Binding-energy predictions of positrons and atoms

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As yet there is no experimental determination of the binding energy of a positron to any neutral atom. However, quantum calculations have given positron binding energies for 12 atoms (including positronium) and have shown that 14 atoms do not bind a positron. We find that the known binding energies can be fitted to a simple expression involving only the polarizabilities, ionization potentials, and the numbers of valence *s* electrons of the atoms, and we use this relationship to predict positron-atom binding energies for other atoms. Positronium-atom binding is not treated here.

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I. INTRODUCTION

The positron is the antiparticle of the electron, and positronium, Ps, is an atom consisting of a positron and an electron. Modern sources of positrons [1–3] have opened several fields to new applications [4] that will be enriched by knowledge of accurate binding energies of positrons and positronium atoms to atoms and molecules. Among these fields are quantum dots [5], superconductors [6], surfaces and coatings [7], and more. A large amount of research work shows that a positron or positronium can form a bound state with some atoms and molecules and not with others. The data for atoms, all of which come from quantum calculations, are shown in Fig. 1, where one can see that there are still many atoms that have not been studied. The subject has been reviewed recently [8].

From the theoretical side, determining binding energies with reasonable accuracy requires tedious calculations, and in several attempts to avoid this labor and at the same time provide useful estimates across the periodic chart, authors have resorted to dubious approximations [9,10]. In this article, we do not rely on quantum mechanical models or approximations. Instead, our approach is entirely empirical: We relate known positron-atom binding energies to certain atomic parameters and thereby predict binding energies for other atoms. We draw our inspiration from a work by Danielson *et al.* [11] in which positron-molecule binding energies were shown to depend in a simple way on molecular polarizabilities, dipole moments, and, for aromatic molecules, the numbers of π electrons. Another useful article is a review article by Mitroy *et al.* [12], where Eq. (23) gives us the underlying physical idea for the present work. Here we extend this idea to quantitative predictions.

First we give a general summary and analysis of our work. Then we examine the dependence of positron-atom binding energies on some physical properties, including ionization potential (V_i), static electric dipole polarizability (α), atomic radius, electronegativity, electron affinity, and the numbers and types of valence electrons. Using different combinations of these parameters, we employ MATLAB to carry out numerous linear regressions to fit positron-atom binding energies. We pick the most accurate and reasonable combination in this article and demonstrate its validity, and we use this result to predict binding energies for all the unstudied atoms up to bismuth.

II. DATA ANALYSIS

The current data of one-positron, one-atom systems show some interesting patterns. The binding energies, thresholds, and methods of calculation for such systems are listed in Table I. Only 26 atoms have been studied so far. It is easy to find ranges of atomic properties within which the binding of positrons is confined. These ranges, shown in Fig. 2, are each bracketed by K and some other atom (Xe, Br, or H). In all cases the separation of binding and nonbonding atoms is perfect, with the exception of Au.

For a bound state of a positron-atom system, there are two channels for the dissociation. For the atoms whose ionization potentials are less than 6.803 eV, the lowest dissociation threshold is

$$e^+A \rightarrow A^+ + \mathrm{Ps},$$

and for the others, it is

$$e^+A \rightarrow A + e^+.$$

Consequently, the positron binding energy as a function of ionization potential has a discontinuity in its slope at 6.803 eV owing to the crossing of the levels associated with the two processes above. Danielson *et al.* [11] fitted the binding energy directly, but all of the molecules in their sample had ionization potentials greater than 6.803 eV. This will not work for us—we need a smoothly varying indicator of the binding energy—so we describe the binding as resulting from the quantum mechanical mixing of the structures $\{e^+A\}$ and $\{\mathrm{Ps}A^+\}$. The eigenvalues are given by

$$\begin{vmatrix} -V_i - \varepsilon & \gamma \\ \gamma & -6.803 - \varepsilon \end{vmatrix} = 0, \tag{1}$$

where V_i is the ionization potential, 6.803 is the ionization potential of positronium, ε is the ground-state energy, and γ is the interaction energy, all in electron volts. We ignore overlap between the two interacting structures. The eigenvalue ε and the interaction energy γ are both smooth functions of the ionization potential and other parameters, but we fit γ^2 because this enables us to treat atoms that do not bind positrons as well as those that do. Then we calculate ε from

$$\varepsilon = \frac{-6.803 - V_i - \sqrt{(V_i - 6.803)^2 + 4\gamma^2}}{2} \tag{2}$$

