cubic ellipsoid nuclear model: the atomic covalent radius function

Ronen Yavor

Abstract

This research explains and calculates the atomic covalent radius and combines it with the cubic ellipsoid nuclear model [1].

According to the cubic 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 we get the following outcomes:

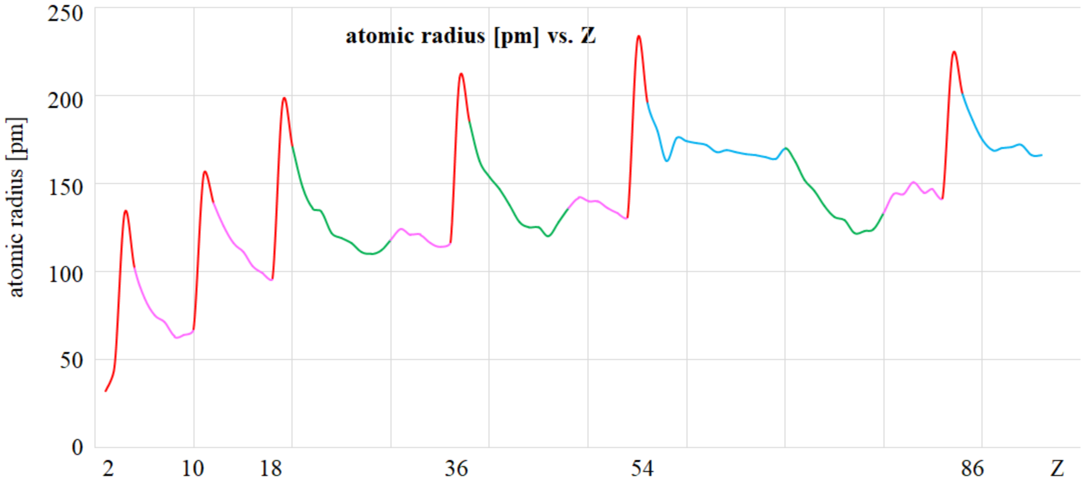
- The protons seem to affect only the electrons of their correlated shell.
- A physical theoretical atomic covalent radius function was constructed to meet this idea.
- The nuclear structure determines the atomic shape and the electronic shielding; this explains the variation of the atomic radius from the calculated value and links between the nuclear and atomic structure.

Remark: by "shell" the electrons or protons of the elements of a common row in the periodic table are meant.

Content

Introduction

The following graph shows the experimental data of the atomic covalent single bond radius as a function of the atomic number [3].



atomic covalent radius vs. atomic number Z (Covalent single bond [3]).
sub-orbitals: ***S***, ***P***, ***D***, ***F***.

The atomic covalent radius shows the following pattern:

- while moving from one row (period) of the periodic table to the next one, the size of the atom grows.
- along a row the size of the atom shrinks.

In this research we try to show how the nuclear geometric structure, according to the cubic ellipsoid model, determines the atomic covalent radius.

Common calculation of the atomic radius

A calculation process of the atomic radius is described in the article of Ghosh and Raka Biswas [4].
The idea is using a Slater-type orbitals as an approximation, that each electron in the multiple electron system has its own one-electron functions.

$$R_{nl}(r) = (2x)^{n+1/2}[(2n)!]^{-1/2}r^{n-1}e^{-xr}$$

with:

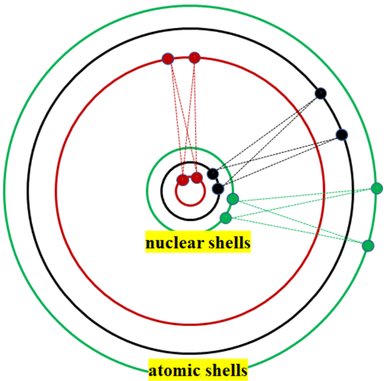
- n: the principal quantum number of the electron
- r: distance from the nucleus
- x: the orbital exponent and given by: $x = \frac{Z-s}{n^*}$
- Z: atomic number
- S: the screening constant
- n^*: the effective principal quantum
- $(Z - s)$ is further identified as effective nuclear charge Z^*

We want to take in this research a simpler approach.
The aim is not to reach a best fit of the electronic functions, but to learn more about the mechanism that governs the atom.

