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Calculation of the Electron Binding Energies and X-Ray Energies for the Superheavy Elements 114, 126, and 140 Using Relativistic Self-Consistent-Field Atomic Wave Functions*

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Relativistic Hartree–Fock–Slater atomic wave functions have been calculated for the superheavy elements $Z = 114$ and 126. The calculations have been made both for the atom and for singly ionized states with holes in the K or L shells. A Wigner-Seitz boundary condition is used, and results for both point and finite nuclei are presented. From these solutions, binding energies and x-ray energies have been evaluated. Similar calculations have been made on Au and U, and have been compared with experiment so as to ascertain what degree of confidence one may have in these computations. A discussion is made of the importance of finite nuclear size in determining the K-shell binding energy, and a solution for element 140 was obtained to demonstrate the atomic stability in the present approximation of elements above $Z = 137$. Finally, the probability for finding an electron within the nuclear radius is given for each of the elements studied, and a brief discussion is given concerning the stability of the superheavy elements against electron capture.

I. INTRODUCTION

There has recently been much speculation[1] about the formation of the superheavy elements ($Z = 114$, $A = 298$) and ($Z = 126$, $A = 310$), which because of their doubly magic numbers may exist with relatively long half lives. If such isotopes could be made, there is the likelihood that in the decay of the excited nuclear states, inner-shell vacancies of the atom, particularly the K shell, would be formed that would subsequently lead to the emission of characteristic x rays. The energy of an internally converted electron will also depend on the binding energies. These x-ray and binding energies might be used to identify the elements if they exist, perhaps in remnants of supernovae or as a product of heavy ion bombardment. In addition, a comparison of the experimental x-ray energies with calculations based on a finite nucleus might yield an estimate of the nuclear size.

We have calculated relativistic self-consistent-field (SCF) wave functions for the elements $Z = 114$ and 126. For these calculations, we have solved the Dirac equation numerically for a self-consistent field with spherical symmetry and Wigner-Seitz boundary conditions. A Slater-type electron exchange approximation, and both point and distributed nuclear charges were used. From the eigenvalues of the solutions for neutral atoms, one can estimate the energies of the x rays which would be emitted following an inner-shell vacancy. In addition, $K\alpha_{1,2}$ x-ray energies have been calculated from the difference in the total energies of the appropriate one-hole configurations. Calculations on gold and uranium have also been made, and have been compared with the experimental results to determine the accuracy of our program for x-ray energy calculations. Finally, an evaluation is made of the dependence of the atomic binding energies on the nuclear size and diffusivity.

In a discussion of superheavy elements, those with $Z > 137$ have always been of special interest. The Darwin-Gordon[2,3] solution of the Dirac equation for a point nuclear charge breaks down for $Z > 1/\alpha$, where α is the fine-structure constant. An earlier investigation[4] by Werner and Wheeler has shown that, with a nuclear charge distribution of finite size, a K-shell electron may exist with a stable electronic configuration where $Z > 1/\alpha$. There remained, however, a degree of uncertainty on account of the approximate nature of that investigation, which did not include, among other things, a self-consistent treatment for the electronic shell structure. Our self-consistent solution for a finite size nucleus remains valid for $Z > 1/\alpha$, and we have computed an ion with $Z = 140$.

II. WAVE FUNCTIONS AND EIGENVALUES

The wave functions and eigenvalues have been obtained using the same theory and code which was applied to calculate the Mössbauer isomer shift for metallic gold[6] and the shake-off probability for elements with $2 \leqslant Z \leqslant 92$.[7] The code gives the eigensolutions of the Dirac equation with a self-consistent potential including a Slater-type exchange term. These solutions are similar to those obtained by Liberman *et al.*[8] In the calculations we have employed either a point or a finite nuclear charge distribution; and have used a Wigner-Seitz boundary condition, rather than the usual free-atom boundary condition.

For the computations reported in this paper, we required a self-consistency of 1 part in 10^5 (or better) in the contribution to the potential from each subshell as well as for the potential due to the total electron cloud. Subshell eigen energies were iterated to a relative deviation of less than 5 parts in 10^6. Computations were done on a CDC 1604-A computer. Details of this code for the calculation of wave functions may be found elsewhere.[6,9] Three points need special comments here. These pertain to the use of (i) the Wigner-Seitz boundary condition, (ii) the Slater exchange potential, and (iii) the finite nuclear size.