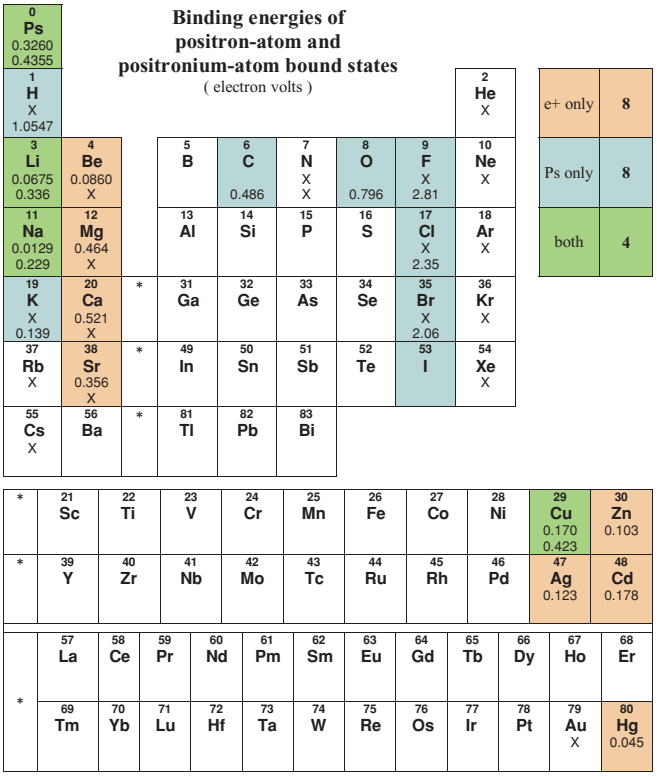

FIG. 1. (Color online) Under the atomic number and chemical symbol of each atom, we give the binding energies of e^+A and then the binding energies of PsA. "X" means the atom does not bind a positron or Ps, and a blank means we have no knowledge.

and the binding energy (in electron volts) from

$$E = -\varepsilon - \max\{V_i, 6.803\}. \quad (3)$$

The upper root [plus sign in front of the radical in Eq. (2)] may indicate resonances, but they are probably not physically meaningful.

III. RESULTS

Until now, 12 atoms have been found to bind with positrons (Table I). We do not use the binding energy of Hg in our fitting because of its great uncertainty, and we introduce K and Br into the fitting with artificial negative binding energies from effective-range theory in order to tie down the two ends of the binding range. Negative binding energies are unphysical, but they are useful for our present purposes. For those two atoms we take the binding energy to be $-1/a^2$, where a is the positron scattering length. We get: E(K) = –0.5442 eV [32] and E(Br) = –0.1048 eV [24], from which corresponding values of γ^2 are easily calculated.

Thus we do the fitting with K and Br and all the binding atoms, except Ps (an atypical atom) and Hg. After numerous sets of fitting with different physical properties and various combinations, we find that the fitting of γ^2 with V_i,α,$\alpha \cdot V_i$, and number of valence s electrons (N_S) is the best. The result is

$$\gamma^2 = -0.2793V_i - 0.1466\alpha + 0.0238V_i\alpha + 0.3646N_S + 1.6757. \quad (4)$$

TABLE I. The binding energies, thresholds, and methods of calculation for all studied positron-atom systems. Hyll means an expansion in a Hylleraasian basis, rel is relativistic treatment, SVM is stochastic variational method, FC_n is fixed core with n particles treated explicitly, CI is configuration interaction, ∞ indicates an extrapolation to convergence of a basis expansion, MBPT is many-body perturbation theory, $ModPot_n$ indicates a model potential with n particles explicitly treated, FNC indicates the atom fails a necessary test for binding a positron, and PO indicates the method of polarized orbitals.