The research

How to approach the atomic covalent radius calculation

We use the assumption of our former study [1] that the nuclear shells correlate with the atomic shells and make the following thought experiment as a preparation for the development of an atomic radius function:
The noble gases have a very weak interaction with other atoms, so we assume that closed nuclear shells don't influence beyond their corresponding atomic shells.
From the graph of the atomic covalent radius it seems, that the radius of each row is above the value of the radius that closes the last row before it.
We make therefore an additional assumption that each nuclear shell influences only the electrons above the last closed shell.
As a result we get to the assumption, that each nuclear shell influences only its corresponding atomic shell.
Remark: we note that the expression "shell" refers here actually to the "row" in the periodic table, because the shells usually refer to the division according to the atomic energy levels or principal quantum number and these are different.
We get to the conclusion, that, at least according to this simplified model, each atomic shell is influenced only by its correlated nuclear shell.
The following illustration depicts schematically this idea.



each nuclear shell affects only its corresponding atomic shell

Remark: at this stage we actually ignore shielding effects.

Constructing the atomic covalent radius function

We use the last section to create the atomic covalent radius function.
Following definitions are used:

- 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.
- r_{shell_k}: the atomic radius of the full atomic shell k.

We estimate the force of the outermost nuclear shell on the outermost atomic shell.
Along a specific row (or shell) we suspect that the force that the nucleus acts on the electrons grows with the number of protons in the shell:
$F(Z) \sim Z_{shell_k}$.
We also expect the following connection between the force and the radius:
$F \sim \frac{1}{r_{shell_k}^2}$
which leads to $r_{shell_k} \sim \frac{1}{\sqrt{F}}$ or $r_{shell_k} \sim \frac{1}{\sqrt{Z_{shell_k}}}$ meaning:
$r_{shell_k} = \frac{a}{\sqrt{Z_{shell_k}}} + constant$.
We thus try the following simplified atomic covalent radius formula:
$r(Z) = \frac{a}{\sqrt{Z_{shell_k}}} + r_{shell_{k-1}}$

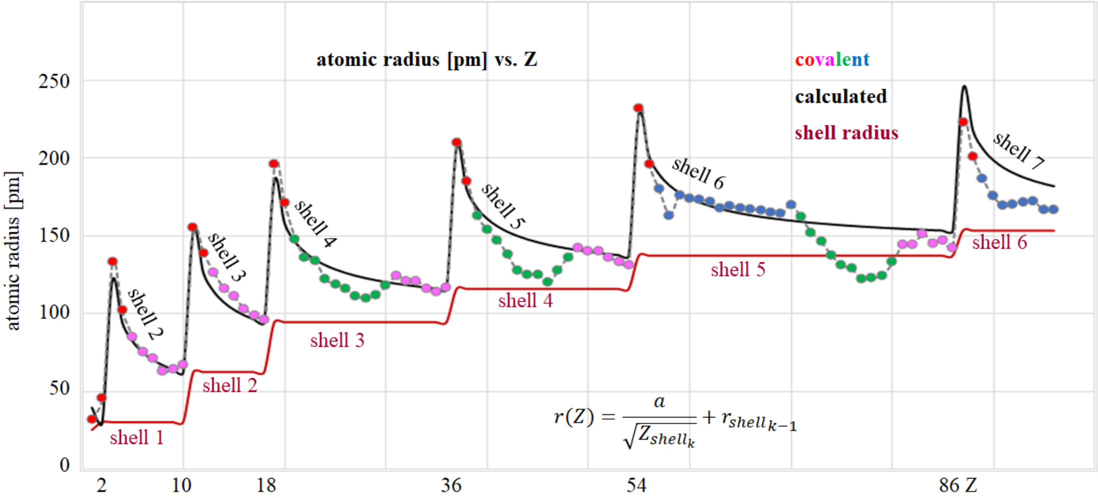
Remark: the function begins from the second row. For the first row we take the experimental data.

Testing the function leads to a rough estimation of its parameters:

- $r_{shell_1} \approx 30\ pm$ this is taken from the experimental data.
- $a \approx 90\ pm$ this is gained via trials.

Analysis of the atomic covalent radius function

The atomic covalent radius function agrees well with the experiment. The variation seems to be mainly due to the various proton positions in the nucleus, that possibly cause shielding effects and are not considered in the function.



