cubic ellipsoid nucleus - atomic physics - part 2: the ionization energy

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Abstract

This research explains and calculates the atomic first ionization energy and combines it with the ellipsoid nuclear model [10].
According to the ellipsoid nuclear model, the nucleus consists of nuclear shells that correlate with the atomic shells (unlike the common nuclear shell model); based on this assumption and the former article regarding the atomic radius [11], we get the following results:

- The protons have no effect on the electrons beyond their correlated atomic shell.
- Moreover possibly the protons only affect the electrons that correlate with their shell.
- A physical theoretical atomic ionization energy function was constructed to meet these requirements.
- The nuclear structure determines the atomic shape and the electronic shielding; this explains the variation of the atomic ionization energy from the calculated value and links between the nuclear and atomic structure.

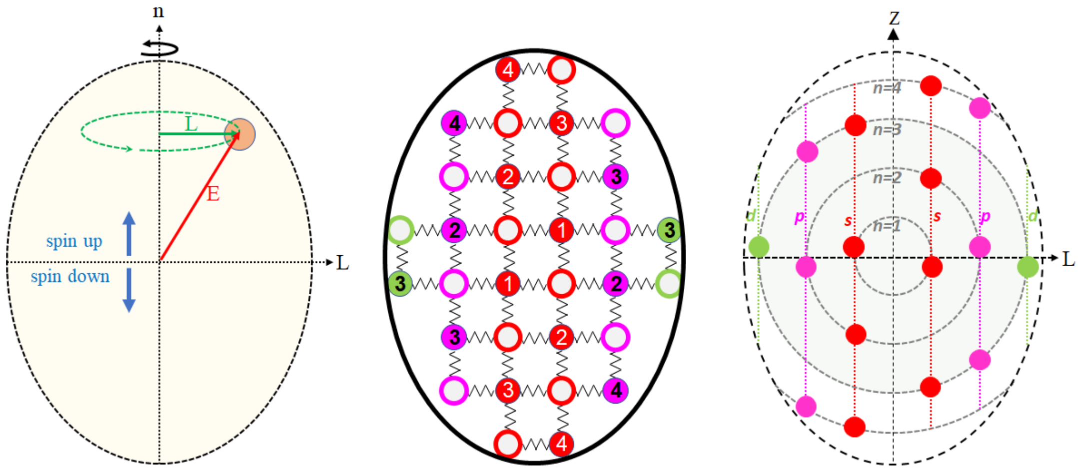
Content

The model at a glance

According to the model these are the shape and properties of the nucleus:

- the nucleus has an ellipsoid shape.
- the nucleon bonds build a cubic system.
- protons are connected to neutrons (**p-n**).
- neutrons are connected mainly to protons.
- the protons are populated and organized in shells in the nucleus in analogy to those of the electrons in the atom.
- the energy layers (principal quantum number **n**) grow with the distance from the origin.
- the perpendicular distance from the **z**-axis in the **x-y**-plane reflects the angular momentum (**L**, sub-orbitals).
- the upper half of the ellipsoid is referred to as spin-up and the lower part as spin-down.
- the nucleus possibly rotates around its **z**-axis.

The following drawings describe the idea via cross sections in the **x-z**-plane of the nucleus.

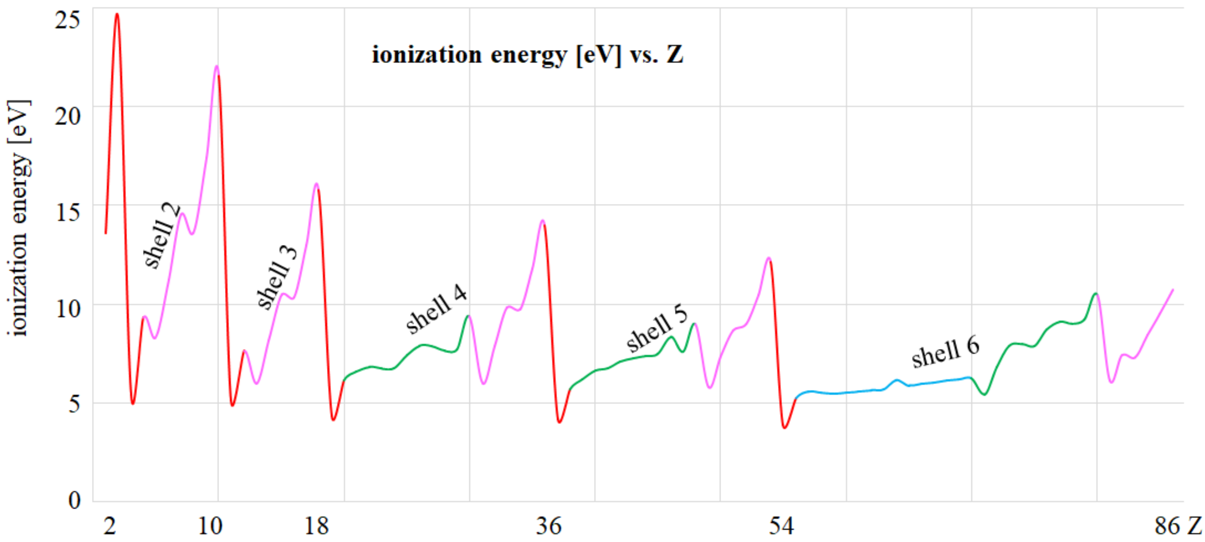


1: a nucleon in the nucleus *2: the bonds between the nucleons* *3: the energy levels of the nucleus*