System	Threshold	E (eV)	Method
Binding atoms			
e^+Ps	$e^+ + Ps$	0.3260	$Hyll_{rel}$ [13]
e^+Li	$Ps + Li^+$	0.0675(3)	SVM [14]
e^+Be	$e^+ + Be$	0.0860(3)	SVM [15]
e^+Na	$Ps + Na^+$	0.0129(5)	$SVMFC_2$ [16]
e^+Mg	$e^+ + Mg$	0.464(6)	$SVMFC_3$ [17]
e^+Ca	$Ps + Ca^+$	0.521(10)	$CI_\infty FC_3$ [17]
e^+Cu	$e^+ + Cu$	0.170(15)	$MBPT_{rel}$ [18]
e^+Zn	$e^+ + Zn$	0.103(2)	$CI_\infty FC_3$ [19]
e^+Sr	$Ps + Sr^+$	0.356(13)	$CI_\infty FC_3$ [17]
e^+Ag	$e^+ + Ag$	0.123(16)	$MBPT_{rel}$ [20]
e^+Cd	$e^+ + Cd$	0.178(3)	$CI_\infty FC_3$ [21]
e^+Hg	$e^+ + Hg$	0.045(20)	MBPT [10]
Nonbinding atoms			
e^+H	$e^+ + H$	Unbound	FNC [22]
e^+He	$e^+ + He$	Unbound	FNC [23]
e^+N	$e^+ + N$	Unbound	FNC [23]
e^+F	$e^+ + F$	Unbound	$ModPot_1$ [24]
e^+Ne	$e^+ + Ne$	Unbound	FNC [23]
e^+Cl	$e^+ + Cl$	Unbound	$ModPot_1$ [24]
e^+Ar	$e^+ + Ar$	Unbound	$ModPot_1$ [25], PO [26]
e^+K	$Ps + K^+$	Unbound	$SVMFC_2$ [27]
e^+Br	$e^+ + Br$	Unbound	$ModPot_1$ [24]
e^+Kr	$e^+ + Kr$	Unbound	$ModPot_1$ [25], PO [28]
e^+Rb	$e^+ + Rb$	Unbound	$SVMFC_2$ [27]
e^+Xe	$e^+ + Xe$	Unbound	$ModPot_1$ [25], PO [28]
e^+Cs	$Ps + Cs^+$	Unbound	$SVMFC_2$ [27]
e^+Au	$e^+ + Au$	Unbound	$MBPT_{rel}$ [20]

The fitting results are shown in Fig. 3. Units of the numerical coefficients above follow from the units of γ^2, α, and V_i, which are eV^2, $Å^3$, and eV, respectively.

The data used for the fit and our calculated binding energies are shown in Table II. The principal source of uncertainties in our calculated binding energies is the polarizabilities, which are not precisely known for all atoms. We test our fitting equation with the atoms which have been determined not to bind with positrons. If the model is valid, then γ^2 of unbound atoms will be negative; for Hg, it will be positive. The result (Table III) is in accordance with our prediction. The model appears to be reliable.

As shown in Table IV and Figs. 4 and 5, we predict that among the 58 atoms not previously studied, 24 will bind a positron, 6 will not, and 28 more are indeterminate. The latter are those with uncertainties larger than or equal to our predicted binding energies. Figure 5 shows the cusp in binding energies as a function of ionization potentials, which we find also in Ref. [12]. The very large positron affinities of atoms with