***graphs**: experimental data of the covalent radius (**S**, **P**, **D**, **F** sub-orbitals). Data from [3]*
calculations: atomic covalent radius and the radius of the last full shell

According to the atomic covalent radius 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.

This strengthen the model assumption, that the nuclear structure determines the atomic properties; it also justifies the conclusion, that the nuclear shells correlate with the atomic shells.

Discussion of the results and conclusions

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

<u>The atomic covalent radius function</u>

- The atomic covalent radius has the form $r(Z) = \frac{a}{\sqrt{Z_{shell_k}}} + r_{shell_{k-1}}$.
- The protons possibly only affect the electrons that correlate with their shell.
- The nuclear structure determines the amount of shielding that the field of the protons experiences; this explains the variation of the atomic radius 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 nuclear structure determines the atomic properties. The model explains the growth of the atom while moving from one row of the periodic table to the next and the decreasing of the atomic covalent radius along the shell itself.
In the appendix the graph of the atomic radius is shown according to the atomic shells and orbitals.

Sources and references

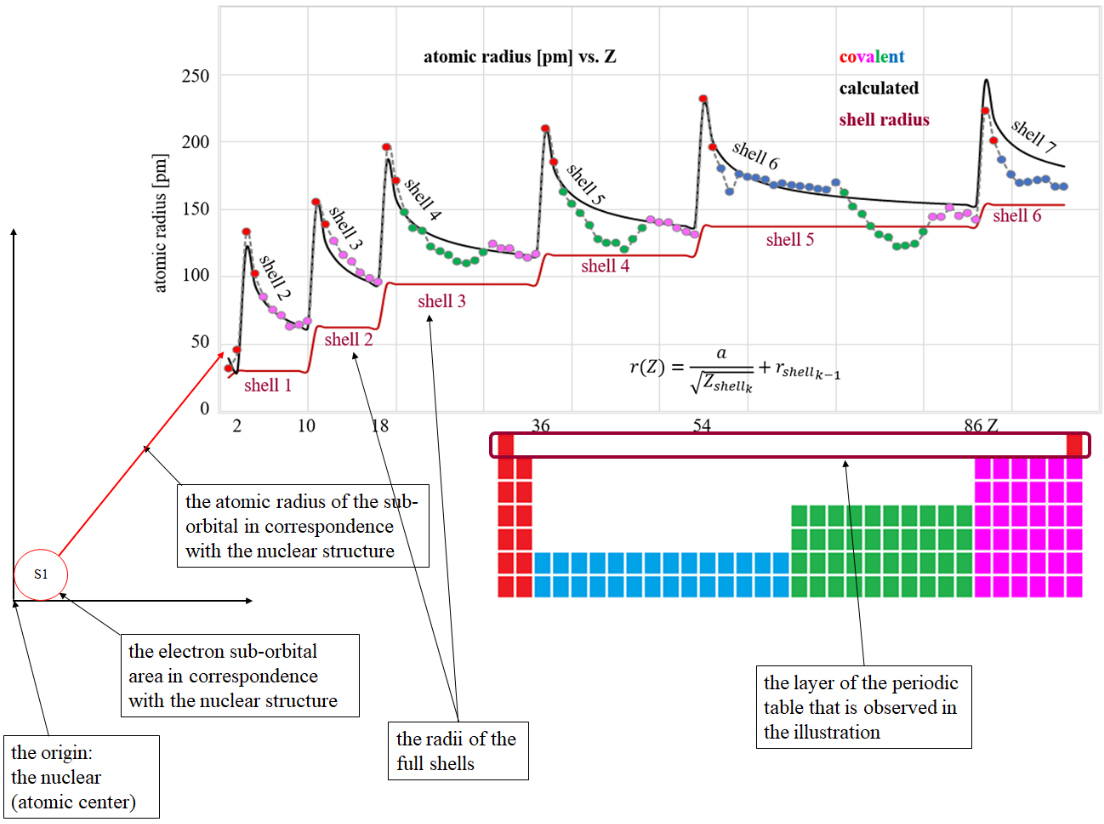
1. *cubic ellipsoid nucleus - part 1 - the model and its mass formula - Ronen Yavor*
2. *Beatriz Cordero, Verónica Gómez, Ana E. Platero-Prats, Marc Revés, Jorge Echeverría, Eduard Cremades, Flavia Barragán and Santiago Alvarez (2008). "Covalent radii revisited". Dalton Trans. (21): 2832–2838*
3. *Pekka Pyykkö, Michiko Atsumi (2009). "Molecular Double-Bond Covalent Radii for Elements Li–E112". Chemistry: A European Journal 15 (46): 12770–12779*
4. *Theoretical Calculation of Absolute Radii of Atoms and Ions. Part 1. The Atomic Radii - Dulal C. Ghosh and Raka Biswas - International Journal of Molecular Sciences*
5. *Atomic radius - Wikipedia*
6. *Atomic radii of the elements (data page) - Wikipedia*
7. *Covalent Radii - libreTexts chemistry*
8. *Rydberg atom - Wikipedia*
9. *Hydrogen atom - Wikipedia*
10. *Ionization energy - Wikipedia*
11. *Ionization Energy in the Periodic Table of Elements - PubChem*
12. *Binding energy - Wikipedia*
13. *van der Waals radius - Wikipedia*
14. *Ionic radius - Wikipedia*
15. *Covalent radius - Wikipedia*
16. *Electron configuration - Wikipedia*
17. *d-block contraction - Wikipedia*
18. *Electronegativity - Wikipedia*
19. *Electron shell - Wikipedia*
20. *Schalenmodell (Atomphysik - German) - Wikipedia*
21. *Core electron - Wikipedia*