A. The Wigner-Seitz Boundary Condition

Instead of calculating wave functions and eigenvalues for a free atom, which would be appropriate to a very dilute gas, we have chosen to use a boundary condition based on a proposal of Wigner and Seitz,[10] restricting the atom to a finite volume of radius R_{WS}. This has two advantages: (1) Such a boundary condition may approximate the "true" situation better in a condensed medium such as a chemical compound or a metal, and (2) such solutions often require less time on the computer for convergence, which may be of particular consequence in the case of a very heavy element.

For Dirac's relativistic radial wave functions, the Wigner-Seitz boundary condition cannot be satisfied simultaneously for both components.[6] In the case of a Schrödinger wave function ψ_S, this boundary condition, which is based on the translational invariance for each atom in a solid lattice may be specified by $(d\psi_S/dr)R_{\mathrm{WS}} = 0$ when quantum number l is even and $\psi_S(R_{\mathrm{WS}}) = 0$ when l is odd, where R_{WS} is the radius of the Wigner-Seitz sphere used to approximate the polyhedral cell for the atom. Since the major component g of the relativistic wave function is predominant in the surface region of the atom, we have chosen to satisfy the Wigner-Seitz boundary condition for the major wave function:

$$dg/dr|_{r=R_{\mathrm{WS}}} = 0 \text{ for even } l$$

$$\text{and } g|_{r=R_{\mathrm{WS}}} = 0 \text{ for odd } l. \qquad (1)$$

B. The Slater Exchange Potential

Since a Hartree-Fock calculation is complex, it is often replaced by an approximate treatment. Slater proposed[11] that the exchange potential at any point in the atom be approximated by that for a free-electron gas having the local charge density. This approximation, at large radii in free atoms, tends to zero as a negative exponential rather than the self-exchange value of $1/r$, causing outer electrons to be less tightly bound than they should be. Latter's modification,[12] which essentially puts a floor of $1/r$ under the Slater exchange potential at large radii, is generally used to correct this problem. When Wigner-Seitz boundary conditions are used, however, it seems more reasonable to use the unmodified Slater potential, since the electron density does not become zero at large radii. We have done this.

One other question concerning Slater's approximation is which value should be assigned to the constant multiplier, in particular, whether it be either 1 or 3/2. Our attitude is that since we are using an approximation, we shall choose the factor which gives better agreement with experimental data for the phenomenon we wish to predict.[13]

C. The Finite Nuclear Size

Most solutions of the Schrödinger and Dirac equations for the electron orbitals in the many-electron problem assume that the nucleus can be represented by a point charge. The effect of the finite nuclear size on any observed phenomenon is then taken into account by a perturbation method, e.g., the treatment of Brix and Kopfermann[14] for the isotope shift in atomic spectra. For superheavy elements, however, these perturbation methods may be inadequate. In the extreme case of $Z > 137$, any such perturbation treatment is impossible because for a point nucleus the Dirac equation does not have a physically acceptable solution.[4] We therefore decided to incorporate the finite nuclear charge distribution in terms of an appropriate potential function $V(r)$ corresponding to a charge density distribution $\rho(r)$,

$$V(r) \equiv (r)^{-1} \int_0^r 4\pi r'^2 \rho(r') dr' + \int_r^\infty 4\pi r' \rho(r') dr'. \qquad (2)$$

We used a modification of the "smoothed uniform" distribution of Yennie, Ravenhall, and Wilson[5,6]

$$\begin{aligned} \rho(r) &= C_N\{1 + \exp[(r - r_0)/a]\}^{-1} && r \geqslant r_m, \\ &= \eta_0 + \eta_2 r^2 && r \leqslant r_m, \qquad (3) \end{aligned}$$

where C_N is a normalization constant, determined from the total charge Z

$$4\pi \int_0^\infty r^2 \rho(r) dr = Z; \qquad (4)$$

r_m is approximately $0.1r_0$, and η_0 and η_2 are chosen such that $\rho(r)$ and $\rho'(r)$ are continuous at $r=r_m$. Besides the nuclear potential, bound electrons are subjected to a SCF potential of the Hartree type, modified by a Slater-type exchange potential.[6]

