Особенности электронного строения и химические свойства сверхтяжелых элементов 7-го и 8-го периодов

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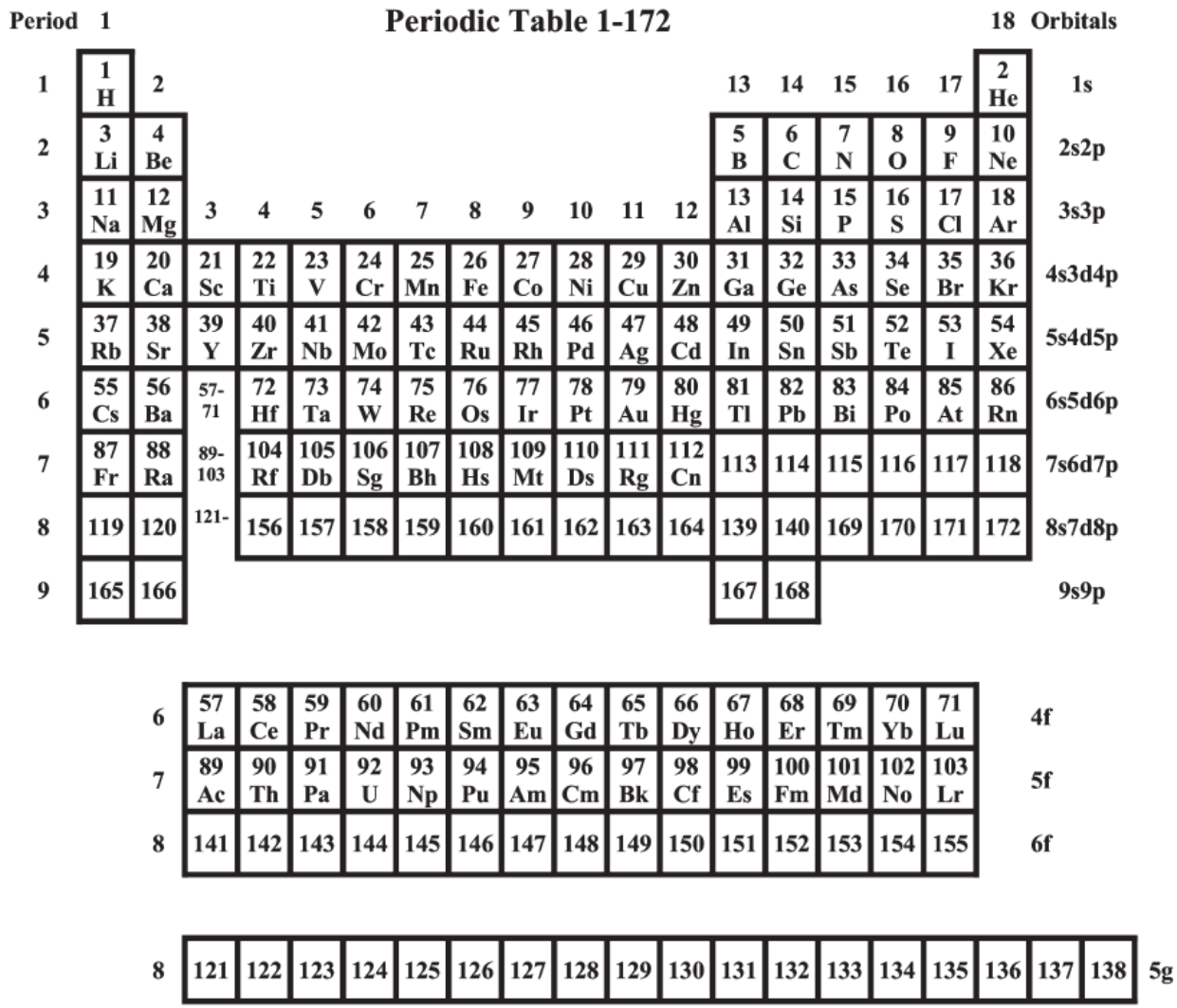
Outline of the Talk

- Introduction
- Ground state electron configurations of superheavy elements (SHE)
- Relativistic effects in the electronic structure of SHE
- Electron density distribution in SHE. Electron localization function (ELF)
- Orbital collapse of the 5g-states
- Summary and Outlook

Introduction. Pyykkö's periodic table



The table is taken from P. Pyykkö Chem. Rev. 112, 371 (2012).

Introduction

In this work, the results of the electronic-structure calculations for a number of super-heavy elements (SHE) of the 7th and 8th periods with atomic numbers Z=111-170 and their lighter homologous are performed [1-3].

- Ground state electron configurations of superheavy elements (SHE)
- Ionization potentials
- Electron affinities
- One-particle electron density
- Root-mean-square radii of the valence states
- Widths of the electron-density distribution of valence shells
- Electron localization functions (ELF)
- Shannon entropy
- Quantum electrodynamics (QED) corrections

1. *M. Y. Kaygorodov et al., Phys. Rev. A 104, 012819 (2021)*
2. *I. I. Tupitsyn et al., Opt. Spectr. 129, 1038 (2021)*
3. *M. Y. Kaygorodov et al., Phys. Rev. A 105, 062805 (2022)*

Introduction. Specific features of electronic structure and chemical properties of super-heavy elements of the 7th and 8th periods

The electronic structure of SHEs is unique in several aspects:

- Strong relativistic effects cause contraction of the s- and p- orbitals
- Spin-orbital splitting of valence p-shells reaches up about 10 eV in Og (Z=118) and about 420 eV for the 7p-orbital and about 75 eV for the 8p-orbital in element with atomic number Z=165.
- As a result, due to the strong relativistic contraction, the radial distribution of the electron density of the valence $7p_{1/2}$-shell of the Og atom starts to overlap with the outer core shells and ELF is close to 0.5 in the valence region.
  In Ref. [1], this effect in Og was interpreted as smearing out the valence electron density distribution and its approaching to the case of the homogeneous electron gas.
- Starting from the Z = 125 element, the 5g-shell with the large angular momentum (l = 4) is occupied with electrons.
- The effective radial potential for the 5g-electron, which includes a large centrifugal repulsive term, has two potential wells which leads to the so-called *orbital collapse*.