Appendix

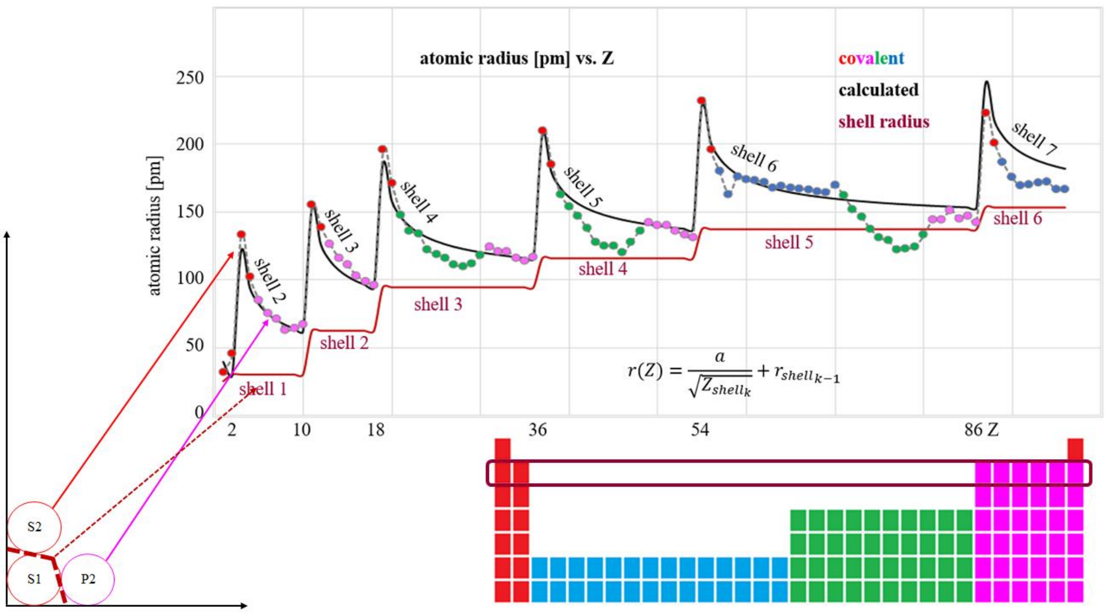
graphs

The following graphs show the atomic covalent radius and the shell radius.

