1. Zinc-like isoelectronic sequence: excitation energies in cm^{-1} from MCDHF calculations and other theories.

Level	VV				CV			Exp[a,b,c]
	$n \le 5$	$n \le 6$	$n \le 7$	$n \le 8$	$n \le 5$	$n \le 6$	$n \le 7$	
$Z = 48$								
$^3P_0$	281609	281639	281650	281652	284469	284413	284446	284831
$^3P_1$	297022	297047	297056	297058	299583	299469	299477	299825
$^3P_2$	353130	353163	353174	353177	356549	356325	356327	356855
$^1P_1$	438218	438107	438089	438084	436094	435342	435089	434699
$Z = 49$								
$^3P_0$	295952	295982	295993	295995	298849	298785	298820	299171
$^3P_1$	312810	312835	312844	312845	315356	315229	315237	315330
$^3P_2$	377053	377086	377098	377100	380537	380297	380301	380737
$^1P_1$	464563	464454	464435	464431	462448	461681	461431	460878
$Z = 50$								
$^3P_0$	310379	310410	310420	310422	313314	313242	313278	313704
$^3P_1$	328722	328748	328756	328757	331248	331110	331118	331470
$^3P_2$	401961	401995	402007	402010	405511	405256	405262	405823
$^1P_1$	491851	491744	491724	491720	489753	488971	488724	488338
$Z = 51$								
$^3P_0$	324895	324927	324938	324939	327867	327788	327825	328203
$^3P_1$	344759	344784	344792	344793	347262	347113	347120	347379
$^3P_2$	427918	427952	427965	427968	431533	431263	431272	431594
$^1P_1$	520150	520044	520025	520021	518075	517281	517036	516560
$Z = 52$								
$^3P_0$	339503	339536	339546	339548	342511	342425	342464	342702
$^3P_1$	360918	360943	360951	360952	363395	363235	363241	363496
$^3P_2$	454985	455020	455033	455036	458664	458381	458391	458711
$^1P_1$	549530	549425	549406	549402	547484	546677	546435	545902
$Z = 53$								
$^3P_0$	354212	354245	354256	354258	357255	357163	357203	357285
$^3P_1$	377204	377229	377236	377237	379653	379482	379487	379730
$^3P_2$	483235	483270	483284	483286	486977	486682	486694	486901
$^1P_1$	580067	579964	579945	579941	578055	577237	576997	576438
$Z = 54$								
$^3P_0$	369020	369053	369064	369065	372097	371998	372040	371982
$^3P_1$	393610	393636	393643	393643	396029	395848	395852	396091
$^3P_2$	512728	512763	512778	512780	516534	516227	516240	516504
$^1P_1$	611829	611728	611708	611704	609856	609027	608790	608091

[a]Churilov *et al.*,[4] [b]Brown *et al.*,[10] [c]NIST[5]

It should be noted that the experimental results in the table are the results for Cd^{18+}–Sn^{20+}, measured by Churilov,[4] while the results for Sb^{21+}–I^{23+} are semi-empirically corrected results given by Brown[10] and the data for Xe^{24+} are cited from NIST.[5] There have been no experimental results for Sb^{21+}–I^{23+} and in Brown's paper the semi-empirically corrected results for Z from 31 to 92 n are nearly equal to the existed experimental results,[7−17] so Brown's results can be seen as a good reference for experiment. In our three models mentioned above, the energy contributions from Breit interaction, quantum electrodynamics (QED) corrections and specific mass shift (SMS) are all included. The mixing coefficients obtained using MCDF and RCI orbital wavefunctions in the block structure format are then converted into non-block format and the orbital wavefunctions of the initial and final states are transformed to a new representation in which the two orbitals are biorthonormal. These biorthonormal wavefunctions are used to evaluate the dipole transition rates. In this implementation of the RCI program, an iterative Davidson method is used together with a spare matrix representation allowing for large expansions. The maximum deviations of VV correction calculations from the experimental and semi-empirically corrected results are 1.04% and 0.31% respectively, those of the CV correction calculations are all 0.74%. It is clear that our CV results are very close to the experimental and semi-empirically corrected results. These energies obtained by three models are very close, which is most likely to be due to slower convergence of correction treatment for GRASP2k, since the effect decreases for higher Z. In order to show that the results are reliable, we plot the difference between theoretical and experimental results versus the atomic number Z for the energy level of $^3P_0$. Included in Fig. 1 are the data from the present calculation, the experimental data, and the values compiled by Biémont[19] and Chen.[25] From Fig. 1, we can conclude that our CV results are very close to experimental results in a difference range from 0.02% to 0.13%. Chen's results accord well with the experimental data than CV results for Cd^{18+}–Sb^{21+}, but their comparison with our CV results shows that the maximum difference is only 0.06%. The previous MCDF results by Biémont are clearly lower than the experimental results.