1. a nucleon (**circle**) is observed inside the ellipsoid (dashed line) that encloses the nucleons and schematically defines the nuclear surface:
   - the distance from the origin represents its energy **E**.
   - the distance from the **z**-axis depicts it angular momentum **L**.
   - the nucleons in the upper half have spin-up, and in the lower one spin-down.
2. the bonds between the nucleons are shown for visibility as springs.
   - **protons**: full circles of the **s**, **p** and **d** sub-orbitals. **neutrons**: hollow circles.
3. the circles of equal energy states **n** in the ellipsoid.
   - the lines mark the development of the **s**, **p** and **d** sub-orbitals along the **z**-axis.
   - the **s** line crosses all **n** circles from 1 to 4 (**s1** to **s4**).
   - the **p** line begins by **n**=2 and reaches till **n**=4 (**p2** to **p4**).
   - the **d** line begins by **n**=3 and reaches the ellipsoid border, before it reaches the **n**=4 circle, and therefore there are no **d4** states at this stage (only **d3**).

Introduction

The following graph shows the experimental data of the atomic first ionization energy of the elements as a function of the atomic number.



atomic first ionization energy vs. atomic number Z [1]; sub-orbitals: ***S***, ***P***, ***D***, ***F***

The atomic first ionization energy shows the following pattern:

- While moving from one row of the periodic table to the next one, the ionization energy decreases.
- Along a row of the periodic table the ionization energy increases.

In this research we try to explain and calculate these phenomena and connect them to the nuclear model.

The research

Constructing the atomic first ionization energy function

Along this work we use the results gained in the former research regarding the atomic radius [11]; similarly, we want to create an atomic ionization energy function. The function should not only be adjusted mathematically, but also have a physical meaning.
The process we take is not precise, yet it seems to deliver results that are good enough to assess the idea.
It is reminded here again that according to the model, the nuclear and atomic shells correspond to each other, and are as they appear in the periodic system.
We define:

- E_0: offset energy [eV]
- Z: the atomic number of the atom observed.
- $k \in \{1, 2, 3, 4, 5, 6, 7\}$ the current nuclear (and atomic) shell.
- Z_{shell_k}: the number of protons (or electrons) currently in the shell, meaning:
- $Z_{shell_k} = Z - Z_{n.g_{k-1}}$.
- $Z_{n.g_{k-1}}$: the (noble gas) atomic number that closes the last row of the periodic table.
- a: the function slope [eV·m].
- b: shielding coefficient.
- $\exp(n, L)$: shielding exponent (depends on the shell n and the sub-orbital l).

and estimate the energy that the outermost nuclear shell exerts on the outermost atomic shell:

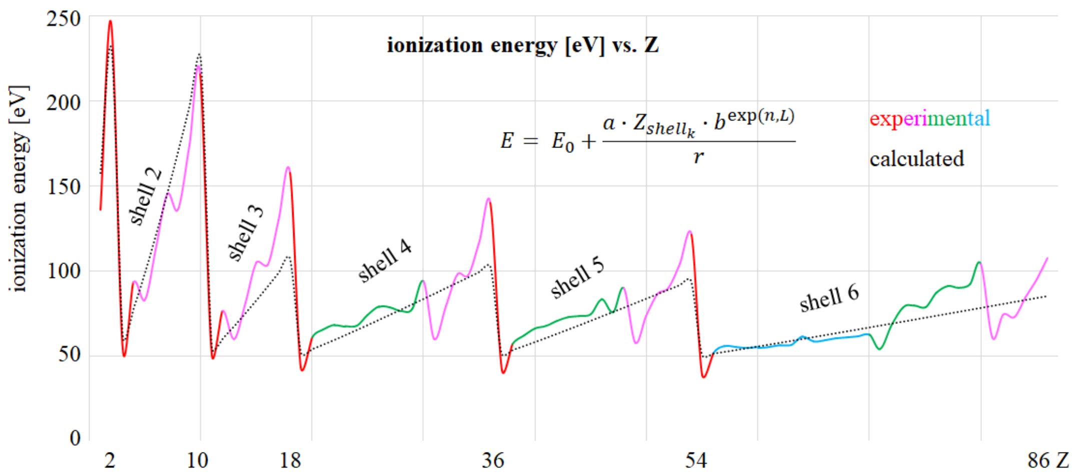
- E decreases with r: $E \sim \frac{1}{r}$
- E grows with Z_{shell_k}: $E \sim Z_{shell}$
- the shielding depends on the atomic shell and sub-orbital.

