

Atomic properties of superheavy elements No, Lr, and Rf

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The combination of the configuration interaction method and all-order single-double coupled-cluster technique is used to calculate excitation energies, ionization potentials, and static dipole polarizabilities of superheavy elements nobelium, lawrencium, and rutherfordium. Breit and quantum electrodynamic corrections are also included. The results for the superheavy elements are compared with earlier calculations where available. Similar calculations for lighter analogs, ytterbium, lutetium, and hafnium, are used to study the accuracy of the calculations. The estimated uncertainties of the final results are discussed.

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I. INTRODUCTION

The study of the superheavy elements (nuclear charge $Z > 100$) is an important multidisciplinary area of research involving nuclear physics, atomic physics, and chemistry (see, e.g., reviews [1–3]). Atomic calculations help to understand the role of the relativistic and many-body effects and provide important information for planning and interpreting the measurements. The need to treat relativistic and correlation effects to a high level of accuracy makes the calculations a very challenging task. Relativistic effects are most important for the structure of the inner electron shells. Their effect on the spectra of neutral atoms, determined by valence electrons, is much smaller. A standard approach based on using Dirac equation and adding Breit and quantum electrodynamic (QED) corrections gives reasonably good results (see, e.g., Refs. [4–7]). Accurate treatment of correlations is a more difficult task. Most of superheavy elements have open shells with many valence electrons and strong correlations between them and between valence electrons and electrons in the core. Therefore, it is particularly important to establish the benchmark values for superheavy systems that have one to four valence electrons which can be treated by the most high-precision approaches. Such calculations also establish the importance of various corrections that may be used for more complicated superheavy atoms. In our previous papers [4–7] we studied the elements with nuclear charge $Z = 112, 119$, and 120 , which are heavier analogs of mercury, francium, and radium respectively. These systems have one or two valence electrons. In the present paper, we calculate the spectra and other atomic properties of superheavy atoms with two, three, and four valence electrons above closed shells: nobelium ($Z = 102$), lawrencium ($Z = 103$), and rutherfordium ($Z = 104$). These elements are heavier analogs of ytterbium, lutetium, and hafnium. No, Lr, and Rf were studied theoretically and experimentally in Refs. [1–3,8–18], but experimental spectra still have not been measured. Present relativistic calculations use the combination of the configuration interaction (CI)

method with the linearized single-double coupled cluster method (CI + SD or CI + all-order) [19]. Correlations between valence electrons are treated with the CI technique while correlations between core and valence electrons are included via the single-double coupled-cluster method. This approach provides the most complete treatment of the interelectron correlations since it includes core-core, core-valence, and valence-valence correlations to all orders. We treat nobelium, lawrencium, and rutherfordium as two-, three-, and four-valence electron systems respectively. Previous calculations for No [8–10] and Rf [16,17] considered these atoms as two-valence electron systems, while calculations for Lr [11–15] treated this atom as a monovalent system. Such treatments omit important correlation effects for Lr and Rf. Comparing present and earlier calculations provides important information on the role of different types of correlation and relativistic corrections. We also present calculations of the few first ionization potentials for No, Lr, and Rf, up to removal of all valence electrons, and calculate static polarizabilities for all three atoms. In the next section we describe the method and present results of calculations for Yb, Lu, and Hf to illustrate the accuracy of the method. In the last section we present results and detailed discussion for No, Lr, and Rf.

II. METHOD OF CALCULATION

The calculations are performed using the configuration interaction method combined with the linearized single-double coupled-cluster method introduced in Ref. [19]. This CI + all-order method yielded accurate atomic properties for a number of divalent systems and trivalent Tl [19–22]. It has been recently applied to the calculations of four-electron systems (Sn-like ions) [23].

We use *frozen core* Dirac-Fock (DF) V^{N-M} potential [24] as the point of departure for all of our calculations, where N is the total number of electrons and M is the number of valence electrons; i.e., the initial DF procedure is carried out for the closed-shell ion, with all valence electrons removed.

For the atoms treated here, $M = 2$ for Yb and No, $M = 3$ for Lu and Lr, and $M = 4$ for Hf and Rf. The effective CI Hamiltonian for states of valence electrons is the sum of single-electron Hamiltonians and an operator representing the interaction between the valence electrons,

$$\hat{H}^{\text{eff}} = \sum_{i=1}^M \hat{h}_1(r_i) + \sum_{i<j} \hat{h}_2(r_i, r_j). \quad (1)$$

The single-electron Hamiltonian for a valence electron has the form

$$\hat{h}_1 = c\alpha\mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + V^{N-M} + \hat{\Sigma}_1, \quad (2)$$

where $\hat{\Sigma}_1$ is the correlation potential operator, which represents the correlation interaction of a valence electron with the core. Its matrix elements are related to the single-excitation amplitudes of the coupled-cluster method via

$$\Sigma_{mv} = \rho_{mv}(\tilde{\epsilon}_v - \epsilon_m), \quad (3)$$

where ρ_{mv} is an excitation coefficient of the atomic wave function for the term with excitation from the valence state v to another excited state m , and ϵ_m are Dirac-Fock energies of corresponding single-electron basis states. The quantities $\tilde{\epsilon}_v$ are discussed in detail in Ref. [19]. Briefly, the CI + all-order approach is based on the Brillouin-Wigner variant of many-body perturbation theory (MBPT) rather than the Rayleigh-Schrödinger variant resulting in the energy dependence of the Σ . Ideally, the energy $\tilde{\epsilon}_v$ should be calculated from the particular eigenvalue of the effective Hamiltonian. In actual calculations, the simplest and the most practical approach is to set the energy $\tilde{\epsilon}_v$ to the Dirac-Fock energy of the lowest orbital for the particular partial wave. For example, we use $\tilde{\epsilon}_v = \epsilon_{6s}$ for all ns orbitals of Yb atom.