In order to study the nature of the analytical solution of the Dirac equation for a nuclear potential with distributed charge and for the self-consistent potential due to other electrons, we note that the nuclear and the SCF potential can be expressed by

$$\sum_{\nu=0}^{n} C_\nu r^{2\nu}$$

near the origin.[6] Thus the solution near the origin is

$$\begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = r^{s-1} \sum_{n=0}^{\infty} \begin{pmatrix} a_n \\ b_n \end{pmatrix} r^n , \qquad (5)$$

$$\text{with } s = |k| = |(l-j)(2j+1)| , \qquad (6)$$

$$a_0/b_0 = (s-k)/(s+k), \qquad (7)$$

and

$$a_n = [(\epsilon/\alpha - \alpha C_0)b_{n-1} - \alpha C_2 b_{n-3} - \alpha C_4 b_{n-5}]/(s+k+n), \qquad (8)$$

$$b_n = [(2-\epsilon)/\alpha + \alpha C_0)a_{n-1} + \alpha C_2 a_{n-3} + \alpha C_4 a_{n-5}]/(s-k+n), \qquad (9)$$

subject to the condition

$$a_{n-i} = b_{n-i} = 0 \text{ for } n<i; \quad i = 1, 3, \text{or } 5.$$

(ϵ and α are, respectively, the eigenvalue and fine-structure constant. We have used $\alpha = 0.007\,297\,2$ and 1 Ry = 13.6053 eV.)

The important difference in the behavior of the wave function for a point and a finite nucleus is that for a point nucleus the first power of r in the Darwin expansion[2] is nonintegral, $(k^2 - \alpha^2 Z^2)^{1/2}$, and both leading coefficients are nonzero; but for a finite nucleus, the first power of r [Eq. (5)] is an integer, $|k| - 1$, and, depending upon the sign of k, either a_0 or b_0 is zero. Moreover the solution exists for $Z > 1/\alpha$, because Z enters only in the magnitude of the finite coefficients C_ν.

In our calculations the nuclear radius r_0 and the diffusivity parameter a are estimated from Elton[15] although the choices are somewhat arbitrary. In the case of elements 114 and 126 the nuclear radius and diffusivity are treated as parameters, solutions being obtained for a variety of values. The Wigner-Seitz radius for gold and uranium is estimated from the molar volume of the metals. For the superheavy elements an arbitrary value of 5 Bohr radii is assigned.

III. RESULTS AND DISCUSSION

To determine the accuracy which might be expected from our codes, we calculated wave functions and eigenenergies for gold and uranium. In these calculations we included the effects of both finite nuclear size and Wigner-Seitz boundary condition. In Table I are given the eigenvalues for the K and L shells of Au and U, using either the Slater exchange multiplier 1 or 1.5. The $K\alpha_1$ and $K\alpha_2$ x-ray energies (representing respectively K-L_{III} and K-L_{II} transitions following a K vacancy) may be estimated from the difference in eigenvalues between the two shells of a neutral atom. (Method I). This follows from the energy cycle of bringing an electron from the continuum into the K hole and then removing from the atom an electron in the L shell. This treatment is, however, only approximate since it neglects the readjustment of the entire atom. A more consistent calculation (Method II) is to take the difference in total energy for the initial and final configuration, i.e., the difference in total energy for the singly charged ion with the hole respectively in the K and L shells. The calculated x-ray energies are also displayed in Table I, together with experimental values for the binding energies and x-ray energies. We see that the best agreement with

TABLE I. Binding energies and $K\alpha$ x-ray energies for Au and U (keV).