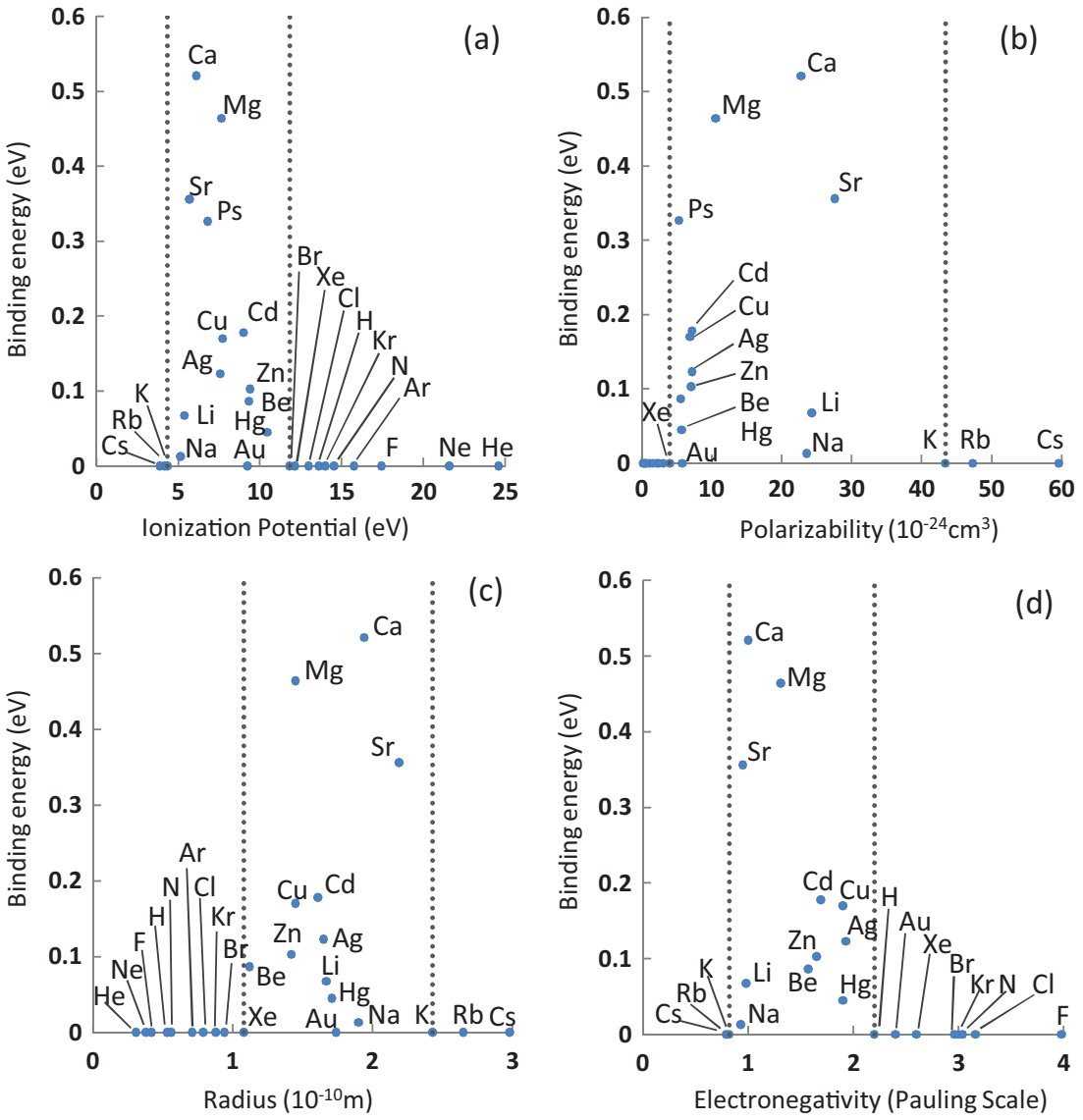

FIG. 2. (Color online) Positron-atom binding energy vs different physical properties, with ranges indicated with vertical dotted lines. (a) Ionization potentials are from Ref. [29]. The range is bracketed by K (4.341 eV) and Br (11.814 eV). (b) The source of polarizabilities is Ref. [30]. The range is bracketed by Xe (4.01 Å^3) and K (43.4 Å^3). The points to the left of Xe are (from left to right) He, Ne, F, H, N, Ar, Cl, Kr, and Br. (c) The source of radii is Ref. [31]. The bracketing atoms are Xe (1.08 Å) and K (2.43 Å). (d) The bracketing atoms are K (0.82) and H (2.2).

ionization potentials close of 6.803 eV is evident and was predicted earlier [10].

Positronium is an atom and so is correctly treated as such here. Ps_2 is also an atom but is not treated here because the addition of a positron gets one involved in exclusion effects that are not present for any other atom.

