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Ionization potentials of superheavy elements No, Lr, and Rf and their ions

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We predict ionization potentials of superheavy elements No, Lr, and Rf and their ions using a relativistic hybrid method that combines configuration interaction (CI) with the linearized coupled-cluster approach. Extensive study of the completeness of the four-electron CI calculations for Hf and Rf was carried out. As a test of theoretical accuracy, we also calculated ionization potential of Yb, Lu, Hf, and their ions, which are homologues of the superheavy elements of this study.

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I. INTRODUCTION

The first ionization potential (IP) of atoms and ions, which is defined as the minimal energy required to remove one electron, is an important characteristic of an element that determines its chemical properties. The IP values presented in tables as experimental ones are usually obtained by extrapolating a sequence of Rydberg levels to $n \to \infty$ (n is principal quantum number). This method has very high accuracy but requires detailed knowledge of the spectra of Rydberg states; otherwise, it cannot be used. For this reason IPs are known to high accuracy for most of neutral atoms and for many ions, the systems with very well studied spectra [1]. For other ions and for superheavy elements (SHEs) the IPs are either not known or known to very poor accuracy only.

The goal of the present work is to address both issues: accurate predictions of IPs for the superheavy atoms and ions and testing the accuracy of the IP predictions for the lighter ions to asses the potential for significant improvement of the IP calculations in ions with one to four valence electrons using state-of-the art methodology.

We focus on the IPs of SHEs (nuclear charge $Z > 100$) as the atomic calculations provide important information for planning and interpreting the measurements for this multidisciplinary area of research involving nuclear physics, atomic physics, and chemistry (see, e.g., reviews [2–4]) The sequence of No ($Z = 102$), Lr ($Z = 103$), and Rf ($Z = 104$) atoms is particulary interesting since these have two, three, and four valence electrons, respectively, and can be modeled with the highest precision relativistic approaches that treat correlation corrections to all orders of perturbation theory [5,6]. In Ref. [7], we studied these systems but calculated ionization potential only using the configuration interaction (CI) + second-order many-body perturbation theory (MBPT) method. In 2015, the first ionization potential of Lr was measured [8], using efficient surface ion-source and a radioisotope detection system coupled to a mass separator. This work opened the way for the first IP measurements of transactinide SHEs on an atom-at-a-time scale. The measurement of the first IP of No is also in progress [9]. Therefore, it is timely to provide accurate predictions for these superheavy atoms and their ions, critically evaluated for their accuracy.

II. COMPUTATIONAL METHODS

Prediction of IPs involves the calculation of the ground-state valence energies of the neutral atoms and ions. For monovalent systems, the IP, i.e., the removal energy of the electron in the ground state is generally calculated directly. For systems with a few valence electrons, two calculations are generally necessary, for the system of interest and the corresponding ion with one electron removed. For example, determining the first IP of divalent Yb I can be accomplished by calculating its two-electron binding energy for the ground $6s^2\ {}^1S_0$ state and a removal energy of Yb II ion in its ground $6s\ {}^2S_{1/2}$ state. The difference of the two values gives the first IP of Yb I. For systems with a few valence electrons, it is important to ensure similar accuracy of these two calculations, as the final IP is very sensitive to any inconsistencies in the computations, both from omitted correlations and other effects and from numerical aspects of both computations. As a result, IPs present excellent benchmarks for tests of computational methods.

We calculate the M-electron IPs of No I, No II, Lr I, Lr II, Lr III, Rf I, Rf II, Rf III, and Rf IV, with the number of valence electrons $M = 1$ to 4, which allowed us to calculate the first IPs for all of the atoms and ions. As a test of theoretical accuracy, we also calculate IPs for their homologues, Yb I, Yb II, Lu I, Lu II, Lu III, Hf I, Hf II, Hf III, and Hf IV. Carrying out these calculations allowed us to both estimate the uncertainties in our IP predictions, based on the comparisons of IPs of Yb, Lu, and Hf with reference data, and to study the differences between SHEs and their lighter homologues. For example, large relativistic corrections in SHEs caused changes in the ground state configurations for several systems that we have studied.