	Calculations[a]			Experimental[b]
		Au		
Binding energies	I(1.5)	I(1)	II(1)	
K	80.958	80.546	80.895	80.725
L_{I}	14.336	14.205	. . .	14.353
L_{II}	13.778	13.631	13.675	13.734
L_{III}	11.922	11.797	11.833	11.919
X-ray energies				
$K\alpha_1$ ($L_{\mathrm{III}} \to K$)	69.036	68.749	69.062	68.804
$K\alpha_2$ ($L_{\mathrm{II}} \to K$)	67.180	66.915	67.220	66.990
		U		
Binding energies	I(1.5)	I(1)	II(1)	
K	116.069	115.527	115.950	115.606
L_{I}	21.752	21.564	. . .	21.757
L_{II}	21.031	20.824	20.872	20.948
L_{III}	17.168	17.001	17.033	17.166
X-ray energies				
$K\alpha_1$ ($L_{\mathrm{III}} \to K$)	99.068	98.526	98.917	98.439
$K\alpha_2$ ($L_{\mathrm{II}} \to K$)	95.038	94.703	95.078	94.665

[a] Calculations based on eigenvalues are given by Method I, and those on the differences of total energies between the initial and final configurations by Method II. Coefficients for exchange potential are in parentheses. For Au: $r_0 = 6.38$ F, $a = 0.567$ F, $R_{\mathrm{WS}} = 3.01$ bohr. For U: $r_0 = 7.33$ F, $a = 0.569$ F, $R_{\mathrm{WS}} = 3.25$ bohr.

[b] J. A. Bearden, Rev. Mod. Phys. 39, 78 (1967); J. A. Bearden and A. F. Burr, *ibid.* 39, 125 (1967).

the experimental x-ray energies comes from using Method I with an exchange coefficient of 1.0. This is, however, probably fortuitous. Whether an exchange coefficient of 1.0 will give the best x-ray energy values in the range of the superheavy elements is as yet open to conjecture. We shall, however, use the value of 1.0 in our calculations of elements 114, 126, and 140.

Before giving the x-ray energies for the superheavy elements, one should first examine the role played by the finite nucleus. In Table II we have shown calculations of the K-shell eigenvalues for elements 114 and 126 as a function of nuclear radius and nuclear surface diffusivity. We see that for these elements one of the greatest errors in the calculation of K x-ray energies will probably come from the assignment of the nuclear radius. In fact, if good experimental results were obtainable for the x-ray energies, fairly good estimates of the nuclear size might be obtained. For example, a variation of 0.1% in the K x-ray energy for element 126 will reflect a change in the nuclear radius of about 0.3 F.

Calculated $K\alpha$ x-ray energies for elements 114 and 126 are given in Table III. For each element, a Wigner-Seitz radius of 5 bohr and exchange coefficient of 1.0 were used. For element 114, the nuclear parameters were $r_0 = 7.35$ F and $a = 0.575$ F, and the outer electron configuration was $5f^{14}6d^{10}7s^2 7p^2$. For element 126, the nuclear parameters were $r_0 = 7.45$ F and $a = 0.575$ F, and the outer electron configuration was $6f^6 7p^6 8s^2$.

Since approximate methods may be used to predict the change in binding energy with Z and nuclear size, we have compared our calculations with such methods for the K-shell binding energy.

TABLE II. (a) The effect of nuclear shape on the K-shell eigenenergy for atomic number 114. $R_{\mathrm{WS}} = 5.0$ bohr, Slater exchange coefficient = 1.0, configuration $5f^{14}$, $6d^{10}$, $7s^2$, $7p^2$. (b) The effect of nuclear shape on the K-shell eigenenergy for atomic number 126. $R_{\mathrm{WS}} = 5.0$ bohr, Slater exchange coefficient = 1.0, configuration $6f^6$, $7p^6$, $8s^2$.

Nuclear Radius (F)	K-shell eigenenergy (keV) Surface Diffusivity (F) 0.500	0.575	0.650
		(a)	
10.00		200.062	
7.35	200.802	200.770	200.734
5.00		201.365	
3.00		201.812	
0		202.807	
		(b)	
10.00		267.605	
7.45	269.767	268.667	269.556
5.00		271.728	
3.00		273.384	
0		278.922	

TABLE III. Binding energies and $K\alpha$ x-ray energies for superheavy elements 114 and 126 (keV).