IV. DISCUSSION

From the fitting results, we can conclude that the binding energies of atoms and positrons are governed by the V_i, α, and the electron configuration. The influence of polarizability is profound, simple, and always attractive at long range:

$$\lim_{r\to\infty} V_{\rm pol}(r) \approx \frac{-\alpha}{2r^4}. \tag{5}$$

This has been understood for a very long time [34] and has been commented on by many authors. The short-range interaction, that of the positron and nucleus, is also profound and simple, but it is always repulsive:

$$\lim_{r\to\infty} V_{\rm pol} = \frac{Z}{r}. \tag{6}$$

The intermediate interaction, much more complicated, arises because of the correlation of the motions of the positron and the atomic electrons. The interplay between these three influences is different for each atom and determines whether a positron can bind. For atoms with ionization potentials less than 6.803 eV, short-range correlation effects are more significant and lead to the formation of virtual positronium that is bound by its large polarizability (5.33 Å^3) to the atomic cation. Ionization potentials are significant in that their propinquity to 6.803 eV is a measure of the strength of the interaction energy γ.

In a new work by Dzuba *et al.* [33], many-body perturbation theory is used to devise a nonlocal potential that accounts for

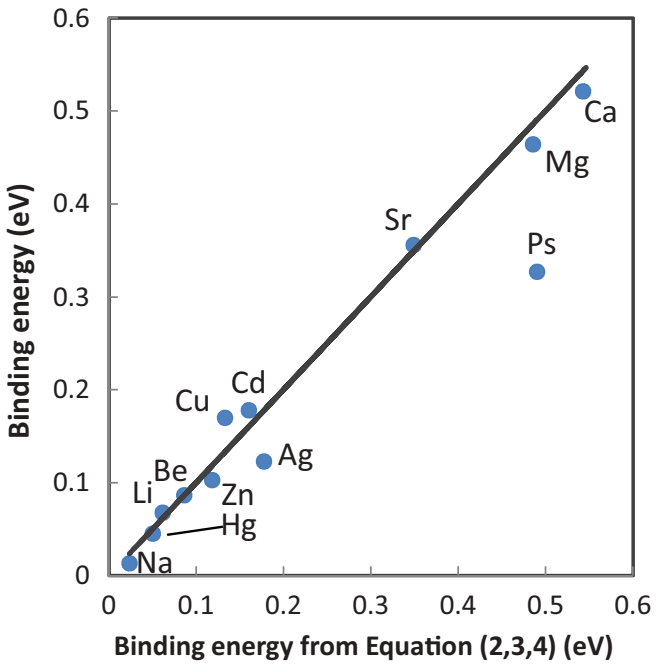

FIG. 3. (Color online) The solid line is the binding energy calculated from the best-fit equation [Eq. (4)]. The solid circles are binding energies from the literature. Ps was not used in the fit but is shown here for reference purposes.

the long-range positron-induced polarization effects discussed above but not the effects of virtual positronium formation. The latter is accounted for approximately and empirically by multiplying the nonlocal potential by the factor 2. Binding energies are predicted for several atoms, mostly transition metals, with ionization potentials greater than about 7.5 eV; the method does not seem to be applicable to atoms with smaller V_is. The results of Dzuba *et al.* are consistent with our work, with only two exceptions: Sn and Pt. These authors ignore relativistic effects and do not provide uncertainties in their predictions. Nevertheless, their predictions for atoms with open *d* subshells are at least as authoritative as our own, and we include them in Table IV for comparison.

We have no data on positron binding to atoms with open *d* and *f* subshells, so our predictions for these atoms are less authoritative. No atom that has unpaired *p* electrons is known to bind a positron, but we predict binding for the entire boron family; for the carbon family, except for C itself; and for the heaviest members of the nitrogen and oxygen families. Good calculations for e^+B,e^+Al, and e^+Si would be valuable tests of our predictions.

Relativistic effects cannot be ignored for atoms with atomic numbers greater than about 30. Dzuba *et al.* [20] compare e^+Ag and e^+Au with nonrelativistic and relativistic calculations that are otherwise comparable. They find that relativistic effects lower the binding energies of e^+Ag by about 0.020 eV and of e^+Au by over 10 times that amount, which is larger than the calculated binding energy in the nonrelativistic approximation.