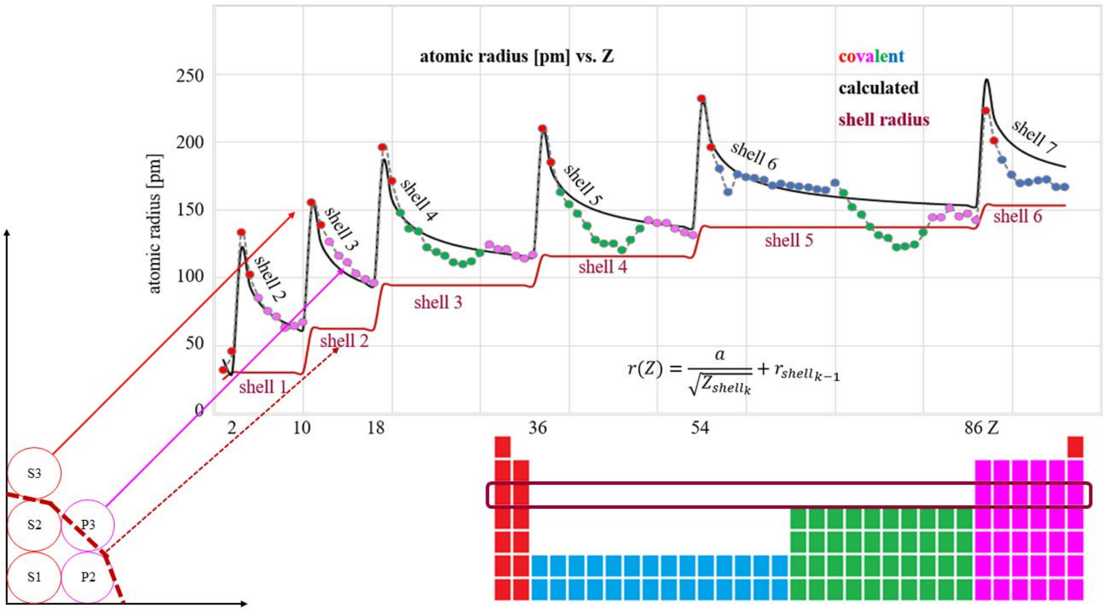
Atomic radius - row (shell) 1



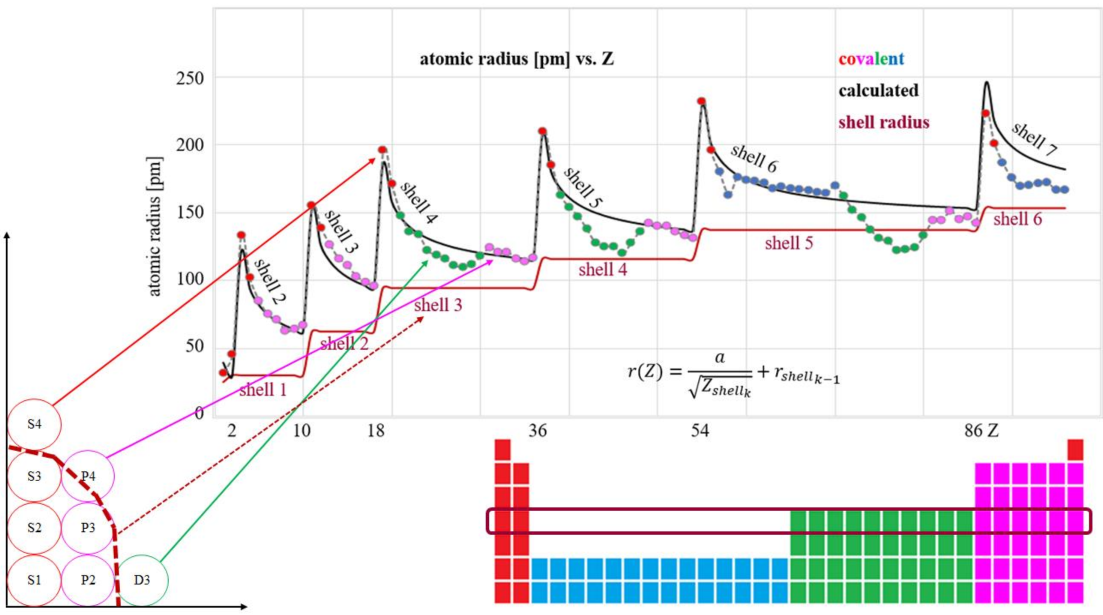
Atomic radius - row 2



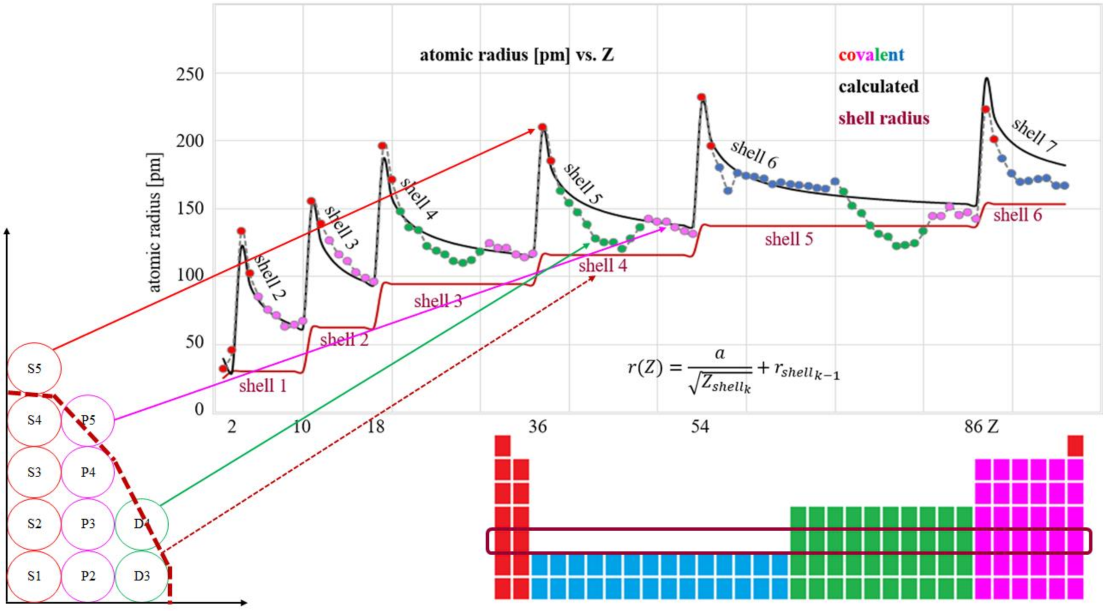