The starting point for all of our calculations is the *frozen core* Dirac-Fock (DF) V^{N-M} potential [10], where N is the total number of electrons. The initial Dirac-Fock procedure is carried out for the closed-shell ion, with all valence electrons removed; with $M = 2$ for Yb and No, $M = 3$ for Lu and Lr, and $M = 4$ for Hf and Rf. The finite single-electron basis set is constructed using the B-spline technique [11]. The basis contains 35 B-splines of order 7 in a cavity of radius $R_{\max} = 60a_B$, where a_B is Bohr's radius. The Breit interaction is included in the present calculations using the approach developed in Refs. [12,13], while quantum electrodynamic (QED) effects are accounted for by using the radiative potential method developed in Ref. [14].

We used linearized coupled-cluster approach [5] (initially developed for accurate treatment of the alkali-metal atoms) to calculate the one-electron ground-state removal energies of monovalent No II, Lr III, Rf IV, Yb II, Lu III, and Hf IV. The details of the method, its applications, and accuracy have been discussed in a review [5]. All other systems considered here have at least two valence electrons, and are treated with the different approach that combines a modified version of the method described above with the CI method [6]. In this method, referred to as CI+all-order, the coupled-cluster calculation is used to construct an effective Hamiltonian that incorporates core-core and core-valence correlations. Then, the effective Hamiltonian is used in the very large-scale CI calculations. Thus CI+all-order method treats correlation corrections in all sectors, core-core, core-valence, and valence-valence, to all orders. We note that only the valence CI calculation needs to be done since core excitations are already accounted for by the effective Hamiltonian. All sums in the all-order terms evaluated for the construction of the effective Hamiltonian are carried out including $l_{\max} = 6$ partial waves. We note that the same effective Hamiltonian is used for the neutral systems and corresponding multivalent ions. For example, the same effective Hamiltonian is used for four-electron Rf I, trivalent Rf II, and divalent Rf III calculations, since we use the same Dirac-Fock starting potential of Rf V with all valence electrons removed. Using the same effective Hamiltonian for all three of these systems brings a high degree of consistency to the binding energy computations and corresponding evaluation of the first ionization potentials, removing some sources of error. The main issue in the computation becomes the saturation of the valence CI space, i.e., ensuring that the uncertainty associated with omitting some many-electron configurations in the CI is small and consistent for all systems. This is particulary difficult to achieve for four-electron Hf and Rf, where the number of configurations is very large and simply increasing the number of configurations without ensuring that dominant configurations are included does not guarantee a high accuracy of the CI calculation. We describe the construction of the Hf CI space and tests that were carried out to ensure convergence of the CI in detail below since efficient construction of configuration space for CI presents an important problem crucial for the high final accuracy of the predicted values.

In principle, the CI calculation should contain all possible multielectron configurations that can be constructed from single-electron basis set wave functions. However, this is impractical even for two electrons since contributions of the $nlml'$ configurations with large principle number n and m are negligible. For two-electron systems, only configurations with large n are excluded without the loss of accuracy. For systems with larger numbers of electrons, further restrictions have to be implemented since the problem of including all possible configurations becomes intractable even for three electrons with reasonable computational resources. Moreover, it is not necessary to include all of the configurations. It is sufficient to select those that provide non-negligible contributions to the low-lying states of interest.

To construct such a set, we start with a few configurations, for example $6s^25d^2$,$6s^26p^2$, $6s5d^3$ for even states of Hf and $6s^26p5d$ and $6s6p5d^2$ for odd states. Then, we make a list of configurations that can be produced by replacing N_e number of electrons from these configurations to N_o basis set orbitals. Generally, it is good to select $N_e = 2$, which would allow single and double excitations from the initial configurations. This limited set is used for the initial computation and its results are used to reorder the configurations by their weights. Then, one more excitation is allowed from about 300 configurations with highest weights, and two excitations are allowed from about 30 most important configurations. The new resulting list of configurations is then merged with the original one, ordered by configuration weights. We find this procedure to be the most efficient and fast construction of the configuration list for an accurate large-scale CI calculation. We tested this procedure in the cases of Hf and Rf. Results of six different calculations of Hf energies with different number of configurations used in the four-electron CI calculations are given in Table I. N_c is the number of four-electrons relativistic configurations; N_d is the corresponding number of determinants (antisymmetrized many-electron basis states). Note that the size of the CI matrix is equal to the number of determinants N_d. The computational time is roughly proportional to N_d^2. Runs 1 to 4 are different initial runs, with 2, 3, or 4 excitations allowed from $6s^25d^2$,$6s^26p^2$, $6s5d^3$, $6s^26p5d$, and $6s6p5d^2$ configurations. Additional restrictions are introduced on how many electrons with the same principal and orbital quantum numbers can be present in the configurations, with only two allowed for orbitals with high principal quantum number (for example, $15d$). Two calculations were carried out with two excitations, Run 1 allowed excitations to 47 orbitals, $15spd14f10g$, and Run 2 to 64 orbitals, $20spd16f10g$. Run 3 allowed up to three excitations to 24 orbitals, $10s9pdfg$ and Run 4 allowed four excitations to 16 orbitals, $8spd7fg$. Run 5 and a final run combined the results of the previous runs with some additional excitations from the dominant configurations but used a different method of constructing the dominant configuration lists. These were two best variants of the calculations. We find similar results from Runs 1 to 4, indicating that it is important to both include a sufficient number of higher orbitals and triple and higher excitations. Results of two best calculations, Run 5 and the final run differ insignificantly, with the differences being much smaller than