One might wonder to what extent Eq. (4) might apply to nearly spherical nonpolar molecules, such as methane and neopentane, and to homonuclear diatomics. We computed with Eq. (4) and found no indication of binding for any of CH_4, neo-C_5H_{12}, H_2, O_2, N_2, F_2, Cl_2, or Br_2. Equation (4), on the other hand, gives for C_{60}, by virtue of its enormous polarizability (550–600 Å^3), an equally enormous binding energy for the positron, ∼40 eV. This figure should be treated with great skepticism, however, since it results from an extrapolation far outside the parameter region used for the fit [Eq. (4)].

TABLE III. Equation (4) for known nonbinding atoms and Hg.

Atoms	V_i (eV)	α (Å^3)	γ^2 (eV^2)
H	13.5984	0.6668(5)	−1.65
Rb	4.1771	46.83(5)	−1.32
Cs	3.8939	59.42(5)	−2.22
N	14.5341	1.13(5)	−1.44
F	17.4228	0.548(5)	−2.34
Cl	12.9676	2.159(5)	−0.88
He	24.5874	0.2049(5)	−4.43
Ne	21.5645	0.3957(10)	−3.52
Ar	15.7596	1.640(2)	−1.65
Kr	13.9996	2.5303(2)	−1.05
Xe	12.1298	4.0099(2)	−0.43
Au	9.2255	5.35(10)	−0.15
Hg	10.4375	5.098(10)	0.04

TABLE II. Data and results. The error is the difference between the present work and literature values of *E*. The tolerance is the sum of the uncertainties of the present work and literature values. The predictions of Li, Sr, Ca, Cu, Be, and Zn are within our tolerances.

			E (eV)			
Atoms	V_i (eV)	α (Å^3)	Present work	Literature values	Error	Tolerance
Na	5.1391	23.6(5)	0.023(8)	0.0129(5)	0.0101	0.0085
Li	5.3917	24.3(5)	0.0617(61)	0.0675(3)	−0.0058	0.0064
Sr	5.6949	27.6(22)	0.349(14)	0.356(13)	−0.007	0.027
Ca	6.1132	22.8(8)	0.543(22)	0.521(10)	0.022	0.032
Ag	7.5762	7.2(2)	0.177(6)	0.123(16)	0.054	0.022
Mg	7.6462	10.6(5)	0.486(12)	0.464(6)	0.022	0.018
Cu	7.7264	6.9(5)	0.135(21)	0.170(15)	−0.035	0.036
Cd	8.9938	7.2(2)	0.159(6)	0.178(4)	−0.019	0.01
Be	9.3227	5.6(1)	0.0858(28)	0.0860(3)	−0.0002	0.0031
Zn	9.3942	7.1(5)	0.118(20)	0.103(2)	0.015	0.022

TABLE IV. All other atoms up to Bi. The energies of the present work are calculated by Eqs. (1)–(4). The uncertainties in the predicted binding energies are from uncertainties in polarizabilities. We calculate uncertainties of the Es from the largest and smallest values of α. We also include the predictions of Ref. [33].