Atomic radius - row 3



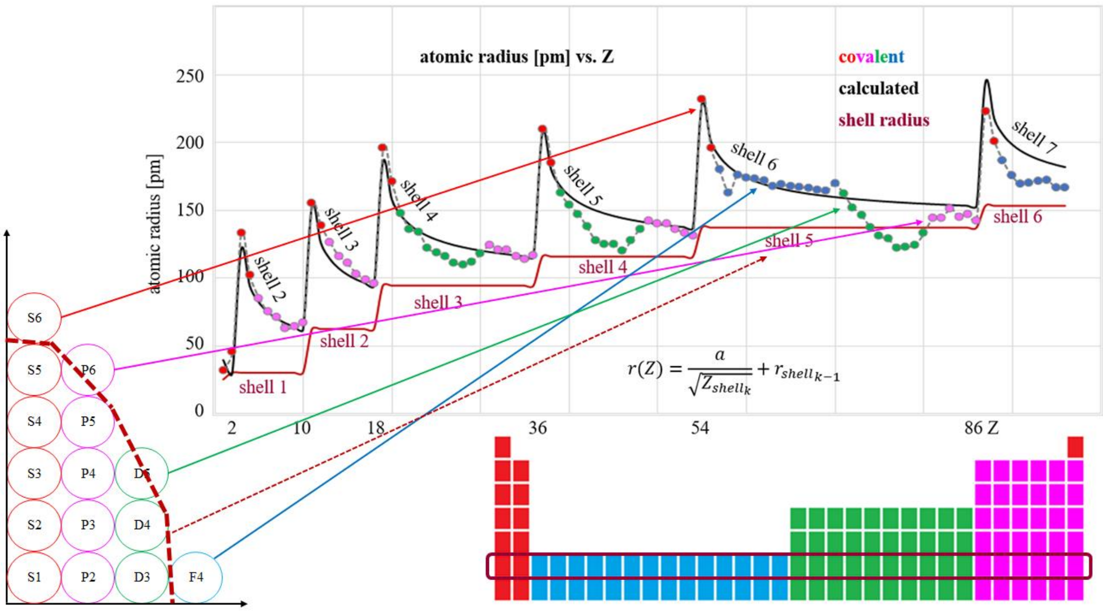
Atomic radius - row 4



Atomic radius - row 5



Atomic radius - row 6



Atomic radius - row 7