We therefore try the simplified function: $E = E_0 + \frac{a \cdot Z_{shell_k} \cdot b^{\exp(n,L)}}{r}$
and obtain by tests the values:

- $E_0 \approx 5\ [eV \cdot m]$
- $a \approx 270\ [eV \cdot m]$
- $b \approx 0.5$
- $\exp(n, L) \approx \{0, 1, 2, 3, 3, 4\}$

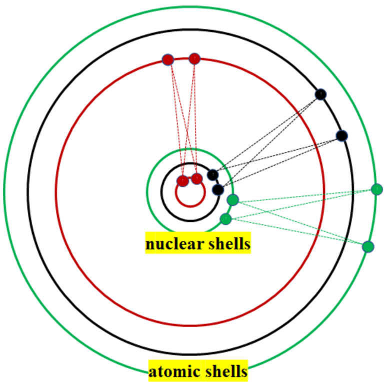
Analysis of the atomic first ionization energy function

The atomic first ionization energy function agrees well with the experiment. The variation seems to be mainly due to shielding effects, that are not taken directly into account in the function.
The shielding is discussed in detail in the appendix.



***graph**: experimental data of the atomic first ionization energy (**S**, **P**, **D**, **F** sub-orbitals); dotted line: calculated function*

According to the atomic first ionization energy function, protons appear to have no effect on electrons beyond their correlated atomic shell; surprisingly it seems that also below their shells they have no influence.
We get to the conclusion, that according to this simplified model at least, each atomic shell is influenced only by its correlated nuclear shell.
The following illustration depicts this idea.



each nuclear shell affects only its corresponding atomic shell

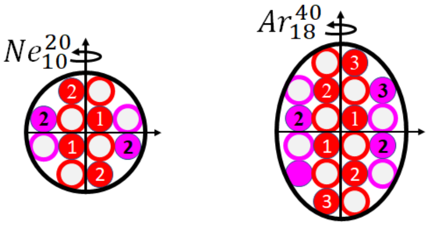
This conclusion agrees with our former research, regarding the atomic radius function [11].

The shielding

The atomic ionization function was defined as:

$$E = E_0 + \frac{a \cdot Z_{shell_k} \cdot b^{\exp\,(n,L)}}{r}$$

The shielding appears in the function as $b^{\exp\,(n,L)}$, where $\exp\,(n,L)$ depends on the sub-orbital and reflects the nuclear structure.
In order to understand the shielding according to the model we observe as an example the nuclei of Neon and Argon; their width remains unchanged while moving from the second row of the periodic table (Neon) to the third row (Argon).
Therefore their screening exponent ($\exp\,(n.L)$) is expected to be quite similar.



the nuclei of Helium and Argon

Similar arguments hold for the fourth and fifth row and for the sixth and seventh row.
The results for the exponents of b are therefore the following:

- the 2'nd and 3'ed row are equal ($exp = 1$)
- the 4'th and 5'th row are equal ($exp = 2$)
- the 6'th and 7'th row are equal ($exp = 3$)

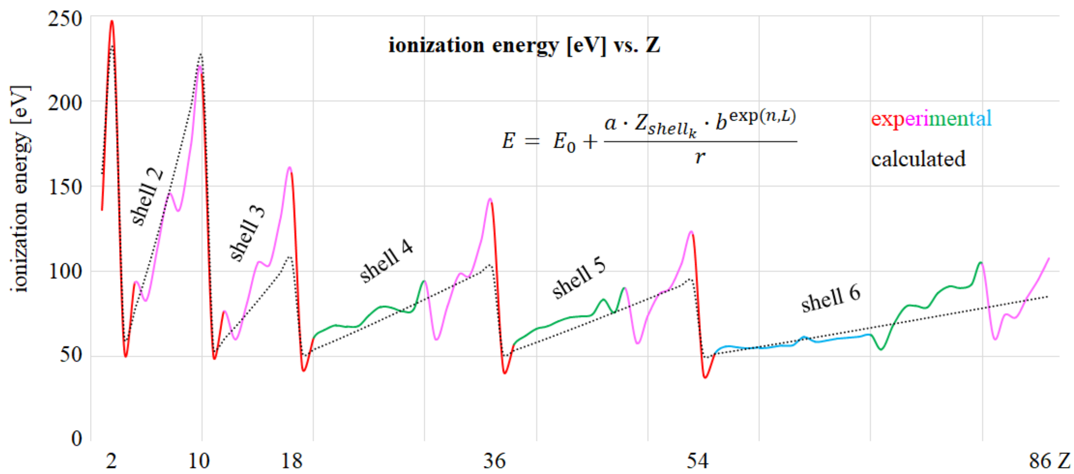
this is a rough estimation that ignores the L dependency of the exponent, but provides results that are good enough for this study, where the discussion is at the level of principles and does not go into precise details.