					E (eV)	
Atomic number	Atom	V_i (eV)	α (Å^3)	γ^2 (eV^2)	Present work	Ref. [33]
5	B	8.298	3.03(5)	0.2404	0.16(1)	
6	C	11.2603	1.76(5)	−0.5274	Unbound	
8	O	13.6181	0.802(5)	−1.2569	Unbound	
13	Al	5.9858	6.8(1)	0.7033	0.54(2)	
14	Si	8.1517	5.38(5)	0.3815	0.25(1)	
15	P	10.4867	3.63(5)	−0.1517	Unbound	
16	S	10.36	2.9(1)	−0.2000	Unbound	
21	Sc	6.5615	17.8(1)	0.7382	0.75(2)	
22	Ti	6.8281	14.6(1)	0.7264	0.84(3)	
23	V	6.7462	12.4(1)	0.6907	0.81(3)	
24	Cr	6.7665	11.6(2)	0.3151	0.54(8)	
25	Mn	7.434	9.4(1)	0.6111	0.53(3)	
26	Fe	7.9024	8.4(1)	0.5437	0.37(3)	0.28
27	Co	7.881	7.5(1)	0.5088	0.36(3)	0.26
28	Ni	7.6398	6.8(1)	0.5087	0.42(3)	0.24
31	Ga	5.9993	8.12(5)	0.6964	0.54(1)	
32	Ge	7.8994	6.07(12)	0.4481	0.33(3)	
33	As	9.7886	4.31(5)	0.0415	0.01(1)	
34	Se	9.7524	3.77(5)	0.0019	0.001(9)	
39	Y	6.2173	22.7(79)	0.6944	0.6(19)	
40	Zr	6.6339	17.9(45)	0.7497	0.8(11)	
41	Nb	6.7589	15.7(39)	0.3726	0.6(14)	
42	Mo	7.0924	12.8(1)	0.3402	0.45(4)	
43	Tc	7.28	11.4(1)	0.6725	0.62(4)	0.46
44	Ru	7.3605	9.6(24)	0.2563	0.30(95)	0.21
45	Rh	7.4589	8.6(22)	0.2206	0.24(86)	0.20
46	Pd	8.3369	4.8(12)	−0.4056	Unbound	
49	In	5.7864	10.2(5)	0.6959	0.48(16)	
50	Sn	7.3439	7.7(5)	0.5686	0.54(1)	0.02
51	Sb	8.6084	6.6(5)	0.3831	0.19(11)	0.05
52	Te	9.0096	5.5(5)	0.2597	0.11(4)	
53	I	10.451	5.35(10)	0.0302	0.01(3)	
56	Ba	5.2117	39.7(5)	0.0460	0.03(1)	
57	La	5.5769	31.1(78)	0.4096	0.3(16)	
58	Ce	5.5387	29.6(74)	0.4145	0.3(16)	
59	Pr	5.473	28.2(70)	0.4097	0.3(15)	
60	Nd	5.525	31.4(78)	0.3811	0.3(17)	
61	Pm	5.582	30.1(75)	0.4259	0.3(16)	
62	Sm	5.6437	28.8(72)	0.4690	0.3(16)	
63	Eu	5.6704	27.7(69)	0.4928	0.4(15)	
64	Gd	6.1498	23.5(59)	0.6765	0.6(14)	
65	Tb	5.8638	25.5(64)	0.5821	0.4(14)	
66	Dy	5.9389	24.5(61)	0.6121	0.5(14)	
67	Ho	6.0215	23.6(59)	0.6403	0.5(14)	
68	Er	6.1077	22.7(57)	0.6659	0.5(15)	
69	Tm	6.1843	21.8(55)	0.6855	0.6(12)	
70	Yb	6.2542	21(53)	0.7005	0.6(12)	
71	Lu	5.4259	21.9(55)	0.5026	0.2(11)	
72	Hf	6.8251	16.2(41)	0.7512	0.8(10)	
73	Ta	7.5496	13.1(33)	0.7260	0.6(8)	0.45
74	W	7.864	11.1(28)	0.6555	0.4(7)	0.46
75	Re	7.8335	9.7(5)	0.6006	0.42(12)	
76	Os	8.4382	8.5(21)	0.5064	0.3(5)	0.47
77	Ir	8.967	7.6(19)	0.4057	0.2(4)	0.46
78	Pt	8.9588	6.5(16)	−0.0310	Unbound	
81	Tl	6.1082	7.6(5)	0.6878	0.57(11)	
82	Pb	7.4167	6.8(5)	0.5349	0.50(15)	
83	Bi	7.2855	7.4(5)	0.5663	0.56(15)	

Binding energies of positron-atom and positronium-atom bound states
(electron volts)

0 Ps 0.3260 0.4355																	
1 H X 1.0547																	2 He X
3 Li 0.0675 0.336	4 Be 0.0860 X		5 B (0.16)	6 C (X) 0.486	7 N X X	8 O (X) 0.796	9 F X 2.81	10 Ne X
11 Na 0.0129 0.229	12 Mg 0.464 X		13 Al (0.54)	14 Si (0.25)	15 P (X)	16 S (X)	17 Cl X 2.35	18 Ar X
19 K X 0.139	20 Ca 0.521 X	*	31 Ga (0.54)	32 Ge (0.33)	33 As (?)	34 Se (?)	35 Br X 2.06	36 Kr X
37 Rb X	38 Sr 0.356 X	*	49 In (0.26)	50 Sn (0.54)	51 Sb (0.19)	52 Te (0.11)	53 I (?) 1.71	54 Xe X
55 Cs X	56 Ba (0.03)	*	81 Tl (0.57)	82 Pb (0.50)	83 Bi (0.56)			