[1] *P. Jerabek, B. Schuetrumpf, P. Schwerdtfeger, and W. Nazarewicz, Phys. Rev. Lett. 120, 053001 (2018).*

Introduction. Methods

In our work, we used two independent theoretical calculation methods.

- **Configuration Interaction Dirac-Fock-Sturm method (CI-DFS)**

  At the first step, to obtain the one-electron wave functions for the occupied atomic shells, we use the Dirac-Fock method. Then the DFS orbitals are obtained by solving the DFS equations for the vacant shells. At the last step, the relativistic CI+MBPT method is used to obtain the many-electron wave functions and the total energies.

- **Fock Space Coupled-Cluster method (FS-CC)**

  DIRAC, a relativistic ab initio electronic structure program, Release DIRAC21 (2021), http://www.diracprogram.org

  FS-CC method, in contrast to the one-configuration coupled-cluster method is capable of providing not only the ground-state energy of an N-electron system, but also an important fraction of system's excitation spectrum, including ionization potentials, electron affinities, etc.

- **To evaluate the QED correction we use the model QED operator approach**[1]

[1] *V.M. Shabaev, I.I. Tupitsyn, V.A. Yerokhin, Comput.Phys.Commun. 189, 175 (2015)*

Ground state configurations

For $Z = 126$ the configurations with the *lowest Dirac-Fcok (DF) energy* within the configuration average approximation are

Configuration	$E_{\mathrm{DF}}^{\mathrm{av}}$ [a.u.]
$8p^1 7d^1 6f^2 5g^2$	-66298.183666
$8p^1 6f^3 5g^2$	.183121
$8p^1 6f^4 5g^1$	.168137
$8p^2 6f^2 5g^2$	.146963
$8p^1 7d^2 6f^1 5g^2$	.114149

- $8p^2 6f^2 5g^2$ Mann et al., 1970 (DF)
- $8p^1 7d^1 6f^2 5g^2$ Fricke et al., 1977 (DFS)
- $8p^1 6f^4 5g^1$ Umemoto and Saito, 1997 (DF+PZ SIC)
- $8p^1 6f^3 5g^2$ (0.98) Nefedov et al., 2006 (MCDF)
- $8p^1 7d^1 6f^2 5g^2$ Zhou et al., 2017 (DF)

Ground state configurations

Таблица: Ground state electron configurations

	Core: [Rn] $5f^{14}$	
Z	Conf.	J
111	$6d^9\ 7s^2$	2.5
112	$6d^{10}\ 7s^2$	0.0
113	$6d^{10}\ 7s^2 7p^1$	0.5
114	$6d^{10}\ 7s^2 7p^2$	0.0
118	$6d^{10}\ 7s^2 7p^6$	0.0
119	$6d^{10}\ 7s^2 7p^6 8s^1$	0.5
120	$6d^{10}\ 7s^2 7p^6 8s^2$	0.0

Ground electron configurations

Таблица: Ground state electron configurations

Z	Conf.	J	Ref[1]	Ref[2]
		Core: [Og] $8s^2$		
125	$5g^1 6f^2 7d^1 8p^1$	8.5	$5g^1 6f^3 8p^1$	$5g^1 6f^2 8p^2$
126	$5g^2 6f^2 7d^1 8p^1$	10	$5g^2 6f^2 7d^1 8p^1$	$5g^2 6f^3 8p^1$
127	$5g^3 6f^2 7d^1 8p^1$	13.5	$5g^3 6f^2 8p^2$	$5g^3 6f^2 8p^2$
		Core: [Og] $8s^2\ 8p^2_{1/2}$		
144	$5g^{18} 6f^1 7d^3$	4.0	$5g^{18} 6f^1 7d^3$	$5g^{17} 6f^1 7d^3$
145	$5g^{18} 6f^3 7d^2$	6.5	$5g^{18} 6f^3 7d^2$	$5g^{18} 6f^3 7d^2$
162	$5g^{18} 6f^{14} 7d^8$	4.0	$5g^{18} 6f^{14} 7d^8$	$5g^{18} 6f^{14} 7d^7 9s^1$
163	$5g^{18} 6f^{14} 7d^9$	2.5	$5g^{18} 6f^{14} 7d^9$	$5g^{18} 6f^{14} 7d^8 9s^1$
164	$5g^{18} 6f^{14} 7d^{10}$	0.0	$5g^{18} 6f^{14} 7d^{10}$	$5g^{18} 6f^{14} 7d^9 9s^1$
165	$5g^{18} 6f^{14} 7d^{10} 9s^1$	0.5	$5g^{18} 6f^{14} 5g^{18} 7d^{10} 9s^1$	—
166	$5g^{18} 6f^{14} 7d^{10} 9s^2$	0.0	$5g^{18} 6f^{14} 5g^{18} 7d^{10} 9s^2$	—