The interaction between valence electrons is the sum of the Coulomb interaction and the correlation correction operator $\hat{\Sigma}_2$:

$$\hat{h}_2(r_i, r_j) = \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \hat{\Sigma}_2(r_i, r_j). \quad (4)$$

The operator $\hat{\Sigma}_2$ represents the screening of the Coulomb interaction between valence electrons by core electrons. Its matrix elements are related to the double-excitation coupled-cluster ρ_{mnvw} coefficients via

$$\Sigma_{mnvw} = \rho_{mnvw}(\tilde{\epsilon}_v + \tilde{\epsilon}_w - \epsilon_m - \epsilon_n). \quad (5)$$

The many-electron wave function for the valence electrons Ψ can be expressed as an expansion over single-determinant wave functions

$$\Psi = \sum_i c_i \Phi_i(r_1, \dots, r_M). \quad (6)$$

The functions Φ_i are constructed from the single-electron valence basis states calculated in the V^{N-M} potential. The coefficients c_i and many-electron energies are found by solving the matrix eigenvalue problem

$$(H^{\text{eff}} - E)X = 0, \quad (7)$$

where $H_{ij}^{\text{eff}} = \langle \Phi_i | \hat{H}^{\text{eff}} | \Phi_j \rangle$ and $X = \{c_1, c_2, \dots, c_n\}$.

We use the linearized coupled-cluster method to calculate the correlation correction operators $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$. The B -spline technique [25] is used to construct a single-electron basis for calculation of $\hat{\Sigma}$ and for building many-electron basis states for the CI calculations. We use 35 B splines of order 7 in a cavity of radius $R_{\text{max}} = 60a_B$, where a_B is Bohr's radius. All sums in the all-order terms are carried out including $l_{\text{max}} = 6$ partial waves. The contributions from $l > 6$ partial waves were estimated and included into the final results.

A. Breit interaction

The Breit interaction is included in present calculations using the approach developed in Refs. [26,27]. We treat Breit interaction in the zero-energy transfer approximation. The Breit Hamiltonian includes magnetic interaction between moving electrons and retardation

$$\hat{H}^B = -\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1 \cdot \mathbf{n})(\boldsymbol{\alpha}_2 \cdot \mathbf{n})}{2r}. \quad (8)$$

Here $\mathbf{r} = \mathbf{n}r$, r is the distance between electrons, and $\boldsymbol{\alpha}$ is the Dirac matrix.

Similar to the way Coulomb interaction is used to form self-consistent Coulomb potential, Breit interaction is used to form self-consistent Breit potential. In other words, Breit interaction is included into self-consistent Hartree-Fock procedure. Thus the important relaxation effect is included. The resulting interelectron potential in Eq. (2) consist of two terms

$$\hat{V} = V^C + V^B, \quad (9)$$

where V^C is the Coulomb potential and V^B is the Breit potential. Coulomb interaction in the second-order correlation operator $\hat{\Sigma}$ is also modified to include Breit operator (8). The contribution of the Breit interaction to the energy levels of all atoms considered here is small, generally less than 100 cm^{-1} .

B. QED corrections

We use the radiative potential method developed in Ref. [28] to include quantum radiative corrections. This potential has the form

$$V_{\text{rad}}(r) = V_U(r) + V_g(r) + V_e(r), \quad (10)$$

where V_U is the Uehling potential, V_g is the potential arising from the magnetic form factor, and V_e is the potential arising from the electric form factor. The V_U and V_e terms can be considered as additions to nuclear potential while inclusion of V_g leads to some modification of the Dirac equation (see Ref. [28] for details). We find that the QED corrections are small in comparison with the higher-order correlation corrections and can be omitted at the present level of accuracy. We compared the results with and without QED for No as an illustration.

C. Calculation of polarizabilities

Polarizabilities characterize interaction of atoms with external electric field. The Stark energy shift of atomic state JLn in the static electric field ε is given by

$$\Delta E(JLn) = -\left(\alpha_0 + \frac{3M^2 - J(J+1)}{J(2J-1)}\alpha_2\right)\frac{\varepsilon^2}{2}, \quad (11)$$

where α_0 and α_2 are scalar and tensor electric-dipole polarizabilities and M is the projection of the total angular momentum J on the direction of electric field. Scalar polarizability is given by

$$\alpha_0(JLn) = \frac{2}{3(2J+1)} \sum_{J'L'n'} \frac{\langle JLn || \mathbf{D} || J'L'n' \rangle^2}{E_{n'} - E_n}, \quad (12)$$

where $= -e \sum_i \mathbf{r}_i$ is the electric dipole operator. Tensor polarizability α_2 is nonzero only for atomic states with $J \geq 1$. The expression for α_2 differs from Eq. (12) by an angular coefficient:

$$\begin{aligned} \alpha_2(JLn) = & \sqrt{\frac{10J(2J-1)}{3(2J+3)(2J+1)(J+1)}} \\ & \times \sum_{J'L'n'} (-1)^{(J+J')} \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J' \end{Bmatrix} \\ & \times \frac{\langle JLn || \mathbf{D} || J'L'n' \rangle^2}{E_{n'} - E_n}. \end{aligned} \quad (13)$$