the influence of the radius on the ionization energy function

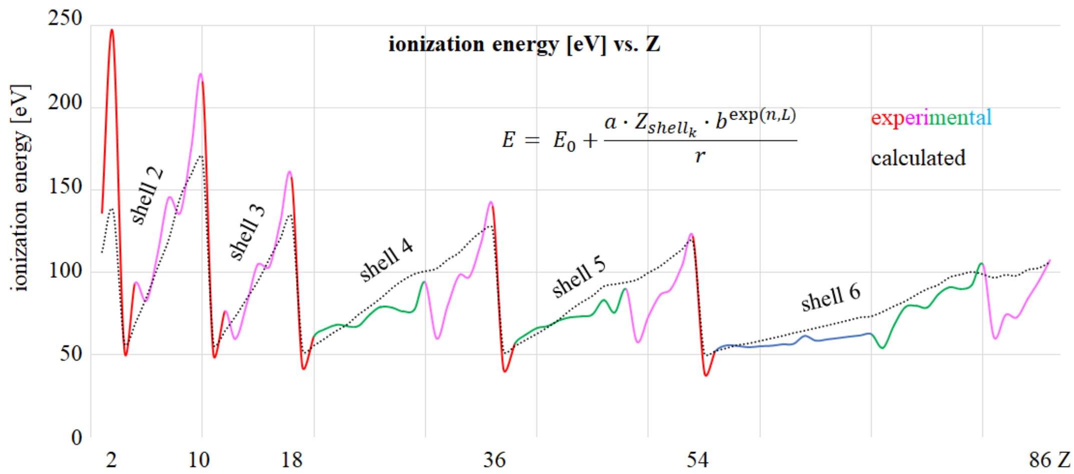
The atomic ionization energy function was defined as: $E = E_0 + \frac{a \cdot Z_{shell_k} \cdot b^{\exp(n,L)}}{r}$

For the atomic radius we could take the calculated values as found in the previous work [11] or use instead the experimental data [4].

The following graphs compare between these two options.



the ionization energy function using the ***calculated*** *values for the atomic radius.*



the ionization energy function using the ***experimental*** *values for the atomic radius.*

We see that although the difference is small, using the experimental data for the radius provides a more accurate graph progression.

Since we want to process the data purely theoretically, we will use the calculated value for the radius in the following graphs.

We remind that the purpose of this work is to discuss the principles and not the exact results, so it sufficient to explain the tendencies of the function as a result of the nuclear ellipsoid theory.

Discussion of the results and conclusions

The focus of this study is neither to define the precise atomic ionization energy function, nor to find its exact parameters, but analyzing the mechanism that governs this process in the light of the cubic ellipsoid nuclear model.
Main statements of this research are:

- The atomic first ionization energy has the form $E \sim \frac{Z_{shell}}{r}$ with:
  Z_{shell} the current number of protons (electrons) in the shell and r the atomic radius.
- The protons have no effect on the electrons beyond their correlated atomic shell.
- More precisely the protons possibly only affect the electrons that correlate with their shell.
- The nuclear structure determines the atomic shape and the amount of shielding that the field of the protons experiences; this explains the variation of the atomic first ionization energy from the calculated values and links between the nuclear and atomic structure.

These results seem to strengthen the ellipsoid nuclear model assumption that the shells of the nucleus and the atom correlate and that the structure of the nucleus determines the shape of the atom.
In the appendix the graph of the atomic first ionization energy is discussed according to the atomic shells and orbitals.

Sources and references

1. *Ionization energy - Wikipedia*
2. *Binding energy - Wikipedia*
3. *Atomic radius - Wikipedia*
4. *Atomic radii of the elements (data page) - Wikipedia*
5. *Rydberg atom - Wikipedia*
6. *Hydrogen atom - Wikipedia*
7. *Electronegativity - Wikipedia*
8. *Electron shell - Wikipedia*
9. *Schalenmodell (Atomphysik) - Wikipedia*
10. *cubic ellipsoid nucleus - part 1 - the model and its mass formula - Ronen Yavor*
11. *cubic ellipsoid nucleus - atomic physics - part 1 - the atomic radius - Ronen Yavor*