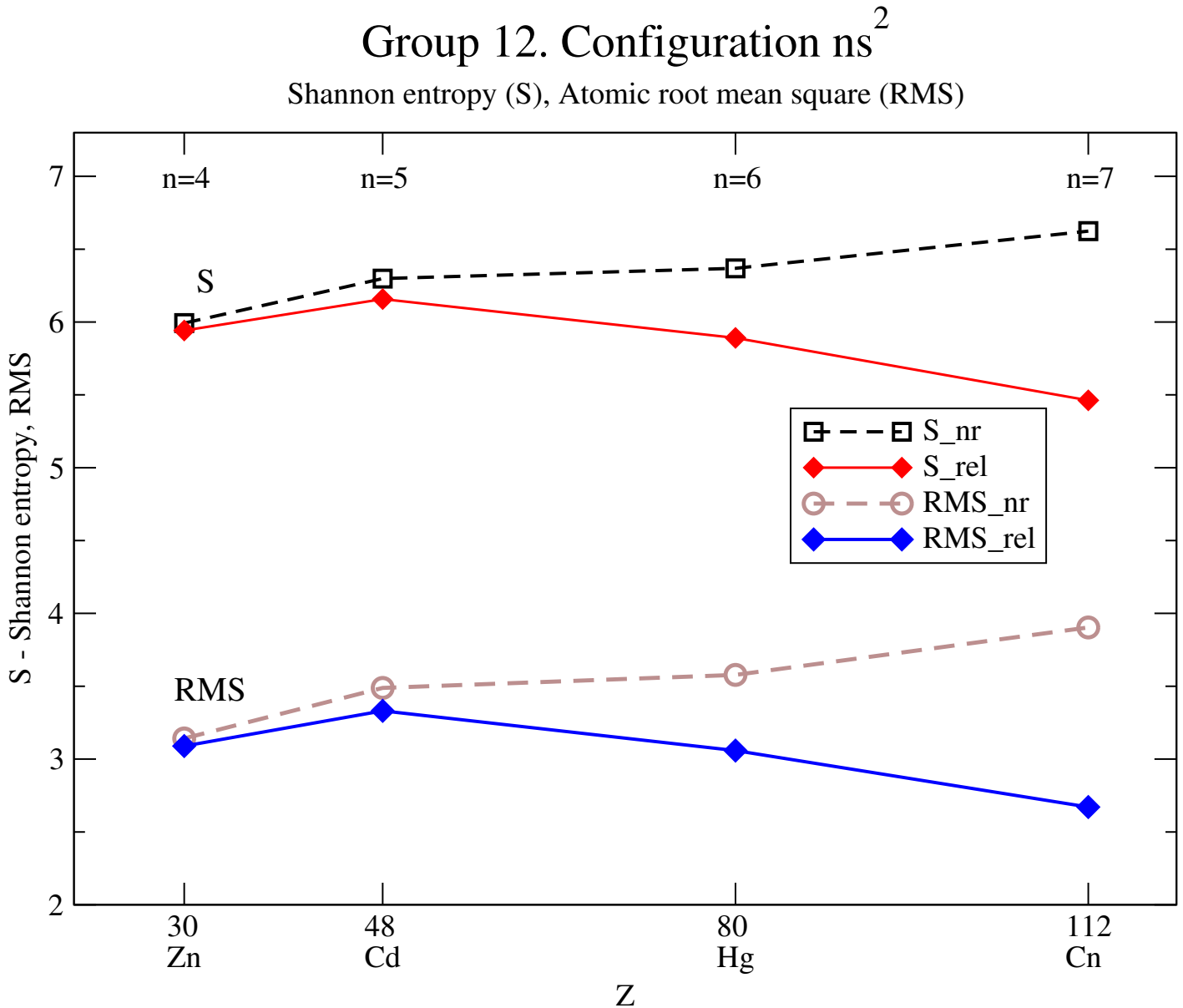
[1] B. Fricke and G. Soff, Atomic Data and Nuclear Data Tables 19, 83 (1977).

[2] V.I. Nefedov, M. Trzhaskovskaya, Dokl. Phys. Chem. 408, 149 (2006).

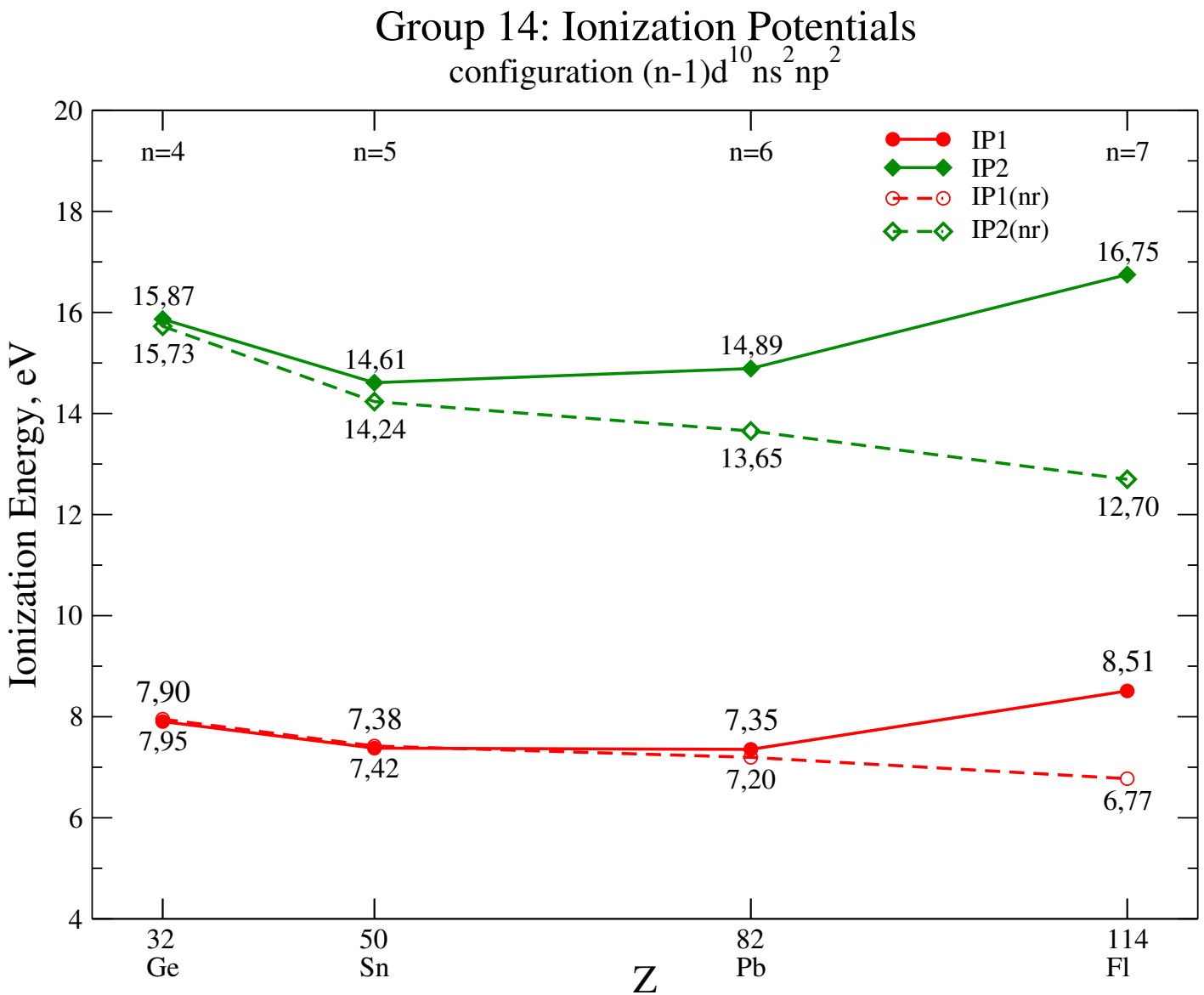
Spin-orbit splitting

Таблица: Spin-orbit splitting Δ_{SO} [eV]