TABLE I. Convergence of the calculated Hf energy levels (in cm^{-1}) with the number of configuration functions. N_o is the number of orbitals used in the construction of the configuration list used in the CI; N_e is the number of allowed excitations from the initial configurations. N_c is the number of four-electrons relativistic configurations; N_d is the corresponding number of determinants. The experimental energies are rounded values from the NIST ASD [1], the value for the ground state $5d^26s^2$ being the sum of ionization potentials of Hf I–IV (see Table II). The last five columns give the differences of Run 1–Run 5 values from the final results.

Configuration		Expt.	Run 1	Run 2	Run 3	Run 4	Run 5	Final	Run 1	Run 2	Run 3	Run 4	Run 5
N_c			18 867	34 403	31 032	17 998	27 955	35 600	Differences with the "Final" run				
N_d			516 419	872 452	1 941 424	1 278 986	1 159 894	1 505 340					
N_o, N_e			47, 2	64, 2	24, 3	16, 4							
$5d^26s^2$	$^3F_2$	632000	621721	622158	621912	622077	622829	622943	1222	784	1030	866	113
$5d^26s^2$	$^3F_3$	2357	2328	2338	2325	2318	2328	2334	6	−5	9	16	5
$5d^26s^2$	$^3F_4$	4568	4636	4662	4604	4584	4597	4598	−38	−64	−6	14	1
$5d^26s^2$	$^3P_0$	5522	6013	5949	5977	5670	5655	5600	−413	−348	−377	−69	−55
$5d^26s^2$	$^1D_2$	5639	6098	6024	6067	5871		5819	−279	−205	−247		−51
$5d^26s6p$	$^3D_1$	14018	12995	13072	13131	13485	13621	13610	615	538	479	125	−12
$5d^26s6p$	$^3F_2$	14435	13300	13381	13419	13758	13924	13911	611	529	491	152	−13
$5d^26s6p$	$^3F_3$	14542	13481	13557	13618	13956	14123	14105	624	548	487	149	−18
$5d^26s6p$	$^3D_2$	16163	15103	15187	15240	15590		15728	625	541	488	139	

the uncertainty in the core-valence contributions. Our study showed that we have sufficiently saturated the configuration space for Hf, which is further confirmed by a similar accuracy of our values for the first IP of Hf and trivalet Lr. A similar study was conducted for Rf.

III. RESULTS AND ESTIMATES OF UNCERTAINTIES

The final values for the ground-state energies (E_M) of Yb, Lu, Hf, No, Lr, and Rf neutral atoms and positive ions and corresponding first IPs are given in Table II. The quantity $I_{\text{calc}} = E_{M-1} - E_M$ gives the calculated IP, where M is the number of valence electrons. The $^1S_0$ closed-shell core energies are set to zero. We note that wrong electronic configurations and terms were listed for Hf III and Hf IV in [7], with also a typo in the term labels listed for Hf I and Rf I ground states.

The calculated energies given in Table II were converted from atomic units (a.u.) to cm^{-1} using the conversion factor 219474.6313702(17) from 2014 CODATA fundamental constants [16].

The CI+all-order results are in better agreement with experiment than the CI+MBPT values of [7], both owing to a more complete inclusion of the correlation correction in this approach and use of a larger-scale CI set constructed as described above for Hf and Rf.