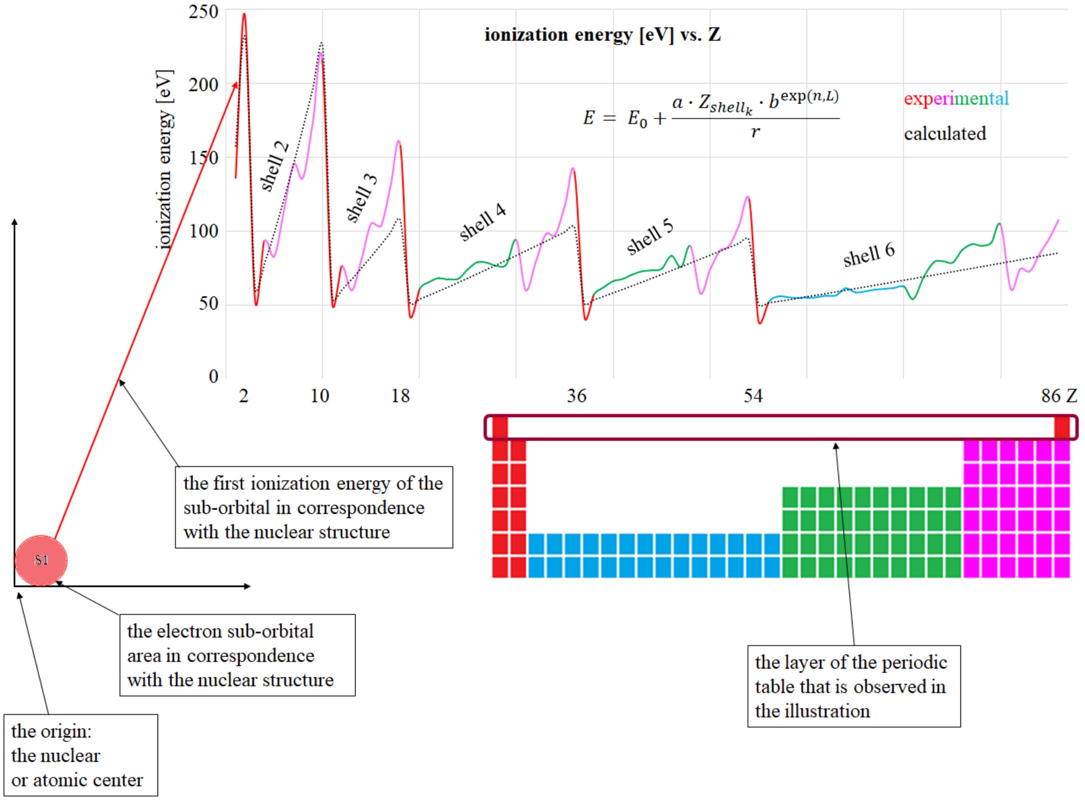
Appendix

graphs

The graphs show the comparison between the measured and the calculated ionization energy. In addition connection to the atom shielding is illustrated.

Atomic ionization energy - row 1

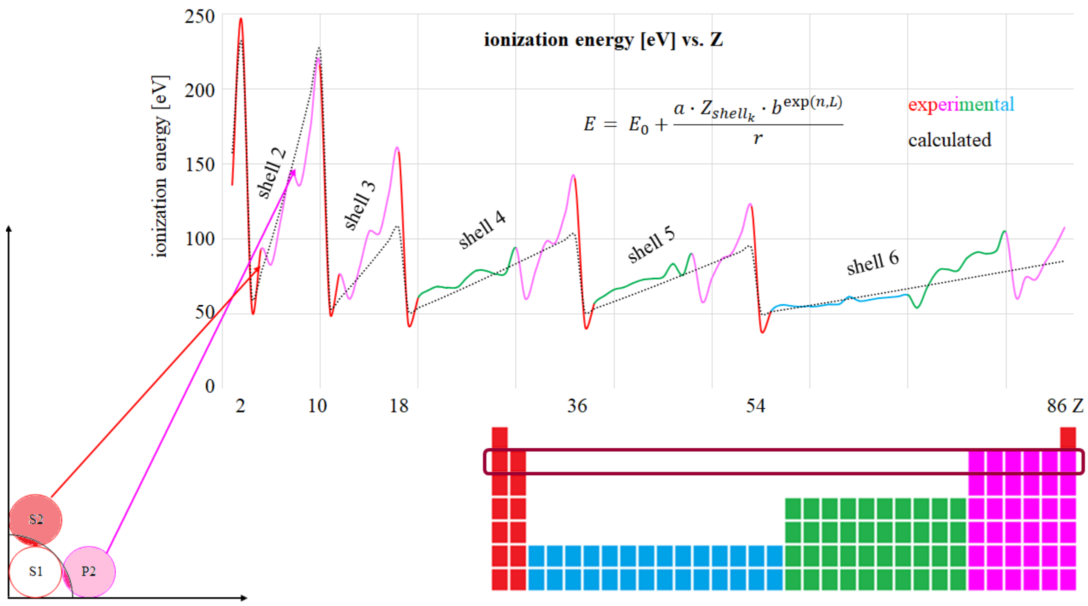
Only the **S**-1 orbital is present. There is no shielding, so the ionization energy is larger than for the following elements.