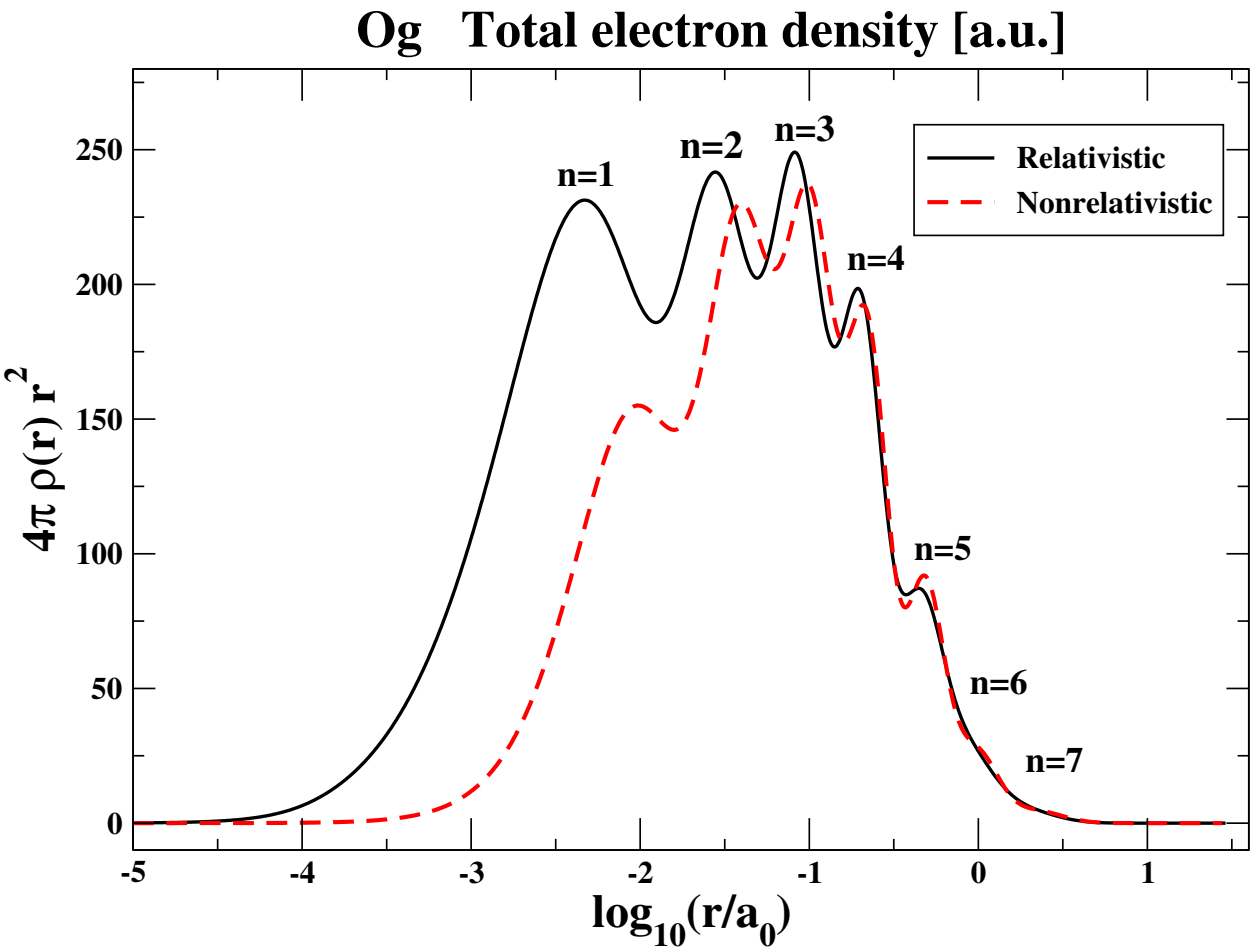
Z	$7p_{1/2}$	$7p_{3/2}$	Δ_{SO}
114	10.4	4.5	5.9
116	14.3	6.1	8.2
118	20.1	8.3	11.8
	$8p_{1/2}$	$8p_{3/2}$	
125	5.3	2.4	2.9
144	13.8	2.7	11.1
145	16.2	2.7	13.5
164	69.9	3.6	66.3
165	79.7	5.0	74.7
166	90.1	6.6	83.5


Group 12. Configuration ns2
Shannon entropy (S), Atomic root mean square (RMS)
n=4
n=5
n=6
n=7
S
RMS
S_nr
S_rel
RMS_nr
RMS_rel
S - Shannon entropy, RMS
7
6
5
4
3
2
30
Zn
48
Cd
80
Hg
112
Cn
Z

14th group of elements



Electron density distribution



Radial electron density $4\pi\rho(r)r^2$ plot for Og in both relativistic and non-relativistic approximations.

There is no visible peak in the valence shell region. Electron density alone does not show any valence shell structure

Nonrelativistic Electron Localization Function (ELF)

The electron localization function is defined by [4]

$$\mathrm{ELF}(\boldsymbol{r}) = \left(1 + \left[\frac{D(\boldsymbol{r})}{D_0(\boldsymbol{r})}\right]^2\right)^{-1}, \tag{1}$$

where

$$D(\boldsymbol{r}) = \frac{1}{2}\left[\tau - \frac{1}{4}\frac{|\boldsymbol{\nabla}\rho(\boldsymbol{r})|^2}{\rho(\boldsymbol{r})}\right], \qquad \text{and} \qquad \tau = \sum_{i,\sigma} |\boldsymbol{\nabla}\varphi_{i\sigma}(\boldsymbol{r})|^2 . \tag{2}$$

Here ρ is total density and τ the kinetic energy density.

$D_0(\boldsymbol{r})$ corresponds to a uniform electron gas (Thomas-Fermi) kinetic energy density

$$D_0(\boldsymbol{r}) = \frac{3}{10}(3\,\pi^2)^{2/3}\rho^{5/3}(\boldsymbol{r}) . \tag{3}$$

The ELF values lie by definition between zero and one. Small values are typical for the region between two electron shells. In a homogeneous electron gas ELF = 0.5.