Binding energies	Method I	Method II
	114[a]	
K	200.770	201.389
L_{II}	40.209	40.295
L_{III}	28.210	28.252
X-ray energies		
$K\alpha_1$ ($L_{\mathrm{III}} \to K$)	172.560	173.137
$K\alpha_2$ ($L_{\mathrm{II}} \to K$)	160.562	161.094
	126[b]	
K	269.667	270.418
L_{II}	58.305	58.403
L_{III}	35.715	35.735
X-ray energies		
$K\alpha_1$ ($L_{\mathrm{III}} \to K$)	233.952	234.683
$K\alpha_2$ ($L_{\mathrm{II}} \to K$)	211.362	212.015

[a] $r_0 = 7.35$ F, $a = 0.575$ F, exchange coefficient = 1, $R_{\mathrm{WS}} = 5$ bohr.

[b] $r_0 = 7.45$ F, $a = 0.575$ F, exchange coefficient = 1, $R_{\mathrm{WS}} = 5$ bohr.

The K binding energy has been estimated from Dirac's solution for a one-electron ion[16] with a point nucleus using as the nuclear charge $Z - \sigma$, where σ, the screening constant, has been estimated[9] to be 0.7 for heavy elements. The change in binding energy due to nuclear size has been obtained from the method of Breit[17] based on first-order perturbation theory, where the $1s$ electron densities were taken from our relativistic SCF wave function for a point nucleus. We see from Table IV that the more approximate methods yield only crude estimates, and for elements with Z above 137, calculations based on a point nucleus give imaginary eigenvalues while the use of a finite nucleus yields real eigenvalues.

Physically it is very easy to understand why the finite nuclear charge distribution allows a stable electronic configuration even when $Z > 137$. In Fig. 1 we have plotted for $Z = 140$ the net equivalent charge seen by an electron at point r, which is $rV(r)$. As the electron moves within the nuclear radius toward the center, it effectively sees less positive charge, analogous to the classical case of the charge seen by a test charge inside a homogeneous charged sphere. In the same figure, the modified major and minor components rg and rf have been plotted for the $1s_{1/2}$ electron. The maxima of the major and minor components lie well outside the nucleus, and only a very small fraction of the electron density distribution lies within the nucleus. This fact refutes the usual heuristic argument based on the Darwin expansion that as

TABLE IV. Comparison of K binding energies (keV), using SFC wave functions and approximate methods.

Element	E (point nucleus) HFS[a]	E (point nucleus) Approximate[b]	E (point nucleus) $-E$ (finite nucleus) HFS[a]	E (point nucleus) $-E$ (finite nucleus) Approximate[b]
Au	80 591	91 629	0.045	0.051
U	115 708	129 906	0.181	0.34
114	202 807	223 523	2.037	4.5
126	278 922	304 559	9.255	37.2
140	?[c]	?[c]	?[c]	?[c]

[a] Based on Hartree-Fock-Slater solutions for finite size (cf. Table I and Table II) and the corresponding case for point nucleus. The calculation of 140 is based on the same parameters as 126 except for the nuclear charge.

[b] Approximate calculation for point nucleus based on Dirac solution for one electron and finite Z. Finite nuclear correction obtained from first-order perturbation theory.

[c] Impossible to make calculations based on point nucleus.

Z is increased close to 137, the K electron will be completely absorbed into the nucleus – that is not the case at all. Rather, the finite nuclear charge distribution pushes the electron out slightly in comparison with a point charge.

It is of interest to compare the probabilities of finding an electron inside the nucleus for the elements calculated with a finite nucleus. The probability, given by

$$P=N_{nlj}\sum_{nlj}\int_0^{r_0}(f^2+g^2)r^2dr, \tag{10}$$

where N_{nlj} is the number of electrons in shell nlj, is listed for each element in Table V. The probability increases with Z, but not precipitously. To a first approximation, the rate for allowed electron capture is, in addition to other factors, directly proportional to the probability for finding an electron in the nucleus.[18] Apart from nuclear considerations and taking into account the contribution of electron charge density within the nucleus only, Table V suggests that the superheavy elements would not be so unstable with regard to electron capture that it would be the determining factor in their detection. For example, there is only about a 20 times greater probability for finding an electron inside the nucleus in element 126 than in uranium, which implies the same enhancement for electron capture.