*	21 Sc (0.75)	22 Ti (0.84)	23 V (0.81)	24 Cr (0.54)	25 Mn (0.53)	26 Fe (0.37)	27 Co (0.36)	28 Ni (0.42)	29 Cu 0.170 0.423	30 Zn 0.103
*	39 Y (?)	40 Zr (?)	41 Nb (?)	42 Mo (0.46)	43 Tc (0.62)	44 Ru (?)	45 Rh (?)	46 Pd X	47 Ag 0.123	48 Cd 0.178

*	57 La (?)	58 Ce (?)	59 Pr (?)	60 Nd (?)	61 Pm (?)	62 Sm (?)	63 Eu (?)	64 Gd (?)	65 Tb (?)	66 Dy (?)	67 Ho (?)	68 Er (?)
	69 Tm (?)	70 Yb (?)	71 Lu (?)	72 Hf (?)	73 Ta (?)	74 W (?)	75 Re (0.42)	76 Os (?)	77 Ir (?)	78 Pt (X)	79 Au X	80 Hg 0.045

e+ only	32
Ps only	8
both	4

FIG. 4. (Color online) Figure 1 with our predictions added (in parentheses). Positron binding energies for atoms with uncertainties larger than our predicted values are unknown and are indicated with question marks.

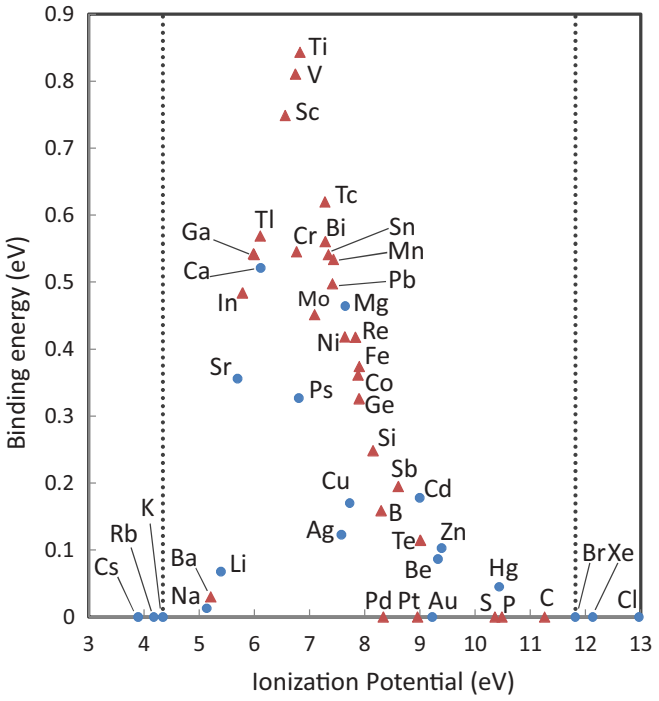

FIG. 5. (Color online) Bonding region of Fig. 2(a), with our predictions added (triangles). The cusp in the binding energy at 6.803 eV is evident. All the predicted binding atoms are in the range of V_is of K and Br.

One might apply a method similar to the one presented here to predict positronium binding to neutral atoms. This is inherently more difficult owing to the unavoidable effects of exclusion that attends the addition of the electron in Ps into a system of atomic electrons.

V. SUMMARY

We have studied the relationship between e^+A binding energies and atomic physical properties using all the available data. We can get good results with the parameters V_i,α, and number of valence s electrons, and we predict binding energies for 23 other atoms. The largest predicted binding energy, 0.84 eV for Ti, is a reflection of the maximum mixing of the structures $\{e^+A\}$ and $\{\mathrm{Ps}A^+\}$ at the crossover point. Positronic titanium, e^+Ti, with five light particles outside its core, is well within reach of present-day high-level codes.

Measurements of positron-atom binding energies are possible with current laboratory technology [8,33,35–37]. We hope the present work will provide motivation to carry out such experiments.

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