[4] *A. D. Becke and K. E. Edgecombe, J. Chem. Phys. v.92, 5397 (1990).*

Relativistic Electron Localization Function (ELF)

$$D(\boldsymbol{r}) = \sum_{\lambda=1,2} \left[W^{\lambda}(r)\, T^{\lambda}(\boldsymbol{r}) - \frac{1}{8} \frac{\left|\boldsymbol{\nabla}\rho^{\lambda}(r)\right|^2}{\rho(r)} \right] , \tag{4}$$

where $\rho(r)$ – total electron density

$$\rho(r) = \sum_{\lambda=1,2} \rho^{\lambda}(r)\,, \qquad \rho^{\lambda}(r) = \frac{4\pi}{r^2} \sum_a q_a \begin{cases} P_a^2(r), & \lambda = 1, \\ Q_a^2(r), & \lambda = 2\,. \end{cases} \tag{5}$$

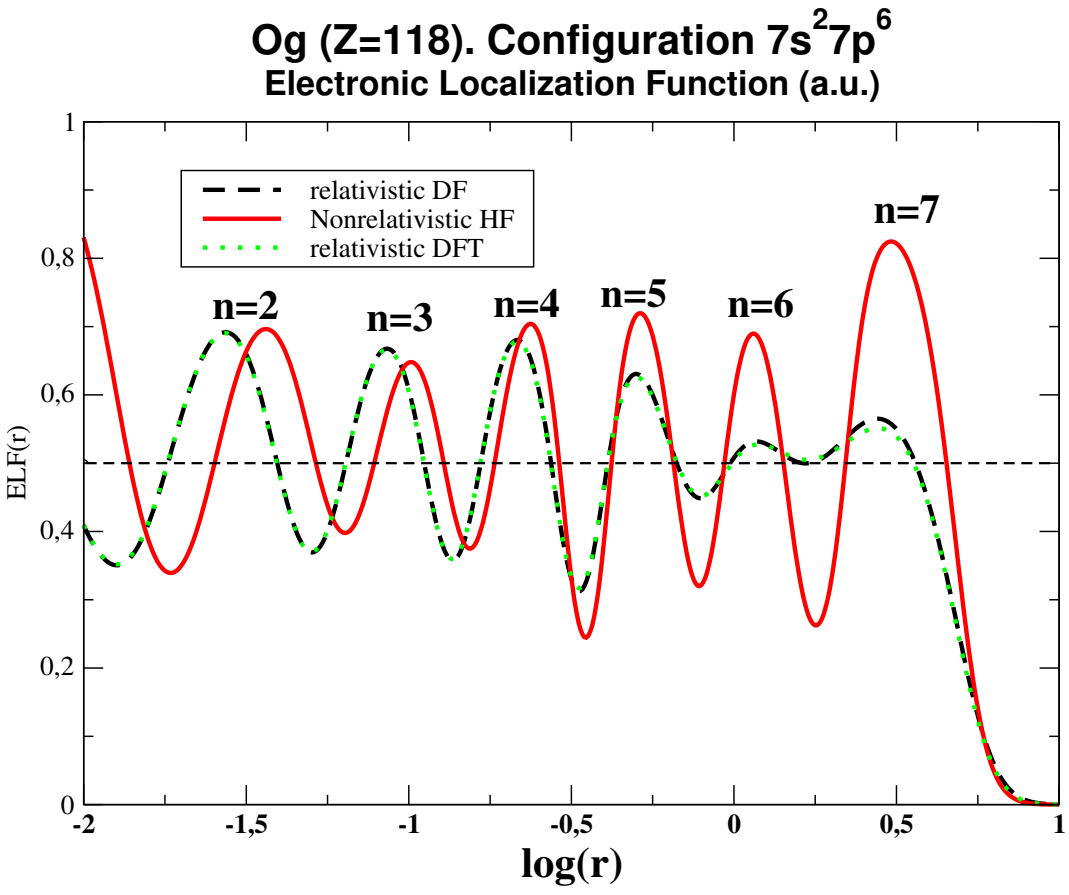
$T^{\lambda}(\boldsymbol{r})$ in formula (4) is the relativistic analogue of the non-relativistic kinetic energy density

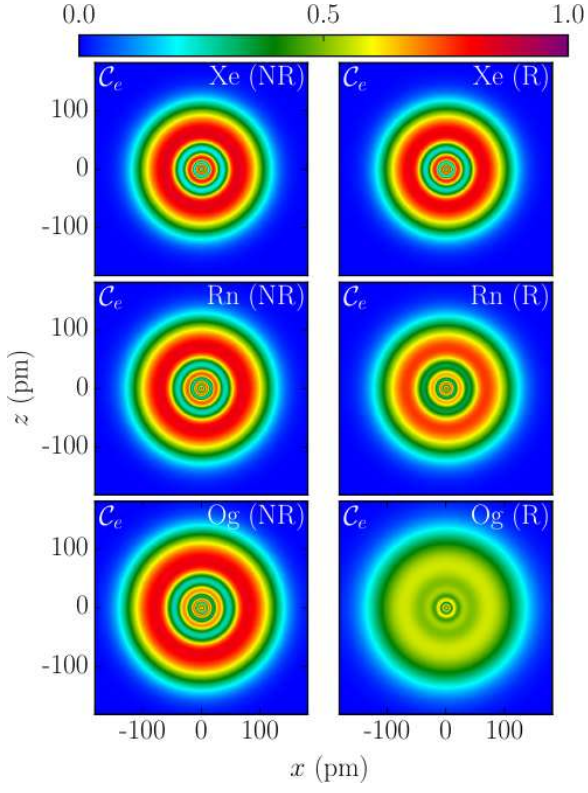
$$T^{\lambda}(\boldsymbol{r}) = \sum_a q_a\, t_a^{\lambda}(\boldsymbol{r})\,, \qquad t_a^{\lambda}(\boldsymbol{r}) = \frac{1}{2}\, \frac{1}{2j_a+1} \sum_{\mu_a,\sigma} |\boldsymbol{\nabla}\phi^{\lambda}_{a\mu_a}(\boldsymbol{r},\sigma)|^2 \tag{6}$$