The expressions (12) and (13) are exact if $|JLn\rangle$ and $|J'L'n'\rangle$ are exact many-electron wave functions. In practice, atomic electrons are divided into core and valence electrons and the expression for scalar polarizability becomes a sum of three terms

$$\alpha_0 = \alpha_c + \alpha_{cv} + \alpha_v. \quad (14)$$

Here α_c is the polarizability of atomic core, and α_{cv} is the contribution caused by Pauli principle, which implies that the excitations from the core cannot go into occupied valence states. Therefore, polarizability of the core is different for the ion, which has no valence electrons and for the neutral atom. This difference is separated into α_{cv} . Usually this contribution is small and needs to be taken into account only in very precise calculations. We neglect it in present work. The term α_v is the dominant contribution due to the valence electrons. The core contribution is given by

$$\alpha_c = \frac{2}{3} \sum_{cm} \frac{\langle cm || \mathbf{d} || m \rangle \langle m || \mathbf{d} + \delta \mathbf{V}_{\text{core}} || c \rangle}{\epsilon_c - \epsilon_m}, \quad (15)$$

where summation goes over core states c and a complete set of single-electron states m . The energies ϵ_c and ϵ_m are the single-electron energies of the basis states. The operator $\mathbf{d} = -e\mathbf{r}$ in Eq. (15) is the single-electron electric dipole operator; $\delta \mathbf{V}_{\text{core}}$ is the correction to the self-consistent core potential due to the effect of electric field. It is also known as the core polarization correction or random-phase approximation (RPA) correction. This correction is calculated by solving the RPA-type equations for atomic core

$$(\hat{H}_0 - \epsilon_c) \delta \psi_c = -\psi_c (\mathbf{d} + \delta \mathbf{V}_{\text{core}}), \quad (16)$$

where \hat{H}_0 is the Hartree-Fock Hamiltonian and $\delta \psi_c$ is the correction to the core state ψ_c due to the effect of external electric field. The equations (16) are solved self-consistently for all states in the core and the correction to the core potential δV_{core} is found. The core contribution is small, ranging from 3.20 a.u. for Hf to 8.46 a.u. for No. The core does not contribute to the tensor polarizability since the total angular momentum of the closed shell core is zero.

The expressions for the valence contributions to the scalar and tensor polarizabilities are very similar to Eqs. (12) and (13) with a few modifications. The many-electron states $|JLn\rangle$ and $|J'L'n'\rangle$ are now the valence states, the summation in the electric dipole operator \mathbf{D} goes over only valence electrons, and every single-electron electric dipole operator d is modified to include core polarization correction, $\tilde{\mathbf{d}} = \mathbf{d} + \delta \mathbf{V}_{\text{core}}$.

To perform summation in Eqs. (12) and (13) over the complete set of many-valence-electrons states we use the method suggested by Dalgarno and Lewis [29]. The summation over intermediate states n is reduced to calculation of the correction $|\tilde{a}\rangle$ to the ground-state wave function. Summation over n includes summation over different values of the total angular momentum which satisfy electric vector selection rules ($J_n = J_a, J_a \pm 1$). The correction $|\tilde{a}\rangle$ can be written as a sum of three terms $|\tilde{a}\rangle = |\tilde{a}\rangle_{J_a} + |\tilde{a}\rangle_{J_a+1} + |\tilde{a}\rangle_{J_a-1}$. Each of these terms $|\tilde{a}\rangle_{J_n}$ satisfy the inhomogeneous equation

$$(H^{\text{eff}} - E_a) |\tilde{a}\rangle_{J_n} = -\tilde{D} |a\rangle_{J_a}. \quad (17)$$

The polarizability is then calculated as

$$\alpha = -2 \langle a | \tilde{D}_z | \tilde{a} \rangle. \quad (18)$$

More detailed formulas including angular coefficients can be found in Ref. [30]. The H^{eff} term in (17) is the effective CI Hamiltonian presented in a matrix form while $|\tilde{a}\rangle_{J_n}$ is a vector of expansion coefficients over single-determinant basis states. Solving the system of linear equations (17) and substituting the result into (18) is equivalent to summation over all possible

TABLE I. Energies (E , cm^{-1}) and g factors of the lowest states of ytterbium (energies are taken from Ref. [31]). Comparison of calculations with experiment [32]. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19).

Conf.	Term	Energy			g factors		
		Expt.	Present	Diff.	Expt.	nr	Present
6s ²	¹ S ₀	0	0	0		0	0
6s6p	³ P ₀ ^o	17288	17561	-273		0	0
	³ P ₁ ^o	17992	18261	-269	1.49282	1.5000	1.4921
	³ P ₂ ^o	19710	20010	-300	1.50	1.5000	1.5000
5d6s	³ D ₁	24489	24505	-16	0.50	0.5000	0.5000
	³ D ₂	24752	24863	-111	1.16	1.1667	1.1634
	³ D ₃	25271	25343	-72	1.34	1.3333	1.3333
6s6p	¹ P ₁ ^o	25068	25816	-748	1.035	1.0000	1.0087
5d6s	¹ D ₂	27678	27991	-313	1.01	1.0000	1.0036
6s7s	³ S ₁	32695	32970	-275	2.01	2.0000	1.9998
6s7s	¹ S ₀	34351	34579	-228		0	0
6s7p	³ P ₀ ^o	38091	38377	-286		0	0
	³ P ₁ ^o	38174	38440	-266	1.14	1.5000	1.4399
	³ P ₂ ^o	38552	38821	-269	1.50	1.5000	1.4999
6s6d	³ D ₁	39809	40053	-244	0.50	0.5000	0.5001
	³ D ₂	39838	40147	-309	1.16	1.1667	1.1414
	³ D ₃	39966	40205	-239	1.33	1.3333	1.3333
6s6d	¹ D ₂	40062	40089	-27	1.03	1.0000	1.1423
6s7p	¹ P ₁ ^o	40564	39150	1414	1.01	1.0000	1.0598
6s8s	³ S ₁	41615	41997	-382	2.02	2.0000	1.9994
6s8s	¹ S ₀	41940	42397	-457		0	0

many electron states which can be constructed from the given single-electron basis.