The column I_{ref} of Table II lists the reference data for IPs. Most of them are taken from the Atomic Spectra Database of the National Institute of Standards and Technology (NIST ASD [1]). One exception is the value for Lu III. Reference [1] gives it as [169010(50)] cm^{-1}, quoted from Sugar and Kaufman [30]. The square brackets around the value denote that it is semiempirical. This reflects the fact that Sugar and Kaufman [30] have used interpolated values of the quantum defect of the $5g$ levels along the Tm I isoelectronic sequence to arrive at this value. However, in the same paper they noted that Kaufman and Sugar [22] obtained a more accurate IP value (quoted here in Table II) derived from the ns Rydberg series, which does not involve any semiempirical adjustments. Another exception is for the IP of Rf II, which was quoted in Ref. [1] from Johnson *et al.* [20]. We replaced it here with the theoretical value from Eliav *et al.* [15], which was a result of a relativistic coupled-cluster calculation similar to ours, but with no account for QED effects.

We estimated the uncertainties of calculations of Eliav *et al.* by extensive comparisons of results published by that group with available reference data for about 50 different spectra. Only two of those results deviate substantially from the reference data in Ref. [1], the IPs of Tl IV and Pr IV. For Tl IV, the NIST ASD [1] quotes 412500(300) cm^{-1} from the thesis of Gutmann [31]. A close examination shows that the $5d^9ns$ series used by Gutmann to derive the IP from the Ritz quantum defect formulas is strongly perturbed at $n = 7$ by interaction with the $5d^96d$ configuration (see percentage compositions of Tl IV levels in Ref. [1]). In addition, positions of three out of four $5d^97s$ levels were revised by Wyart *et al.* [32] by a few hundred cm^{-1}. Thus the IP of Tl IV should be revised, and its present value in ASD [1] should be disregarded. For Pr IV, ASD quotes [314400(200)] cm^{-1} from Sugar and Reader [33]. This value disagrees with the calculations of Eliav *et al.* [34], 311426 cm^{-1}, by about 3000 cm^{-1}. Sugar and Reader derived their semiempirical value by assuming a constant value for the change in effective principal quantum numbers $\Delta n^* = 1.048(2)$ between the $7s$ and $6s$ levels of all doubly and triply ionized lanthanide atoms. Perhaps, this assumption does not hold for Pr IV, which might be due to unusually strong interaction between the $4f7s$ and $5d6p$ configurations, not accounted for in the analysis of the Pr IV spectrum [35].

Excluding the Tl IV and Pr IV data from the comparison, the root-of-mean-square (rms) deviation of the remaining 50 calculated values of Eliav *et al.* from high-quality reference data was calculated separately for electron affinities of neutral atoms and for IPs of atoms and ions. For the former, it is about 200 cm^{-1}, and for the latter, it is about 500 cm^{-1}. We adopted

TABLE II. Calculated ground-state energies (E_M) of Yb, Lu, Hf, No, Lr, and Rf neutral atoms and positive ions. M is the number of valence electrons. The difference $I_{calc} = E_{M-1} - E_M$ gives the IP. It is assumed that $E_0 = 0$ and the corresponding state is the $^1S_0$ state of the closed-shell core, [$4f^{14}$] for Yb, Lu, and Hf, and [$5f^{14}$] for No, Lr, and Rf.