and $W^{\lambda}(r)$ is a weight function that has the form

$$W^{\lambda}(r) = \frac{\rho^{\lambda}(r)}{\rho(r)}\,. \tag{7}$$

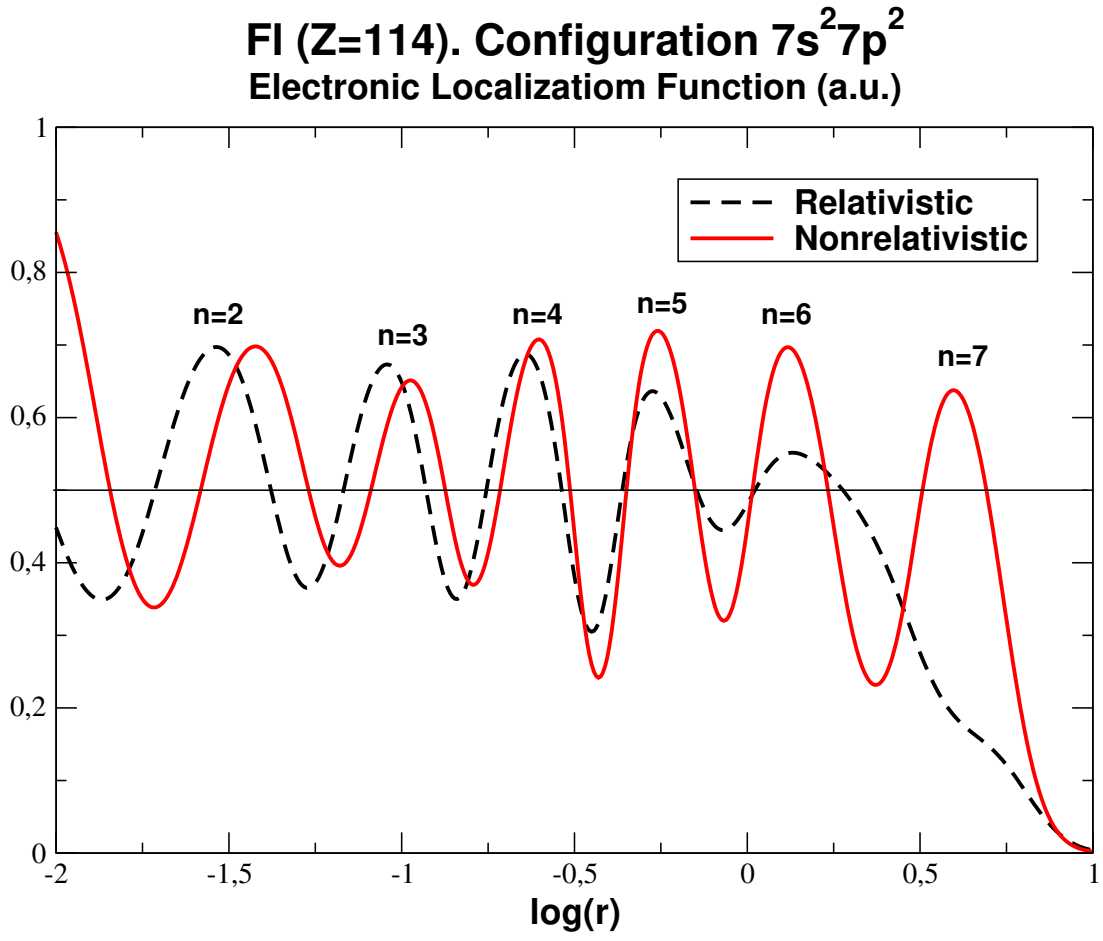
I.I Tupitsyn et al., Optics and Spectroscopy, 130, 1022 (2022)

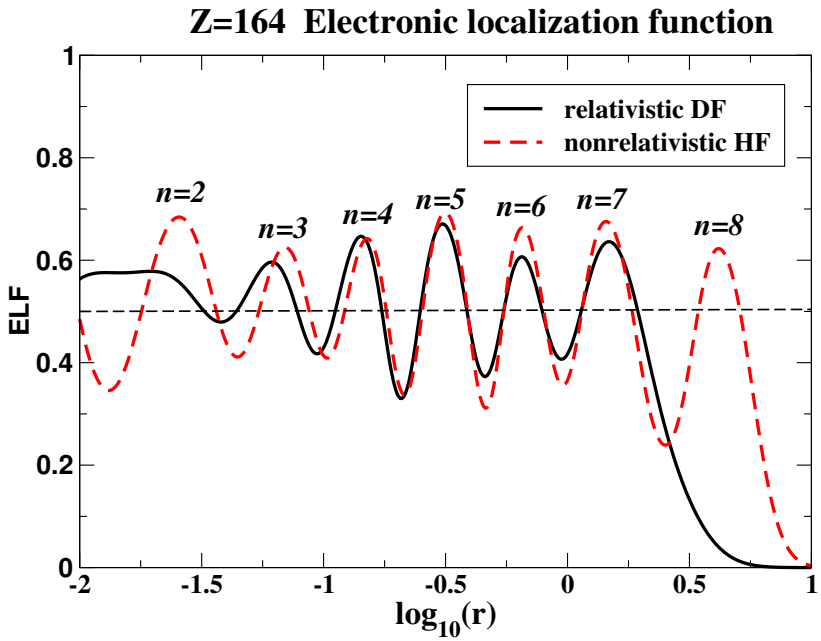


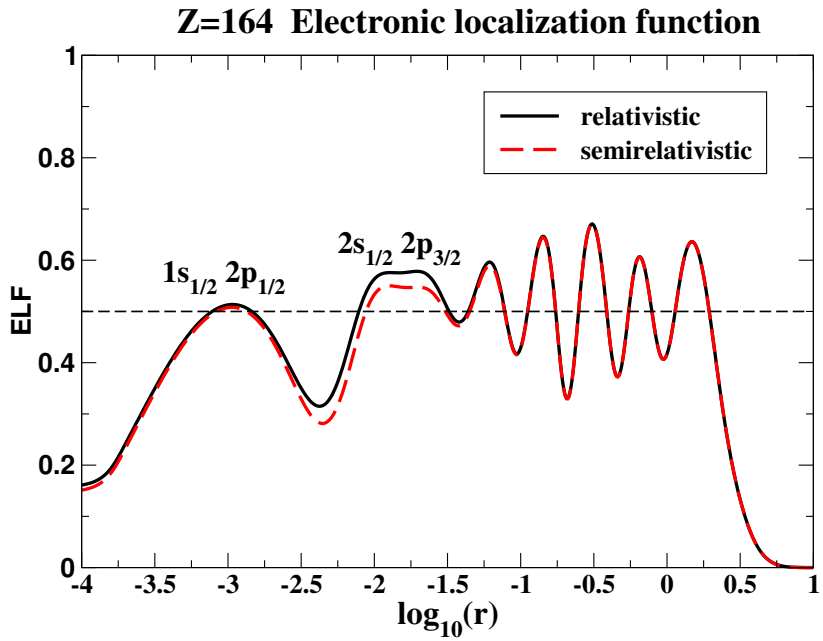


"Spin-orbit splitting in the 7p electronic shell becomes so large (∼10 eV) that Og is expected to show uniform-gas-like behavior in the valence region" [5].