D. Results for Yb, Lu, and Hf

First, we carry out the calculations for “reference” atoms Yb, Lu, and Hf which have the closest electronic structure to the superheavy No, Lr, and Rf, respectively. Since the energies of Yb, Lu, and Hf are known experimentally, such calculation provides the benchmark test of our method. Further comparison of correlation corrections in “reference” and superheavy atoms allows us to predict the accuracy of our approach for superheavy elements.

Our calculated energy levels of Yb, Lu and Hf are compared with experiment in Tables I, II, and III, respectively. Yb energy levels have been presented in Ref. [31]. Comparison shows that relative theoretical errors in excitation energies are rather similar for Yb, Lu, and Hf, with somewhat better accuracy for two-electron Yb.

The difference with experiment is 0.1–1.6% for Yb with the exception of the singlet $6s6p\ ^1P_1$ and $6s7p\ ^1P_1$ states, where it is 3–3.5%. The lower accuracy of the singlet states arises when there is significant difference in the position of the triplet and singlet energy levels, such as in 1P_1 and 3P_1 cases. It is

TABLE II. Energies (E , cm^{-1}) and g factors of the lowest states of lutetium. Comparison of calculations with experiment [32]. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19).

Conf.	Term	Energy			g factors		
		Expt.	Present	Diff.	Expt.	nr	Present
$5d6s^2$	$^2D_{3/2}$	0	0	0	0.79921	0.8000	0.8000
	$^2D_{5/2}$	1993	2014	−21	1.20040	1.2000	1.1999
$6s^26p$	$^2P_{1/2}^o$	4136	3910	226	0.66	0.6666	0.6661
	$^2P_{3/2}^o$	7476	7228	248	1.33	1.3333	1.3333
$5d6s6p$	$^4F_{3/2}^o$	17427	17723	−296	0.59	0.4000	0.4525
	$^4F_{5/2}^o$	18504	18789	−285	1.07	1.0286	1.0586
	$^4F_{7/2}^o$	20432	20731	−299	1.22	1.2381	1.2424
	$^4F_{9/2}^o$	22609	22911	−302	1.30	1.3333	1.3332
$5d^26s$	$^4F_{3/2}$	18851	19182	−331		0.4000	0.4109
	$^4F_{5/2}$	19403	19737	−334		1.0286	1.0305
	$^4F_{7/2}$	20247	20578	−331		1.2381	1.2368
	$^4F_{9/2}$	21242	21591	−349	1.0	1.3333	1.3313
$5d6s6p$	$^4D_{1/2}^o$	20762	20995	−233	0.00	0.0000	0.0353
	$^4D_{3/2}^o$	21195	21448	−253	1.19	1.2000	1.1551
	$^4D_{5/2}^o$	22221	22504	−283	1.39	1.3714	1.3799
	$^4D_{7/2}^o$	23524	23795	−271	1.41	1.4286	1.4171
$5d6s6p$	$^2D_{5/2}^o$	21462	21735	−273	1.23	1.2000	1.2107
	$^2D_{3/2}^o$	22124	22376	−252	0.874	0.8000	0.8591
$5d^26s$	$^4P_{1/2}$	21472	21860	−388		2.6667	2.6098
	$^4P_{3/2}$	22467	22849	−382	1.73	1.7333	1.7016
	$^4P_{5/2}$	22802	23242	−440		1.6000	1.4749
$5d6s6p$	$^4P_{1/2}^o$	24108	24520	−412		2.6667	2.6264
	$^4P_{3/2}^o$	24308	24786	−478	1.67	1.7333	1.6530
	$^4P_{5/2}^o$	25191	25774	−583	1.53	1.6000	1.5267
$5d^26s$	$^2D_{3/2}$	24518	25015	−497		0.8000	0.8379

TABLE III. Energies (E , cm^{-1}) and g factors of the lowest states of hafnium. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19). Comparison of calculations with experiment [32]. Result with “**” is by Sansonetti and Martin [33].