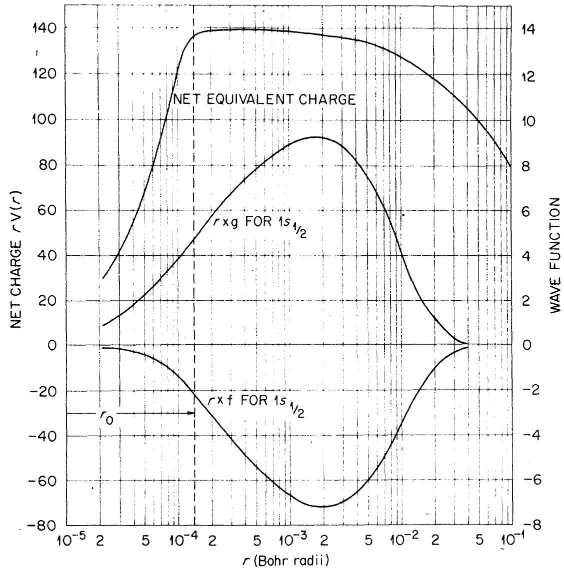

FIG. 1. Results from the solution of element 140 (cf. Table VI for parameters). Upper curve: plot of net equivalent charge (proton + electron + exchange potential) as a function of radial distance r, when the net equivalent charge is r times the potential acting upon a test charge at r. r_0 = nuclear radius. Lower curves: the major ($r\times g$) and minor ($r\times f$) components of the $1s_{1/2}$ wave function $[\int(g^2+f^2)\,r^2dr=1]$ as a function of r.

Since this is one of the first SCF relativistic calculation made of the superheavy elements,[19] it was thought interesting to include the eigenvalues and mean radii for all the shells, although for the outer shells such values have only a specialized meaning dependent on the choice of configuration and Wigner-Seitz boundary condition. In fact it is possible to obtain eigenvalues with the opposite sign, i.e., unbound states, for some of the orbitals because these electrons are artificially constrained within the Wigner-Seitz sphere. (For convenience, we have assigned in this paper a positive sign to the binding energies and eigenvalues of bound states.) For the lower shells (i.e., K, L, M, and N) the eigenvalues may be used with confidence for calculating x-ray energies. The nature of the outermost shell does not greatly affect the energies of the inner shell. Compare, for example, the calculations for the two configurations of element 126 in Table VI. In addition, the difference in energy between the eigenvalues of nearly all but the outermost shell (and, in consequence, the evaluation of the x-ray energies) remains essentially constant. The same result has also been noted for changes in the ionization state[20] and Wigner-Seitz radius.[6]

Before concluding, we wish to point out that some types of error which are negligible when computing eigenenergies of light atoms are quite important for the superheavy elements. For example, the large relativistic effect observed within the framework of the Dirac equation makes one wonder about the importance of higher-order relativistic effects such as the vacuum polarization and fluctuation. Any estimate of such effects within the framework of existing perturbation theory does not have any meaning for these elements. Particularly this cannot be carried out

TABLE V. Probability of finding an electron inside the nuclear radius.

Atomic Number	r_0 (F)	Probability[a] (%)
79	6.38	0.0014
92	7.33	0.0058
114	7.35	0.038
126	7.45	0.12
140	7.45	0.43

[a] Cf. Eq. (10).

TABLE VI. Eigenvalues and mean radii for elements 114, 126, and 140. ϵ = eigenvalue; $\bar{r}$ = mean radius = $\int_0^\infty r\psi^2 dr$, where $\epsilon > 0$ corresponds to a bound state.