Atomic ionization energy - row 2

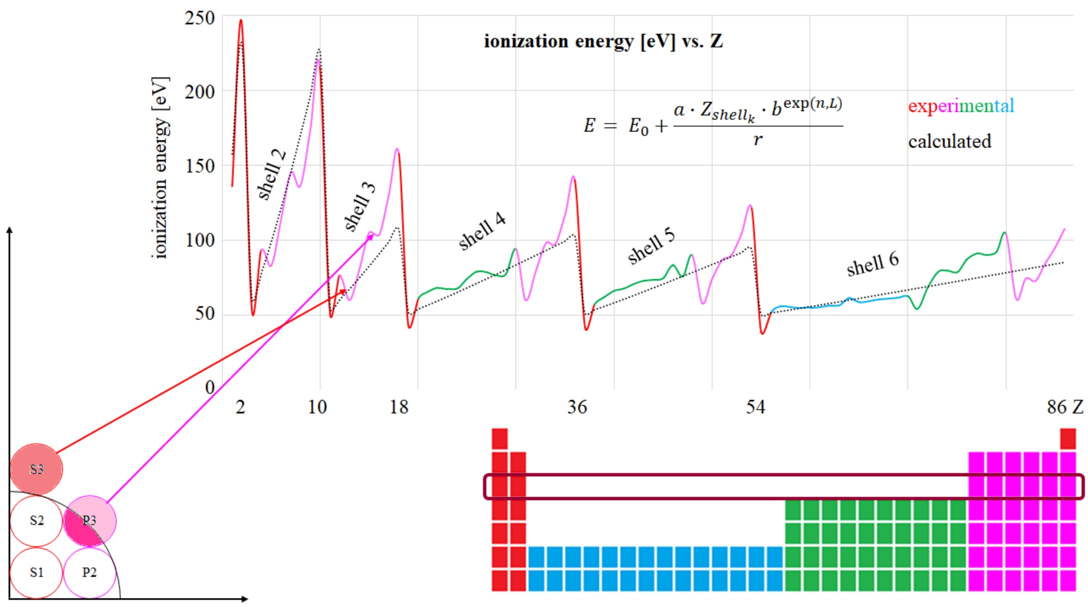
The S-2 and P-2 orbitals are shielded almost equally by the S-1.

The ionization energy grows linearly with the number of protons in the nucleus.



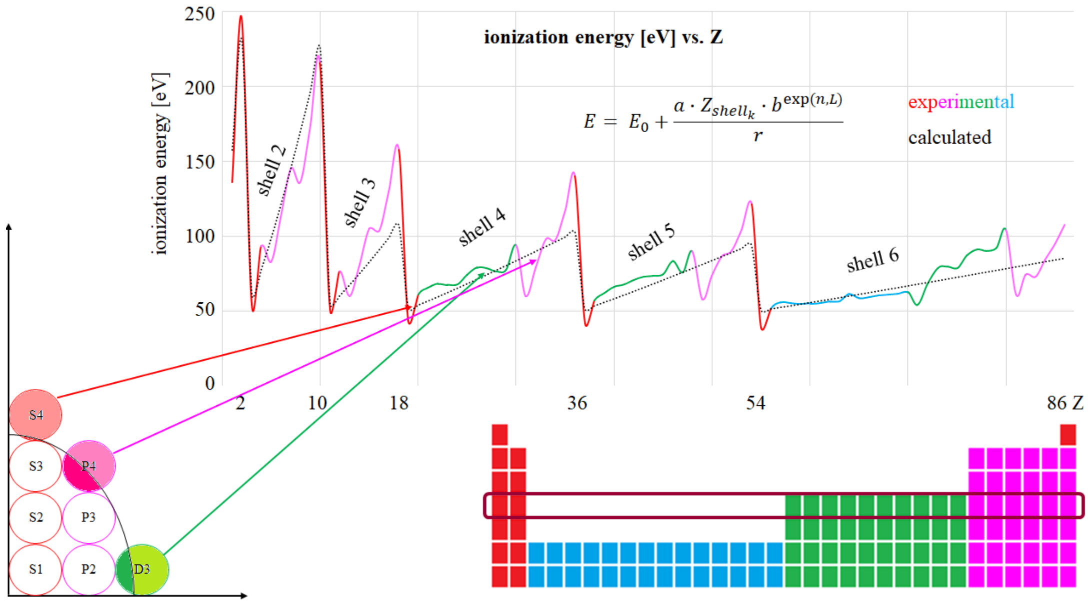
Atomic ionization energy - row 3

The P-3 orbital is less shielded than the S-3 orbital, but the difference is small, so basically the ionization energy grows with the number of protons.