Conf.	Term	Energy			g factors		
		Expt.	Present	Diff.	Expt.	nr	Present
$5d^26s^2$	3F_2	0.	0		0.695	0.667	0.6936
	3F_3	2357	2343	14	1.083	1.083	1.0832
	3F_4	4568	4617	−49	1.240	1.250	1.2425
$5d^26s^2$	3P_0	5522	5611	−89	0.00	0.00	0.00
	3P_1	6573	6594	−21	1.500	1.500	1.5000
	3P_2	8984	9151	−167	1.300	1.500	1.2783
$5d^26s^2$	1D_2	5639	5842	−203	1.165	1.000	1.1947
$5d6s^26p$	$^1D_2^o$	10509*	10095	414		1.000	0.8173
$5d^26s^2$	1G_4	10533	11411	−878	1.008	1.000	1.0073
$5d6s^26p$	$^3D_1^o$	14018	13718	300	0.55	0.500	0.5384
	$^3D_2^o$	16163	15840	323	1.17	1.167	1.1714
	$^3D_3^o$	18381	18084	297	1.29	1.333	1.2980
$5d^36s$	5F_1	14092	14445	−353	0.00	0.00	0.0217
	5F_2	14741	15079	−338	1.00	1.000	1.0038
	5F_3	15673	15996	−323	1.25	1.250	1.2485
	5F_4	16767	17099	−332	1.36	1.350	1.3445
$5d6s^26p$	$^3F_2^o$	14435	14019	416	0.89	0.666	0.8914
	$^3F_3^o$	14542	14210	332	1.08	1.083	1.0877
	$^3F_4^o$	18225	17887	338	1.24	1.250	1.2451
$5d6s^26p$	$^3P_1^o$	18143	17932	211	1.43	1.500	1.4401
	$^3P_2^o$	19791	19584	207	1.41	1.500	1.4192
$5d^26s6p$	$^5G_2^o$	18011	17996	15	0.40	0.333	0.3874
	$^5G_3^o$	19293	19262	31	0.95	0.917	0.9375
	$^5G_4^o$	20960	20935	25	1.16	1.150	1.1597

1.1–2.2% for Lu, with the exception of $6s^26p$ states, where it is 3–5%.

An explanation for poor accuracy for the $^1P_1^o$ states of ytterbium was given in Ref. [34]. It is caused by the mixing of these states with the odd state at $E = 38422\ \text{cm}^{-1}$. This state is assumed to belong to the $4f^{13}5d^26s$ configuration [32]. It has an excitation of the core electron from the $4f$ subshell. Such states are not included into the configuration interaction (CI) matrix. Core-valence excitations are treated perturbatively via the correlation operator $\hat{\Sigma}$ (3,5). This might be insufficient when mixing is strong. Judging by the single-electron spectra, excitation energy from the $5f$ state of No is expected to be about 10% smaller than in Yb. Since the lowest excitation correspond to the $5f$ - $6d$ transition, some odd states of No might be affected by mixing with these states in a similar way as for Yb. Core excitation energies for Lu, Hf, Lr, and Rf are large and unlikely to have pronounced effect on the calculations.

A common problem of the CI calculation with four valence electrons is a rapid increase of the number of many-electron basis states with the increase in the number of valence electrons usually leading to omitting configurations which correspond to multiple excitations of valence electrons from the ground state to high-lying states. This helps to reduce the CI matrix to a manageable size but leads to deterioration of the accuracy

TABLE IV. Energies (E , cm^{-1}) and g factors of the lowest states of nobelium. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19). Comparison with theoretical results presented by Borschevsky *et al.* [9] and Liu *et al.* [10].

Conf.	Term	Energy		Energy		g factors	
		Present	+Lamb	Ref. [9]	Ref. [10]	Present	nr
7s2	1S_0	0	0	0	0	0	0
7s7p	$^3P_0^o$	19682	19567	18879	19798	0	0
	$^3P_1^o$	21156	21042	20454	21329	1.4577	1.500
	$^3P_2^o$	26225	26113	25374	26186	1.4998	1.500
7s7p	$^1P_1^o$	30304	30203	30056	30069	1.0409	1.000
7s6d	3D_1	28587	28436	28338		0.5000	0.500
	3D_2	29098	28942	28778		1.1606	1.167
	3D_3	30322	30183	29897		1.3332	1.333
7s6d	1D_2	33657	33504	32892		1.0071	1.000
7s8s	3S_1	35815	35731	35092		1.9994	2.000
7s8s	1S_0	37444	37360	36538		0.0000	0.000
7s8p	$^3P_0^o$	41365	41266	40576		0.0000	0.000
	$^3P_1^o$	41481	41382	40692		1.4083	1.500
	$^3P_2^o$	42582	42484	42837		1.4999	1.500
7s8p	$^1P_1^o$	43011	42910	42285		1.0917	1.000
7s7d	3D_1	43522	43422	42726		0.5002	0.500
	3D_2	43581	43481	42758		1.1452	1.167
	3D_3	43830	43730	43033		1.3333	1.333
7s7d	1D_2	44099	43999	43079		1.0216	1.000
7s9s	3S_1	44894	44794	44247		1.9994	2.000
7s6f	$^3F_2^o$	46795	46695			0.6669	0.667
	$^3F_3^o$	46788	46688			1.0072	1.083
	$^3F_4^o$	46810	46710			1.2500	1.250
7s6f	$^1F_3^o$	46806	46706			1.0762	1.000

of the calculations. However, we were able to saturate the four-electron CI space by carrying out several very large CI

calculations with different types of excitations, then selecting the configuration with the largest weights from each of the runs, and combining them to produce nearly complete configuration space. Comparing results with increasing number of selected important configurations produced estimated uncertainty due to configuration space of less than 50 cm^{-1} for most states. As a result, we do not observe significant deterioration of results between Lu and Hf. The difference with experiment is 0.1–2.9% for Hf with the exception of the singlet 1D_2 and 1G_4 states, where it is 4% and 8%, respectively. Note, that in contrast to Yb, mixing with states having a hole in the $4f$ subshell cannot explain poor accuracy for these states. Core excitation energy is large for Lu and Hf, and corresponding states that lie high in the spectrum cannot be strongly mixed with low states.

We also present the values of calculated and nonrelativistic magnetic g factors in Tables I, II, and III. Nonrelativistic (nr) values are given by

$$g_{\text{nr}} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}, \quad (19)$$

where J is total angular momentum of the atom, L is its angular momentum, and S is the spin ($\mathbf{J} = \mathbf{L} + \mathbf{S}$). The g factors are useful for identification of the states.