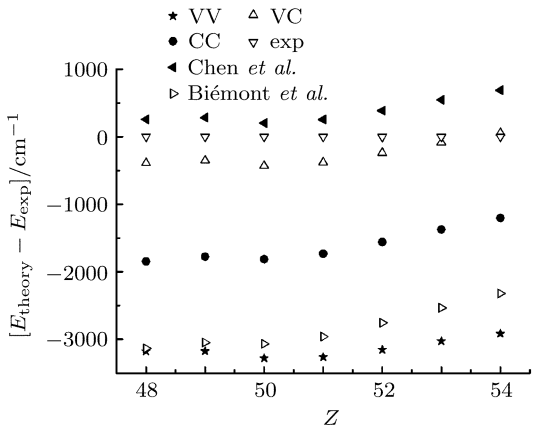


Fig. 1. Difference between the available theoretical and experimental values and the present values for the $^3P_0$ along the sequence versus atomic number Z.

As we know, the $4s^2\ ^1S_0$–$4s4p\ ^1P_1$ resonance transition of zinc-like ions is often prominent in tokamak discharges. It is therefore useful to diagnose these hot plasmas. Also, in order to check the reliability of our calculation, we compare our results of wavelength λ for Zinc-like ions with nuclear charges ranging from $Z = 48$ to $Z = 54$. In Fig. 2, the experimental results are given by Churilov *et al.*[4] and the other theoretical results are reported by Brown *et al.*,[10] Sugar *et al.*[12] Biémont,[19] and Chen and Cheng.[25]

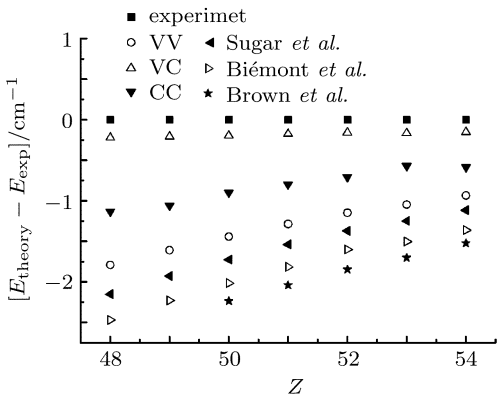


Fig. 2. Difference between the available theoretical and experimental values and the present VV, VC, and CC results for the transition $4s^2\ ^1S_0$–$4s4p\ ^1P_1$ versus atomic number Z.

Sugar's data obtained by using the advanced version of the Desclaux code are somewhat higher than the experimental results, which range from 1.117 Å to 2.152 Å (1 Å = 0.1 nm). Brown *et al.* have calculated the transition wavelengths for Sn^{20+}–Xe^{24+} by using the HULLAC code. The difference between the experimental and Brown's data is in a range from 1.523 Å to 2.238 Å. It is clear that the calculated values including the CV correction are in general in good

agreement with the experimental results; the biggest difference is only 0.2 Å, while the biggest difference for VV is 1.7 Å and for CC is 1.1 Å. And we can find that the difference between the theoretical and the experimental results decreases with the increase of Z number. It should be noted that the Desclaux code is an MCDF program, why are the Sugar's data higher than ours? We think that in their calculations, they considered only the Lamb-shift, but they did not take into account the other QED corrections which have been proved to be important in many studies.[25,26] Since in Brown *et al.*'s[10] paper, they calculated only 84 levels belonging to 10 configurations for the type $4l4l'$, which is not sufficient for the complex configuration. In our previous work and Chen and Cheng's paper,[25] we find that the $n \geq 5$ layer electrons have influence on the E1 transitions.

The transition energy for the spin-forbidden line term splitting $E(^1\mathrm{P}_1)$–$E(^3\mathrm{P}_1)$ from the current calculation is shown in Table 2. We also present the results from Chen, Biémont, Brown and experiment. From Table 2, we find that the difference increases steadily along the sequence. It is interesting that data for Sb^{21+} do not obey the trend. From Table 2, our CV data are generally in agreement with experimental results and semiempirically corrected results given by Brown *et al.*[10]

Better QED (self-energy and vacuum polarization) calculations are important for improving the atomic theory at higher Z. In Table 3, we compare QED energies calculated here with those given by Chen *et al.*[25] and Blundell *et al.*[24] Here our results are divided into three parts according to VV, CV, and CC corrections. Our QED energies for CV and CC lie between the other two theoretical predictions. The CV results are slightly closer to Chen's results, with the differences ranging from 0.001 eV to 0.007 eV, while our CC results are close to the results given by Blundell *et al.*[24] The maximum difference is 0.019 eV. We know that in QED calculation, frequency-dependent, retarded Breit corrections, diagonal and off-diagonal contributions should be considered. The details of these calculations can be found in Ref. [22]. In view of the difficulty closer of these QED calculations, the agreement among theories is quite reasonable.

Table 2. Term splitting $^1\mathrm{P}_1$–$^3\mathrm{P}_1$ (the unit is in cm^{-1}).