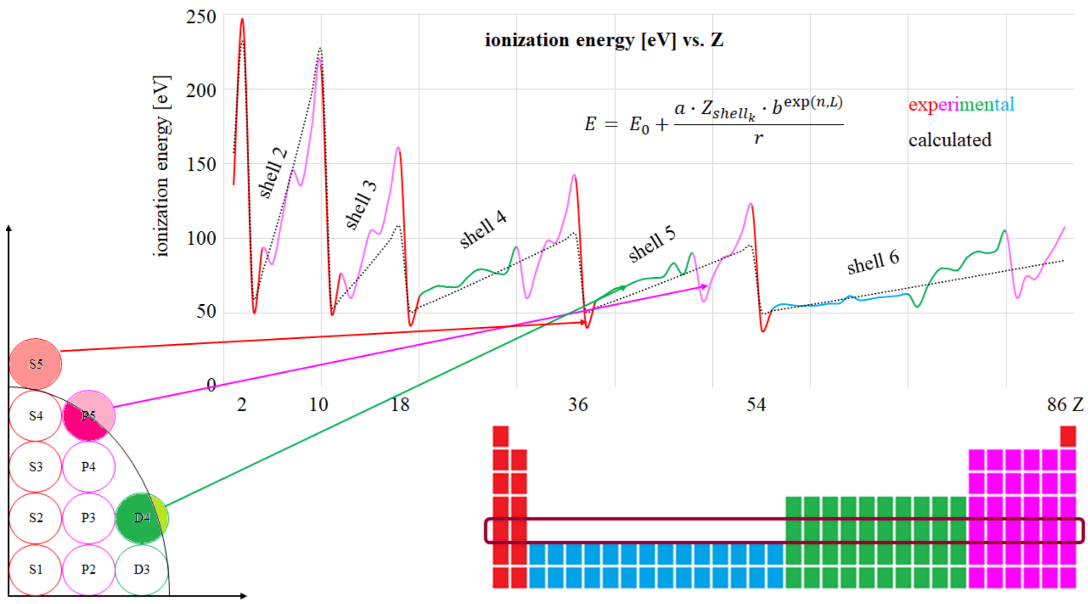
Atomic ionization energy - row 4

The **D**-3 is less shielded and therefore its ionization energy is a bit above the curve.



Atomic ionization energy - row 5

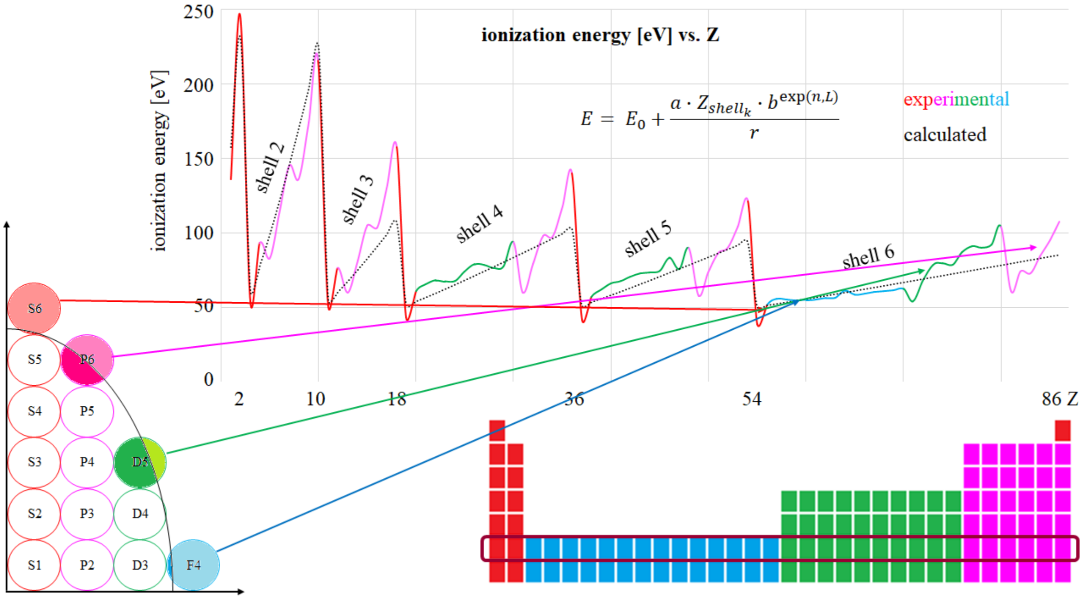
The **D**-4 is less shielded and therefore its ionization energy is a bit above the curve.



Atomic ionization energy - row 6

The **F**-4 orbital is shielded and so lies somewhat nearer to the curve.

The **D**-5 and **P**-6 lie above, because they are less shielded.



data

the ionization energy function was defined as:

$$E = E_0 + \frac{a \cdot Z_{shell_k} \cdot b^{\exp(n,L)}}{r}$$

with:

- E_0: offset energy [eV]
- Z: the atomic number of the atom observed.
- $k \in \{1, 2, 3, 4, 5, 6\}$ the current nuclear (and atomic) shell.
- Z_{shell_k}: the number of protons (or electrons) currently in the shell, meaning:
- $Z_{shell_k} = Z - Z_{n.g_{k-1}}$.
- $Z_{n.g_{k-1}}$: the (noble gas) atomic number that closes the last row of the periodic table.
- a: slope [eV·m]
- b: shielding coefficient.
- $\exp(n, L)$: shielding exponent (depends on the shell n and the sub-orbital l)

and the values:

- $E_0 \approx 5\ [eV \cdot m]$
- $a \approx 270\ [eV \cdot m]$
- $b \approx 0.5$
- $\exp(n, L) \approx \{0, 1, 2, 3, 3, 4\}$

Data Table

The following table contains the data.
Legend:

- exp_{shell}: the shielding exponent (of b)
- *cov. radius*: the covalent atomic radius [4]
- *calc. radius*: the calculated atomic radius [11]
- *ion. Energy [eV]*: the ionization energy in eV []
- *calc ion. Energy [eV] calc. radius*: the calculated ionization energy in eV, using the calculated radius from [11]
- *calc ion. Energy [eV] cov. radius*: the calculated ionization energy in eV, using the covalent radius from [4]