114^a			126^b			126^c			140^d		
Shell	ϵ (eV)	$\bar{r}$ (bohr)	Shell	ϵ (eV)	$\bar{r}$ (bohr)	Shell	ϵ (eV)	$\bar{r}$ (bohr)	Shell	ϵ (eV)	$\bar{r}$ (bohr)
$1s_{1/2}$	200 770.2	0.009 494	$1s_{1/2}$	269 667.2	0.007 562	$1s_{1/2}$	269 651.5	0.007 562	$1s_{1/2}$	388 124.7	0.005 462
$2s_{1/2}$	41 150.2	0.038 89	$2s_{1/2}$	58 603.4	0.030 95	$2s_{1/2}$	58 586.9	0.030 10	$2p_{1/2}$	97 940.0	0.013 77
$2p_{1/2}$	40 208.6	0.029 93	$2p_{1/2}$	58 305.4	0.022 42	$2p_{1/2}$	58 289.2	0.022 42	$2s_{1/2}$	91 310.5	0.022 69
$2p_{3/2}$	28 209.9	0.043 70	$2p_{3/2}$	35 715.1	0.038 80	$2p_{3/2}$	35 698.3	0.038 80	$2p_{3/2}$	45 883.4	0.034 14
$3s_{1/2}$	11 067.5	0.103.42	$3s_{1/2}$	16 139.8	0.084 45	$3s_{1/2}$	16 121.4	0.084 44	$3p_{1/2}$	26 433.1	0.054 86
$3p_{1/2}$	10 582.4	0.095 27	$3p_{1/2}$	15 734.9	0.076 11	$3p_{1/2}$	15 716.8	0.076 10	$3s_{1/2}$	25 546.6	0.064 87
$3p_{3/2}$	7673.00	0.1198	$3p_{3/2}$	10 171.4	0.105 47	$3p_{3/2}$	10 152.1	0.105 46	$3p_{3/2}$	13 837.1	0.092 03
$3d_{3/2}$	6887.25	0.1020	$3d_{3/2}$	9243.29	0.089 23	$3d_{3/2}$	9224.67	0.089 22	$3d_{3/2}$	12 716.6	0.077 33
$3d_{5/2}$	6401.56	0.1086	$3d_{5/2}$	8473.00	0.096 47	$3d_{5/2}$	8454.10	0.096 45	$3d_{5/2}$	11 469.4	0.085 34
$4s_{1/2}$	3185.16	0.2220	$4s_{1/2}$	4916.16	0.1822	$4s_{1/2}$	4894.17	0.1821	$4p_{1/2}$	8322.70	0.1316
$4p_{1/2}$	2942.38	0.2170	$4p_{1/2}$	4663.80	0.1754	$4p_{1/2}$	4642.02	0.1754	$4s_{1/2}$	8258.56	0.1426
$4p_{3/2}$	2108.53	0.2617	$4p_{3/2}$	3017.48	0.2275	$4p_{3/2}$	2994.67	0.2274	$4p_{3/2}$	4532.39	0.1963
$4d_{3/2}$	1725.13	0.2528	$4d_{3/2}$	2553.34	0.2178	$4d_{3/2}$	2530.74	0.2177	$4d_{3/2}$	3965.86	0.1865
$4d_{5/2}$	1593.16	0.2645	$4d_{5/2}$	2332.57	0.2301	$4d_{5/2}$	2309.81	0.2300	$4d_{5/2}$	3590.03	0.1996
$4f_{5/2}$	1090.29	0.2435	$4f_{5/2}$	1730.81	0.2088	$4f_{5/2}$	1708.42	0.2087	$4f_{5/2}$	2869.14	0.1790
$4f_{7/2}$	1051.22	0.2489	$4f_{7/2}$	1663.65	0.2144	$4f_{7/2}$	1641.15	0.2143	$5s_{1/2}$	2822.47	0.2760
$5s_{1/2}$	838.59	0.4376	$5s_{1/2}$	1457.59	0.3540	$5s_{1/2}$	1435.04	0.3542	$5p_{1/2}$	2770.42	0.2654
$5p_{1/2}$	728.06	0.4433	$5p_{1/2}$	1327.27	0.3529	$5p_{1/2}$	1304.76	0.3532	$4f_{7/2}$	2753.44	0.1850
$5p_{3/2}$	485.19	0.5304	$5p_{3/2}$	812.92	0.4478	$5p_{3/2}$	792.19	0.4489	$5p_{3/2}$	1521.36	0.3772
$5d_{3/2}$	322.89	0.5584	$5d_{3/2}$	604.22	0.4615	$5d_{3/2}$	583.91	0.4631	$5d_{3/2}$	1253.78	0.3824
$5d_{5/2}$	288.96	0.5840	$5d_{5/2}$	540.83	0.4856	$5d_{5/2}$	521.11	0.4876	$5d_{5/2}$	1135.44	0.4060
$6s_{1/2}$	156.46	0.8860	$6s_{1/2}$	361.08	0.6755	$6s_{1/2}$	346.59	0.6810	$6s_{1/2}$	983.10	0.5076
$6p_{1/2}$	115.42	0.9394	$6p_{1/2}$	303.37	0.6945	$6p_{1/2}$	289.40	0.7011	$6p_{1/2}$	937.43	0.5010
$5f_{5/2}$	96.435	0.6671	$5f_{5/2}$	286.79	0.5171	$5f_{5/2}$	267.96	0.5217	$5f_{5/2}$	808.58	0.4155
$5f_{7/2}$	89.047	0.6830	$5f_{7/2}$	270.73	0.5295	$5f_{7/2}$	252.22	0.5345	$5f_{7/2}$	776.15	0.4266
$6p_{3/2}$	62.628	1.167	$6p_{3/2}$	161.86	0.8938	$6p_{3/2}$	152.62	0.9076	$6p_{3/2}$	536.31	0.7057
$6d_{3/2}$	15.421	1.509	$6d_{3/2}$	84.872	1.010	$6d_{3/2}$	77.609	1.035	$6d_{3/2}$	422.67	0.7576
$7s_{1/2}$	12.024	2.191	$6d_{5/2}$	71.084	1.073	$6d_{5/2}$	64.722	1.101	$6d_{5/2}$	388.82	0.8038
$6d_{5/2}$	11.173	1.651	$7s_{1/2}$	57.789	1.384	$7s_{1/2}$	54.499	1.413	$7s_{1/2}$	380.16	0.9278
$7p_{1/2}$	2.6025	2.464	$7p_{1/2}$	38.537	1.506	$7p_{1/2}$	35.928	1.544	$7p_{1/2}$	355.43	0.9376
			$7p_{3/2}$	13.137	2.108	$7p_{3/2}$	12.268	2.157	$6f_{5/2}$	262.46	0.9288
			$8s_{1/2}$	5.936	2.416	$8s_{1/2}$	5.857	2.405	$7p_{3/2}$	235.47	1.3070
			$6f_{5/2}$	−1.355	1.701	$6f_{5/2}$	−3.457	1.838	$8s_{1/2}$	190.35	1.6270
						$5g_{7/2}$	−5.488	0.7590			