[5] *Jerabek et al., PRL 120, 053001 (2018).*


Fl (Z=114). Configuration 7s²7p²
Electronic Localizatiom Function (a.u.)
Relativistic
Nonrelativistic
n=2
n=3
n=4
n=5
n=6
n=7
1
0,8
0,6
0,4
0,2
0
-2
-1,5
-1
-0,5
0
0,5
1
log(r)





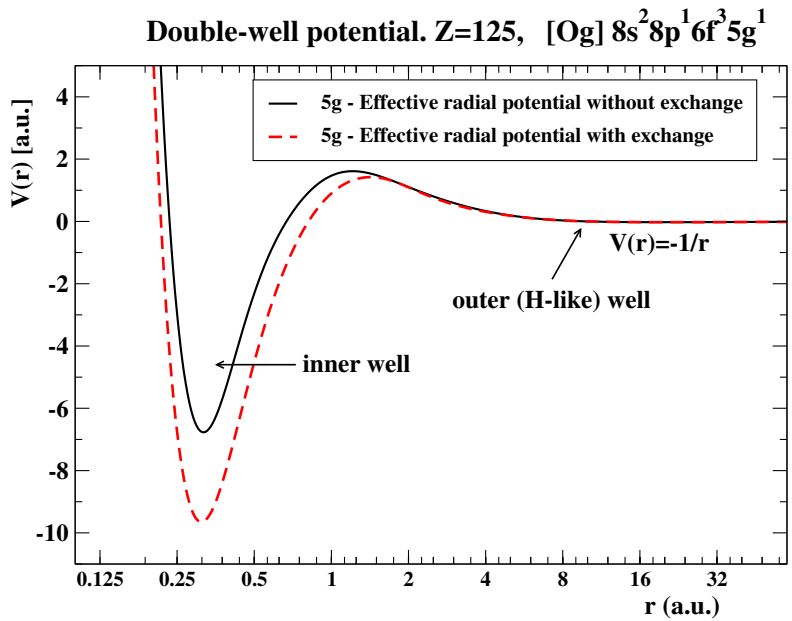
Z164 Electron configuration: [Og]$5g^{18}6f^{14}7d^{10}$.

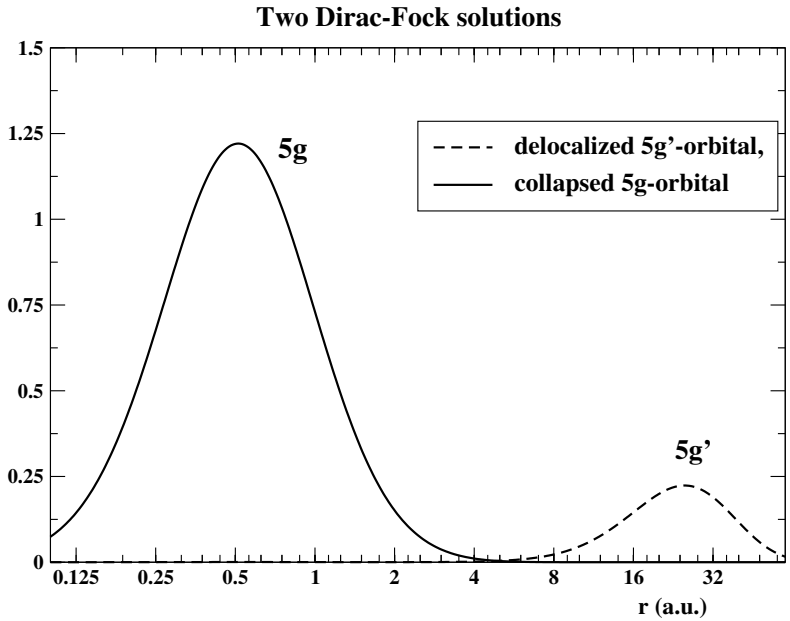
One-electron energies ε and mean radii of the core electrons

	ε [keV]	<r> [a.u.]
1s 1/2	-770.6	0.0028
2p 1/2	-343.0	0.0038
2s 1/2	-196.3	0.0130
2p 3/2	-66.2	0.0279