III. RESULTS AND DISCUSSION

A. Energy levels of No, Lr, and Rf and estimates of their uncertainties

Calculated energy levels and magnetic g factors for No, Lr, and Rf are presented in Tables IV, V, and VI together with the results of earlier calculations [8–17]. We observe good agreement between the theoretical results for most of the states. We compare No results with and without the QED correction in Table IV. The value of the QED correction is of the order of 100 cm^{-1} for most of the states while maximum value of the correction is slightly larger than 200 cm^{-1} . This is smaller than

TABLE V. Calculated energies (E , cm^{-1}) and g factors of the lowest states of lawrencium. Comparison with other calculations. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19).

Config.	Term	J	Present work			Other energy			
			Energy	g	g_{nr}	Ref. [12]	Ref. [13]	Ref. [14]	Ref. [15]
7s ² 7p	$^2P^o$	1/2	0	0.6652	0.6666	0	0	0	0
		3/2	8495	1.3333	1.3333	8273	8935	8138	8389
7s ² 6d	2D	3/2	1555	0.8002	0.8000	1263	1127	1331	1408
		5/2	5423	1.2001	1.2000	5062		4187	5082
7s7p6d	$^4F^o$	3/2	21288	0.4803	0.4000			20886	
		5/2	23530	1.0668	1.0286			23155	
		7/2	28320	1.2468	1.2381			27276	
		9/2	34212	1.3266	1.3333			32775	
7s ² 8s	2S	1/2	20253	2.0163	2.0000			20405	20131
7s ² 8p	$^2P^o$	1/2	25912	0.6161	0.6666				26104
		3/2	27079	1.3174	1.3333				27491
7s6d ²	4P	1/2	25409	2.4737	2.6667				
3/2		26327	1.5286	1.7333					
5/2		27397	1.3148	1.6000					

the uncertainty due to correlations (see the difference between theory and experiment for Yb, Lu, and Hf in Tables I, II, III). Therefore, we do not include QED corrections for Lr and Rf.

The accuracy of the calculations was discussed in the previous section for the case of Yb, Lu, and Hf atoms. However, since relativistic and correlational effects are larger in the superheavy elements it is reasonable to assume that the uncertainties for No, Lr, and Rf are slightly larger than for Yb, Lu, and Hf. We verified that the contribution of the Breit interaction to the energy levels in Tables I–VI is small in all cases (generally less than 100 cm^{-1}).

To estimate the accuracy of our values, we directly compare the correlation effects in Lu and Lr, since these dominate the uncertainty of the calculations. We carry out an additional calculations for both atoms using a combination of the configuration interaction and second-order many-body perturbation theory (CI + MBPT) methods [35]. In this approach, the Σ_1 and Σ_2 of the effective Hamiltonian are built using the second-order perturbation theory instead of the coupled-cluster method. The difference of the CI + MBPT and CI + all-order values gives the estimate of the third and higher-order corrections. We note that Lu and Lr have different types of ground-state configurations, $6s^2 5d^2 D_{3/2}$ and $7s^2 7p^2 P_{1/2}$. Therefore, we first directly compare the higher-order corre-

lation contributions to the three-electron removal energies of Lu and Lr, which are given in Table VII. Columns CI + MBPT and CI + all give trivalent removal energies calculated in the respective approximations. The difference of these values give the estimate of the higher-order correlation correction given in column labeled “Diff.” The last column labeled “Diff*” gives the higher-order correlations relative to the corresponding ground states. We find that while the energies are similar for Lu and Lr, the higher-order correlation corrections significantly increase from Lu ($2000\text{--}3200 \text{ cm}^{-1}$) to Lr ($3800\text{--}6300 \text{ cm}^{-1}$). However, we observe that the correlation increases for all of the states and when the ground-state values are subtracted out, the remaining higher-order corrections, listed in the last column of Table VII, are very similar for Lu and Lr. Only for the three states, $7s^2 6d^2 D_{3/2}$ and $7s 6d^2 D_{3/2,5/2}$, the remaining contributions are larger than for Lu cases, which may result in somewhat lower accuracy for their states.

Therefore, we expect 1–2% accuracy of the energy levels in No, 1–3% in Lr, and 2–5% for Rf for most of the states presented here.

B. Ionization potentials

Calculations in the V^{N-M} approximation are very similar for a neutral atom and negative and positive ions [24]. The number of valence electrons is the only parameter in the effective CI Hamiltonian (1), which changes while moving from a neutral atom to an ion or from one ion to another.

TABLE VI. Energies (E , cm^{-1}) and g factors of the lowest states of rutherfordium. Nonrelativistic values of g factors (g_{nr}) are given by Eq. (19). Comparison with results by Eliav *et al.* [16] and Mosyagin *et al.* [18].