[a] Calculation based on relativistic Hartree-Fock-Slater (HFS) solutions where $r_0 = 7.35$ F, $a = 0.575$ F, $R_{WS} = 5.0$ bohr radii. Exchange coefficient = 1.0, configuration $5f^{14}$, $6d^{10}$, $7s^2$, $7p^2$.

[b] Calculation based on relativistic HFS solution where $r_0 = 7.45$ F, $a = 0.575$ F, $R_{WS} = 5.0$ bohr radii. Exchange coefficient = 1.0, configuration $6f^6$, $7p^6$, $8s^2$.

[c] Calculation same as b except configuration $5g^2$, $6f^4$, $7p^6$, $8s^2$.

[d] Calculation based on relativistic HFS solution where $r_0 = 7.45$ F; $a = 0.575$ F, $R_{WS} = 5.0$ bohr radii, exchange coefficient = 1.0, configuration $6f^6$, $7p^6$, $8s^2$ (+14 ion).

for $Z = 140$. A possible estimate of these in terms of perturbation calculations based on our computed wave functions is beyond the scope of this paper, although it may be necessary if the experimentally observed x rays have resolutions better than 1%.

CONCLUSION

It is now possible to obtain relativistic SCF atomic wave functions for the superheavy elements, including exchange and finite nuclear size. It has been further shown that such calculations can also be made for elements higher than 137. If and when these elements are produced, good values of the x-ray energies and binding energies will be available to help in their identifications. Further, if good experimental binding energies are obtained, it will provide an important challenge to atomic structure calculations because of the great enhancement of effects caused by the relativistic velocity of the inner-shell electrons and the no longer negligible nuclear size.

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