symbol	Z	$Z_{n.g}$	Z_{shell}	sub orbital	exp_{shell}	calc radius	calc E [eV]	Ionization Energy [eV]
H	1	1	1	s	0	25	15.8	13.6
He	2	1	2	s	0	30	23.0	24.6
Li	3	2	1	s	1	120	6.1	5.4
Be	4	2	2	s	1	94	7.9	9.3
B	5	2	3	p	1	82	9.9	8.3
C	6	2	4	p	1	75	12.2	11.3
N	7	2	5	p	1	70	14.6	14.5
O	8	2	6	p	1	67	17.1	13.6
F	9	2	7	p	1	64	19.8	17.4
Ne	10	2	8	p	1	62	22.5	21.6
Na	11	10	1	s	2	152	5.4	5.1
Mg	12	10	2	s	2	125	6.1	7.6
Al	13	10	3	p	2	114	6.8	6.0
Si	14	10	4	p	2	107	7.5	8.2
P	15	10	5	p	2	102	8.3	10.5
S	16	10	6	p	2	99	9.1	10.4
Cl	17	10	7	p	2	96	9.9	13.0
Ar	18	10	8	p	2	94	10.8	15.8
K	19	18	1	s	3	184	5.2	4.3
Ca	20	18	2	s	3	157	5.4	6.1
Sc	21	18	3	d	3	146	5.7	6.6
Ti	22	18	4	d	3	139	6.0	6.8
V	23	18	5	d	3	134	6.3	6.7
Cr	24	18	6	d	3	130	6.6	6.8
Mn	25	18	7	d	3	128	6.9	7.4
Fe	26	18	8	d	3	125	7.2	7.9
Co	27	18	9	d	3	124	7.5	7.9
Ni	28	18	10	d	3	122	7.8	7.6
Cu	29	18	11	d	3	121	8.1	7.7
Zn	30	18	12	d	3	120	8.4	9.4
Ga	31	18	13	p	3	119	8.7	6.0
Ge	32	18	14	p	3	118	9.0	7.9
As	33	18	15	p	3	117	9.3	9.8
Se	34	18	16	p	3	116	9.6	9.8
Br	35	18	17	p	3	115	10.0	11.8
Kr	36	18	18	p	3	115	10.3	14.0
Rb	37	36	1	s	3	205	5.2	4.2
Sr	38	36	2	s	3	178	5.4	5.7
Y	39	36	3	d	3	167	5.6	6.2
Zr	40	36	4	d	3	160	5.8	6.6
Nb	41	36	5	d	3	155	6.1	6.8
Mo	42	36	6	d	3	152	6.3	7.1
Tc	43	36	7	d	3	149	6.6	7.3
Ru	44	36	8	d	3	147	6.8	7.4
Rh	45	36	9	d	3	145	7.1	7.5
Pd	46	36	10	d	3	143	7.4	8.3
Ag	47	36	11	d	3	142	7.6	7.6
Cd	48	36	12	d	3	141	7.9	9.0

symbol	Z	$Z_{n.g}$	Z_{shell}	sub orbital	exp_{shell}	calc radius	calc E [eV]	Ionization Energy [eV]
In	49	36	13	p	3	140	8.1	5.8
Sn	50	36	14	p	3	139	8.4	7.3
Sb	51	36	15	p	3	138	8.7	8.6
Te	52	36	16	p	3	137	8.9	9.0
I	53	36	17	p	3	137	9.2	10.5
Xe	54	36	18	p	3	136	9.5	12.1
Cs	55	54	1	s	4	226	5.1	3.9
Ba	56	54	2	s	4	200	5.2	5.2
La	57	54	3	f	4	188	5.3	5.6
Ce	58	54	4	f	4	181	5.4	5.5
Pr	59	54	5	f	4	176	5.5	5.5
Nd	60	54	6	f	4	173	5.6	5.5
Pm	61	54	7	f	4	170	5.7	5.6
Sm	62	54	8	f	4	168	5.8	5.6
Eu	63	54	9	f	4	166	5.9	5.7
Gd	64	54	10	f	4	165	6.0	6.2
Tb	65	54	11	f	4	163	6.1	5.9
Dy	66	54	12	f	4	162	6.2	5.9
Ho	67	54	13	f	4	161	6.4	6.0
Er	68	54	14	f	4	160	6.5	6.1
Tm	69	54	15	f	4	159	6.6	6.2
Yb	70	54	16	f	4	159	6.7	6.3
Lu	71	54	17	d	4	158	6.8	5.4
Hf	72	54	18	d	4	157	6.9	6.8
Ta	73	54	19	d	4	157	7.0	7.9
W	74	54	20	d	4	156	7.2	8.0
Re	75	54	21	d	4	156	7.3	7.9
Os	76	54	22	d	4	155	7.4	8.7
Ir	77	54	23	d	4	155	7.5	9.1
Pt	78	54	24	d	4	154	7.6	9.0
Au	79	54	25	d	4	154	7.7	9.2
Hg	80	54	26	d	4	154	7.9	10.4
Tl	81	54	27	p	4	153	8.0	6.1
Pb	82	54	28	p	4	153	8.1	7.4
Bi	83	54	29	p	4	153	8.2	7.3
Po	84	54	30	p	4	152	8.3	8.4
At	85	54	31	p	4	152	8.4	9.5
Rn	86	54	32	p	4	152	8.6	10.7