Conf.	Term	Energy		g factors		nr
		Present	[16]	[18]	Present	
$7s^2 6d^2$	3F_2	0	0	0	0.7291	0.667
	3F_3	4904	4855	4869	1.0834	1.083
	3F_4	8625	7542	8597	1.2062	1.250
$7s^2 7p 6d$	$^3F_2^o$	2547	2210	3923	0.7869	0.667
	$^3F_3^o$	11390	11905	12953	1.1041	1.083
	$^3F_4^o$	20477			1.2489	1.250
$7s^2 6d^2$	3P_0	5034		5932	0.0	0.0
	3P_1	8348	8776	10051	1.4996	1.500
	3P_2	7398	7542	8704	1.1853	1.500
$7s^2 7p 6d$	$^3D_1^o$	8288	8373	9201	0.6794	0.500
	$^3D_2^o$	11273	10905	12889	1.1493	1.167
	$^3D_3^o$	18029			1.2016	1.333
$7s^2 6d^2$	1D_2	13630			1.2531	1.000
$7s^2 6d^2$	1G_4	14476			1.0439	1.000
$7s^2 7p 6d$	$^1D_2^o$	14403			1.0650	1.000
$7s^2 6d^2$	1S_0	18679			0.0	0.0
$7s^2 7p 6d$	$^1F_3^o$	24634			1.1077	1.000
$7s 6d^3$	5F_1	21552			0.0962	0.000
	5F_2	23079			1.0289	1.000
	5F_3	25432			1.2475	1.250
$7s^2 7p 6d$	$^3P_1^o$	16551			1.2712	1.500
	$^3P_2^o$	21480			1.2267	1.500
$7s 6d^2 7p$	$^5G_2^o$	20347			0.5067	0.333
	$^5G_3^o$	23325			0.9523	0.917

TABLE VII. Comparison of higher-order (III⁺) correlation contributions to three-electron removal energies of Lu and Lr. Columns CI + MBPT and CI + all give removal energies calculated in the respective approximations. The difference of these values give the estimate of the higher-order correlation correction given in column labeled Diff. Last column labeled Diff* give the higher-order correlation relative to the corresponding ground states.

Atom	Level	CI + MBPT	CI + all	Diff	Diff*
Lu	$6s^2 5d^2 D_{3/2}$	328791	325983	−2808	0
	$6s^2 5d^2 D_{5/2}$	326610	323981	−2629	179
	$5d^2 6s^4 F_{3/2}$	309931	306716	−3215	−406
	$5d^2 6s^4 F_{5/2}$	309307	306166	−3141	−333
	$5d^2 6s^4 F_{7/2}$	308356	305330	−3026	−217
	$5d^2 6s^4 F_{9/2}$	307222	304323	−2898	−90
	$6s^2 6p^2 P_{1/2}^o$	324182	322187	−1996	812
	$6s^2 6p^2 P_{3/2}^o$	320859	318866	−1993	815
	$5d 6s 6p^4 F_{3/2}^o$	310376	308268	−2107	701
	Lr	$7s^2 6d^2 D_{3/2}$	337828	331718	−6110
$7s^2 6d^2 D_{5/2}$		333287	327872	−5415	−726
$7s^2 8s^2 S_{1/2}$		318449	313137	−5311	−623
$7s 6d^2^4 P_{1/2}$		311742	307921	−3821	867
$7s 6d^2^4 P_{3/2}$		313159	306879	−6280	−1592
$7s 6d^2^4 P_{5/2}$		311830	305825	−6005	−1317
$7s^2 7p^2 P_{1/2}^o$		338055	333366	−4688	0
$7s^2 7p^2 P_{3/2}^o$		329645	324877	−4768	−80
$7s 7p 6d^4 F_{3/2}^o$		316309	311992	−4318	371
$7s 7p 6d^4 F_{5/2}^o$		314099	309752	−4348	341
$7s^2 8p^2 P_{1/2}^o$		312532	307454	−5079	−391
$7s^2 8p^2 P_{3/2}^o$		311250	306266	−4984	−296

TABLE VIII. 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 $\Delta E = E_{M-1} - E_M$ gives the ionization potential.

Atom/ion	Configuration	Term	M	E_M (a.u.)	ΔE (cm ⁻¹)	Expt. ^a (cm ⁻¹)
Yb I	6s ²	¹ S ₀	2	-0.68232	50768	50443
Yb II	6s	² S _{1/2}	1	-0.45101	98985	98207
Lu I	6s ² 5d	² D _{3/2}	3	-1.48938	43289	43763
Lu II	6s ²	¹ S ₀	2	-1.29215	113323	112000
Lu III	6s	² S _{1/2}	1	-0.77581	170270	169014
Hf I	6s ² 5d ²	³ F ₀	4	-2.83907	53431	55048
Hf II	6s ² 5d	² D _{3/2}	3	-2.59562	126748	120000
Hf III	6s ²	¹ S ₀	2	-2.01811	190885	187800
Hf IV	6s	² S _{1/2}	1	-1.14837	252037	269150
No I	7s ²	¹ S ₀	2	-0.72799	54390	
No II	7s	² S _{1/2}	1	-0.48018	105387	
Lr I	7s ² 7p	² P _{1/2} ^o	3	-1.52543	39801	
Lr II	7s ²	¹ S ₀	2	-1.34408	118058	
Lr III	7s	² S _{1/2}	1	-0.80617	176934	
Rf I	7s ² 6d ²	³ F ₀	4	-2.79968	46067	
Rf II	7s ² 5d	² D _{3/2}	3	-2.58979	116925	
Rf III	7s ²	¹ S ₀	2	-2.05704	193246	
Rf IV	7s	² S _{1/2}	1	-1.17654	258220	

^aReference [32].

All other terms, including the Coulomb potential created by core electrons and correlation operator $\hat{\Sigma}$, remain the same. Removing one electron from a neutral atom and comparing the energy of the resulting ground state with the energy of the ground state of neutral atom gives first ionization potential of the atom. Removing one more electron leads to second ionization potential, etc. This process can be repeated until all valence electrons are removed. The number of ionization potentials which can be calculated this way is limited by the number of valence electrons. To illustrate the accuracy of the calculations we calculate ionization potentials for Yb, Lu, and Hf and compare them with experiment. The results are presented in Table VIII. Then in the same table we present ionization potentials for No, Lr, and Rf.