Atom/Ion	Configuration	Term	M	E_M (a.u.)	I_{calc} (cm^{-1})	I_{ref}[a] (cm^{-1})	Ref.	$\Delta I_{\text{calc-ref}}$ (cm^{-1})
Yb I	$6s^2$	$^1S_0$	2	−0.68050	50591	50443.20(10)	[17]	148
Yb II	$6s$	$^2S_{1/2}$	1	−0.44999	98761	98231.75(20)	[19]	530
Lu I	$6s^25d$	$^2D_{3/2}$	3	−1.48409	43296	43762.60(10)	[26]	−467
Lu II	$6s^2$	$^1S_0$	2	−1.28682	112795	[112000(3000)]	[25,28]	
Lu III	$6s$	$^2S_{1/2}$	1	−0.77289	169630	169049(10)	[22]	581
Hf I	$6s^25d^2$	$^3F_2$	4	−2.83969	54570	55047.9(1)	[27]	−478
Hf II	$6s^25d$	$^2D_{3/2}$	3	−2.59105	117821	[120000(4000)][b]	[24]	
Hf III	$5d^2$	$^3F_2$	2	−2.05422	181835	[187800(4000)]	[21]	
Hf IV	$5d$	$^2D_{3/2}$	1	−1.22572	269014	[269150(200)]	[23]	−136
No I	$7s^2$	$^1S_0$	2	−0.72010	53738	[53600(600)]	[29]	138
No II	$7s$	$^2S_{1/2}$	1	−0.47525	104305	[101000(3000)]	[18]	
Lr I	$7s^27p$	$^2P^o_{1/2}$	3	−1.51676	39749	40000(650)	[8]	−251
Lr II	$7s^2$	$^1S_0$	2	−1.33565	117289	[115000(3000)]	[18]	
Lr III	$7s$	$^2S_{1/2}$	1	−0.80124	175852	[173000(3000)]	[18]	
Rf I	$7s^26d^2$	$^3F_2$	4	−2.79617	48579	(48500(500))[b]	[15]	79
Rf II	$7s^26d$	$^2D_{3/2}$	3	−2.57483	115736	(115900(500))[b]	[15]	−164
Rf III	$7s^2$	$^1S_0$	2	−2.04750	192301	[192800(2400)]	[20]	
Rf IV	$7s$	$^2S_{1/2}$	1	−1.17131	257073	[255700(3200]	[20]	

[a] Most of the reference values are taken from the NIST ASD [1]. The original sources of these values are given in the next column. Uncertainty in the unit of the last digit is given in parentheses after the value. Values enclosed in parentheses are purely theoretical; those in square brackets are semiempirical (see text).

[b] Uncertainty is estimated in the present work.

the latter value as an estimate of the average uncertainty of their IP calculations for atoms and ions. The same estimate is given here for the Rf I result from Ref. [15].

The IP of Hf II was given in ASD [1] as [120000] cm^{-1} without an uncertainty. This value was quoted from Meggers and Scribner [24], who approximately estimated the IP based on analogies between the level structure of Hf II and La II, assuming that the e^2D and e^4F terms form series with a^2D and a^4F. If these assumptions are valid, the accuracy of their estimated IP should be around 4000 cm^{-1}, which is a typical uncertainty of IP of the second spectra derived from two-member series.

To compare our results with compiled reference data, we first note that semiempirical data on Lu II, Hf II, Hf III, No II, Lr II, Lr III, Rf III, and Rf IV have very large uncertainties ranging from 2400 cm^{-1} to 4000 cm^{-1}, and they agree with our calculations within these uncertainties. Excluding those low-quality data from the comparison, we obtain the rms deviation of our values from the reference data about 350 cm^{-1}, with no discernible correlation of the magnitude of deviations with the core charge or with the magnitude of IP. Thus we estimate the uncertainty of our calculated values as 350 cm^{-1} for all spectra in Table II.

Our value for the IP of Lr I is in excellent agreement with the 2015 experiment [8], the difference being smaller than the experimental uncertainty. It also agrees with the results of coupled cluster calculations presented in the same work [8]. Similar agreement is found with the result of calculation of Ref. [36] for No I, 53 489 cm^{-1}. We note that our estimate of uncertainty of this value is the same as that for Ref. [15], 500 cm^{-1}, as it was included in our statistical analysis of results of Eliav and co-workers. This is lower that the uncertainty stated in Ref. [36], 0.1 eV (800 cm^{-1}). It is also lower than the uncertainty of the reference value from Sugar [29], 600 cm^{-1}. Nevertheless, in our choice of reference data we give stronger preference to experimental data, if they are available. The semiempirical result of Ref. [29] for No I is essentially based on experimental data on several actinide spectra and withstood a reliability test of several decades.

In summary, we provided accurate predictions for IP of superheavy No, Lr, Rf, and their ions. We expect these values to be accurate to about 350 cm^{-1}. Extensive study of CI convergence was carried out for Hf and Rf to ensure that uncertainty of the CI calculations is significantly below the uncertainty in the treatment of core-valence correlation corrections. We also demonstrated that CI+all-order method is capable of predicting IP of ions with 1 to 4 valence electron to a very good precision, which may be used to provide improved recommended data.

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