Z	VV	VC	CC	Chen	Biémont	Brown	Exp.
48	141026	135612	138393	134573	142214		134874
49	151586	146194	148898	145155	152714		145548
50	194662	189247	191982	188168	195929		188513
51	175227	169916	172473	168867	176250	169181	
52	188450	183194	185681	182143	189422	182406	
53	202704	197510	199929	196460	203625	196708	
54	218061	212938	215290	211889	218934		212000

Table 3. QED corrections (eV) to the $^1\mathrm{P}_1$ excitation energies of Zn-like ions.

Z	VV	CV	CC	Chen	Blundell
51	–0.227	–0.231	–0.238	–0.233	–0.256
52	–0.246	–0.252	–0.259	–0.255	–0.279
53	–0.256	–0.272	–0.284	–0.279	–0.303
54	–0.293	–0.304	–0.309	–0.305	–0.328

Radiative lifetimes of the $^1\mathrm{P}_1$ are compared with other theoretical results from Chen *et al.*[25] and Pascal *et al.*[19] As we know, theoretical energy may not be very accurate, theoretical transition rate, which is scaled as ω^3, is often adjusted by replacing theoretical value with empirical transition energy. For low- to mid-Z ions, the $4s^2\ ^1\mathrm{S}_0$–$4s4p\ ^3\mathrm{P}_1$ spin-forbidden transition is allowed through singlet–triplet mixings and its transition matrix element is proportional to the small $^1\mathrm{P}_1$ mixing coefficient which is in turn scaled approximately as the inverse of the $^{1,3}\mathrm{P}_1$ level splitting. As a result, radiative lifetime is often adjusted for the transition energy $\Delta E = E(^{3,1}\mathrm{P}_1) - E(^1\mathrm{S}_0)$ with the formula

$$\tau_{\mathrm{adjusted}} = \tau_{\mathrm{original}}(\Delta E_{\mathrm{theory}}/\Delta E_{\mathrm{exp}\,t})^3, \qquad (9)$$

while those for the $^3\mathrm{P}_1$ states of low- to mid-Z ions may be further adjusted for the singlet–triplet interval energy $\delta E = E(^1\mathrm{P}_1) - E(^3\mathrm{P}_1)$ with the formula[37]

$$\tau_{\mathrm{adjusted}} = \tau_{\mathrm{original}}(\Delta E_{\mathrm{theory}}/\Delta E_{\mathrm{exp}\,t})^3/(\delta E_{\mathrm{exp}\,t}/\delta E_{\mathrm{theory}})^2. \qquad (10)$$

While in Chen *et al.*'s paper, they found that their results were in agreement with empirical data

even for neutral Zinc in better than 0.5% and they did not make empirical energy adjustment to their results, but we do. For the lifetime of the $^1P_1$ state, the maximum difference between Chen's and ours is 11.6% for VV, 2.03% for CV and 6.61% for CC. It seems that our CV results accord with Chen *et al.*'s very well. But we should point out that if the values in last column are used, the biggest difference is only 1.6%. It is interesting that our CV results are close to Biémont's[19] results except the results for In^{19+}, I^{20+} and Xe^{21+}, while the VV results of these three ions are in good agreement with theirs. Although the Biémont's[19] lifetime for In^{19+} is nearly equal to our VV result, it is still confused, because the lifetime will decrease with the increase of atomic number, which is the trend of our results and Chen *et al.*'s.[25]

Table 4. Lifetimes (in ns) for the 4s2 $^1S_0$–4s4p $^1P_1$ transition in Zn-like ions.

	VV	CV	CC	Chen	Biémont	Others
48	0.0174	0.0193	0.0188	0.0197	0.0174	0.0191[a]
49	0.0158	0.0179	0.0175	0.0178	0.0157	
50	0.0147	0.0159	0.0157	0.0161	0.0159	0.0158[b]
51	0.0132	0.0144	0.0140	0.0146	0.0144	
52	0.0125	0.0130	0.0128	0.0132	0.0130	
53	0.0108	0.0119	0.0113	0.0121	0.0109	0.0117[a]
54	0.0099	0.0107	0.0105	0.0110	0.0098	0.0107[a]

[a] Chou *et al.*,[22] [b] Fischer and Hansen.[38]

4. Conclusions

We use the relativistic multi-configuration Dirac–Hartree–Fock (MCDHF) method to calculate the fine-structure energy levels, the term splitting, the wavelengths, transition rates and lifetimes of the Zinc-like $4s^2$–4s4p transitions in the ions Cd^{18+}–Xe^{24+}. We show different results for fine structure energies by the method including different effects. The results obtained by MCDHF are in excellent agreement with experimental data and cited results. The availability of such data would lead to an improved understanding of the relative importance of different contributions to the energies of highly charged ions. These calculations provide a theoretical benchmark for the comparison between experiment and theory. It is found that the relativistic and configuration interaction effects are dominant in the correct assignment of different transitions and also in the accurate evaluation of atomic transition data of highly ionized atoms. However, because these results are all from single- or few-configuration calculations, it would be imprudent to conclude that it is now more than a trend; more calculations with more configurations are clearly needed. We hope that these results will be useful for analysing the existing and future experimental results.

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