C. Static polarizabilities

Results of calculations of static polarizabilities of Yb, Lu, Hf, No, Lr, and Rf are presented in Table IX. CI + MBPT and CI + all-order results are listed in columns labeled “MBPT” and “All-order,” respectively. The calculations are done as described in Sec. II C. The result for ytterbium agrees precisely with our previous calculations [31,36,37], with experimental constrain presented in Ref. [38], and with most of other accurate calculations (see, e. g., review [40]); the results for lutetium and hafnium agree well with the calculations of Doolen [39]. Estimation of accuracy is based on comparison of the results obtained with the use of different approaches, including comparison with experiment for ytterbium, and on the sensitivity of the results to variation of the parameters of the computational procedure. The theoretical uncertainties presented in the parentheses are on the level of 5% for Yb, Lu, and Hf (see Table IX). We expect similar uncertainty for No and Rf. Lawrencium represents a special case due to anomalously small energy interval between ground ²P_{1/2} state

and first excited ²D_{3/2} state. Note that there is an inversion of the order of these states in Lr as compared to its lighter analog Lu. The inversion is due to relativistic effects [11–15]. Because of small value of this energy interval it is very sensitive to the correlations. Different treatment of correlations leads to significantly different values of the interval (see Table V). This in turn leads to large uncertainty in the value of the polarizabilities of both states of Lr.

The value of the electric dipole transition amplitude between 7p_{1/2} and 6d_{3/2} states of Lr in the calculations is

 TABLE IX. Ground-state scalar α_0 and tensor α_2 polarizabilities of Yb, Lu, Hf, No, Lr, and Rf. CI + MBPT and CI + all-order results are listed in columns labeled “MBPT” and “All-order,” respectively. The last column presents the values of α_0 from other sources. All numbers are in atomic units. To convert them into 10⁻²⁴cm³ one should divide the numbers by 6.749.

Atom/ate		α_0		α_2		α_0 Other
		MBPT	All-order	MBPT	All-order	
Yb	¹ S ₀	141(6) ^a	141(2) ^b	0	0	139.3(4.9) ^c
Lu	² D _{3/2}	137(7)	145	-15(1)	-22	148 ^d
Hf	³ F ₂	103(5)	97	-0.41(2)	-0.92	109 ^d
No	¹ S ₀	112(6)	110	0	0	
Lr	² P _{1/2}	320(80)	323	0	0	
Lr	² D _{3/2}	-12(25)	-12	120(25)	119	
Rf	³ F ₂	107(5)	115	2.3(4)	8.9	

^aAgrees precisely with our previous calculations, Refs. [36,37].

^bReference [31].

^cExperimental constrain, Ref. [38].

^dRelativistic linear response calculations by G. D. Doolen, unpublished, cited from Ref. [39].

given by

$$\langle 7s^2 7p_{1/2} || \mathbf{D} || 7s^2 6d_{3/2} \rangle = 2.02 \text{ a.u.} \quad (20)$$

This allows us to separate the contribution due to this transition from the rest of the sum in Eqs. (12) and (13) and present polarizabilities in the form

$$\alpha_0(7p_{1/2}) = 126 + 1.35/\Delta E, \quad (21)$$

$$\alpha_0(6d_{3/2}) = 67 - 0.677/\Delta E, \quad (22)$$

$$\alpha_2(6d_{3/2}) = 26 + 0.677/\Delta E, \quad (23)$$

where all values are in atomic units and $\Delta E = E(6d_{3/2}) - E(7p_{1/2})$. Sensitivity of the polarizabilities to the value of this energy interval is the main source of uncertainty. The uncertainty assigned to the polarizabilities of lawrencium (Table IX, MBPT column) are based on the variation of the energy interval in different calculations (Table V). The uncertainties for other atoms are smaller due to absence of the resonance contribution. The most accurate values are those obtained in the all-order calculations while the difference between all-order and MBPT results can serve as an estimation of theoretical uncertainty.

Knowing the value of the electric dipole transition amplitude (20) allows us to calculate lifetime of the $6d_{3/2}$ state. It is 0.23 ms if we take the energy interval to be our theoretical value of 1555 cm^{-1} (see Table V). This is a long-lived metastable state. Since lawrencium atoms are not found in nature but produced on accelerators they can probably be produced

in either of the $7p_{1/2}$ or $6d_{3/2}$ states. The interaction with environment is very different for Lr atoms in these two states. It is isotropic for the atoms in the $7p_{1/2}$ state and strongly anisotropic for atoms in the $6d_{3/2}$ state. In the latter case, the polarizability is dominated by the tensor term. The total value is positive ($\alpha \approx 100 \text{ a.u.}$) for the case when total atomic angular momentum is parallel to the electric field ($|M| = J$) and it is negative ($\alpha \approx -160 \text{ a.u.}$) for the case when total atomic angular momentum is perpendicular to the electric field ($M = 0$).

IV. CONCLUSION

Energy levels for lowest states of superheavy elements nobelium, lawrencium, and rutherfordium as well as first few ionization potentials and static polarizabilities have been calculated using the combination of the configuration interaction with the all-order single-double method. The accuracy of the calculations are controlled by performing similar calculations for lighter analogs of the elements, ytterbium, lutecium, and hafnium. These calculations provide benchmark data, critically evaluated for their accuracy, for future experimental studies.

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