mc^2=510.7 keV

Orbital collapse. Two solutions



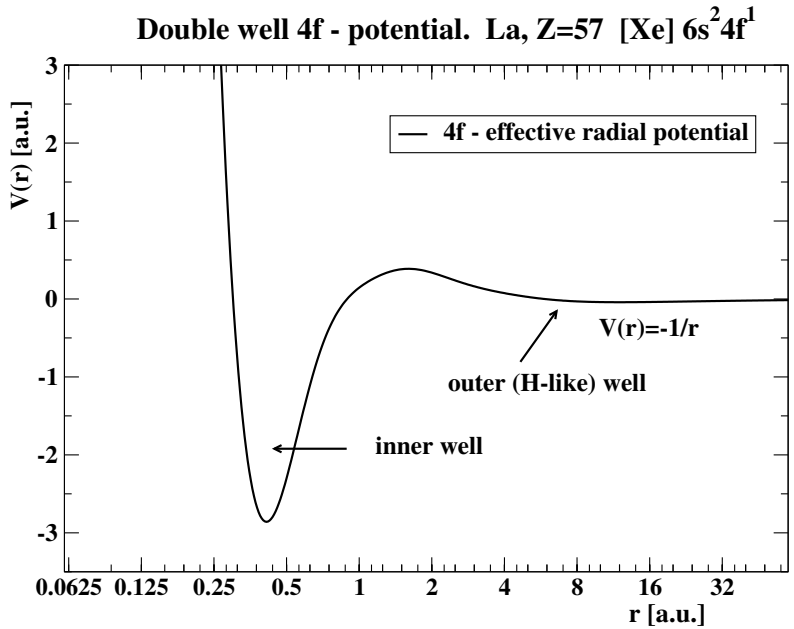


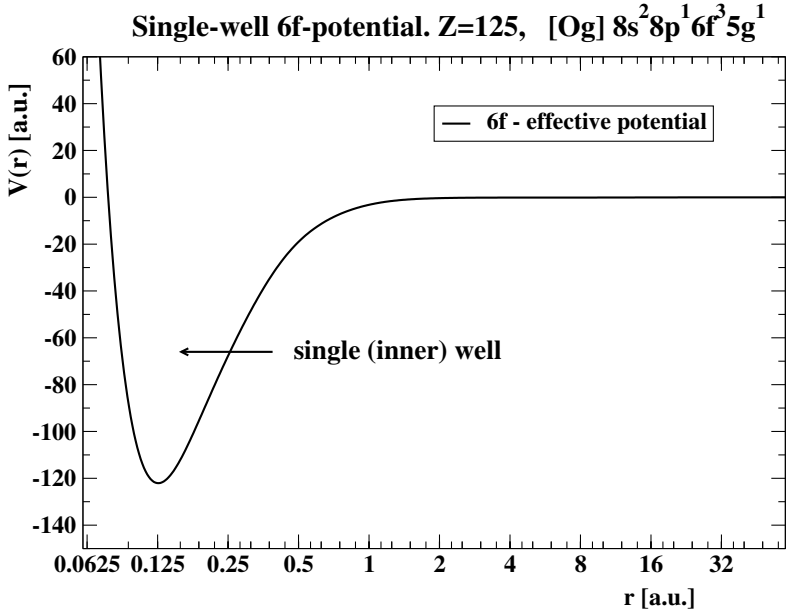
$$
\begin{aligned}
\varepsilon_{5g} &= -0.51464169 \text{ a.u.} & \langle r \rangle_{5g} &= 0.71289 \text{ a.u.} \\
\varepsilon_{5g'} &= -0.02000147 \text{ a.u.} & \langle r \rangle_{5g'} &= 27.4943 \text{ a.u.} \\
\varepsilon^{H}_{5g} &= -0.02000001 \text{ a.u.} & \langle r \rangle^{H}_{5g} &= 27.5000 \text{ a.u.}
\end{aligned}
\tag{8}
$$

Total Energies (J=0.5):

$$
\begin{aligned}
E_{\text{inner}} &= -64846.2788 \text{ a.u.} \\
E_{\text{outer}} &= -64846.0878 \text{ a.u.}
\end{aligned}
\tag{9}
$$

Orbital collapse. Two solutions. La (Z=57)





$$
\begin{aligned}
\varepsilon_{4\mathrm{f}} &= -0.2304 \text{ a.u.} & \langle r \rangle_{4\mathrm{f}} &= 1.27452 \text{ a.u.} \\
\varepsilon_{4\mathrm{f}'} &= -0.03176 \text{ a.u.} & \langle r \rangle_{4\mathrm{f}'} &= 17.1653 \text{ a.u.} \\
\varepsilon_{4\mathrm{f}'}[1] &= -0.0316 \text{ a.u.} & & -- \\
\varepsilon^{\mathrm{H}}_{4\mathrm{f}} &= -0.03125 \text{ a.u.} & \langle r \rangle^{\mathrm{H}}_{4\mathrm{f}} &= 17.9999 \text{ a.u.}
\end{aligned}
\tag{10}
$$

Total Energies (J=0.5):

$$
\begin{aligned}
E_{\mathrm{inner}} &= -8493.5483 \text{ a.u.} & E_{\mathrm{inner}}[3] &= -8493.6247 \text{ a.u.} \\
E_{\mathrm{outer}} &= -8493.4767 \text{ a.u.} & E_{\mathrm{outer}}[3] &= -8493.5512 \text{ a.u.}
\end{aligned}
\tag{11}
$$

1. *I.M. Band and V.I. Fomichev, Phys.Letters A*, **75**, *178 (1980)*

2. *J.-R Connerade and R.C. Kamatak, Handbook on the Physics and Chemistry of Rare Earths, v. 28, p. 1 (2000)*

Thank You for Attention.

Таблица: Comparison of contributions to the Electron Affinities (EA) of Og (Z=118) atom ([Rn]$5f^{14}6d^{10}7s^27p^6$) calculated with the CI-DFS and FSCC methods in the present work [1] with results of Refs. [2-5] (eV). In Ref. [4] a combination of CI with the many-body perturbation theory is used.

Reference	EA_{CI-DFS}	$EA_{FSCC-SD}$	δEA^{T}	δEA^{QED}	EA^{Total}
Kaygorodov *et al.*[1]	0.070(10)	0.070(2)	0.008(3)	−0.002(1)	0.076(4)
Eliav *et al.*[2]					0.056(10)
Goidenko *et al.*[3]		0.064(2)		−0.0059(5)	0.058(3)
Lackenby *et al.*[4]					0.096
Guo *et al.*[5]					0.080(6)

1. *M. Y. Kaygorodov et al., PRA, 104, 012819, (2021).*
2. *E. Eliav, U. Kaldor, Y. Ishikawa, and P. Pyykkö, PRL 77, 5350 (1996).*
3. *I. Goidenko, L. Labzowsky, E. Eliav, U. Kaldor, and P. Pyykkö, PRA 67, 020102 (2003).*
4. *B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum, PRA 98, 042512 (2018).*
5. *Y Guo, et al., arXiv:2107.02164 [physics], (2021)*

Shannon entropy

According to the formula of K. Shannon [1], the amount of information is defined as:

$$S = -\sum_{i=1}^{N} p_i \, \ln p_i \tag{12}$$

where N is the number of random events, p_i is the probability of the i-th event and

$$\sum_{i=1}^{N} p_i = 1 \, . \tag{13}$$

The minimum value of S is reached for the deterministic event when one of the probabilities of p_i is 1, and the rest are zero. In this case, $S = S_{\min} = 0$.

The maximum value of S is reached for an equally probable distribution $p_i = 1/N$. Then, $S_{\max} = \ln(N)$

$$0 \leq S \leq \ln(N) \tag{14}$$

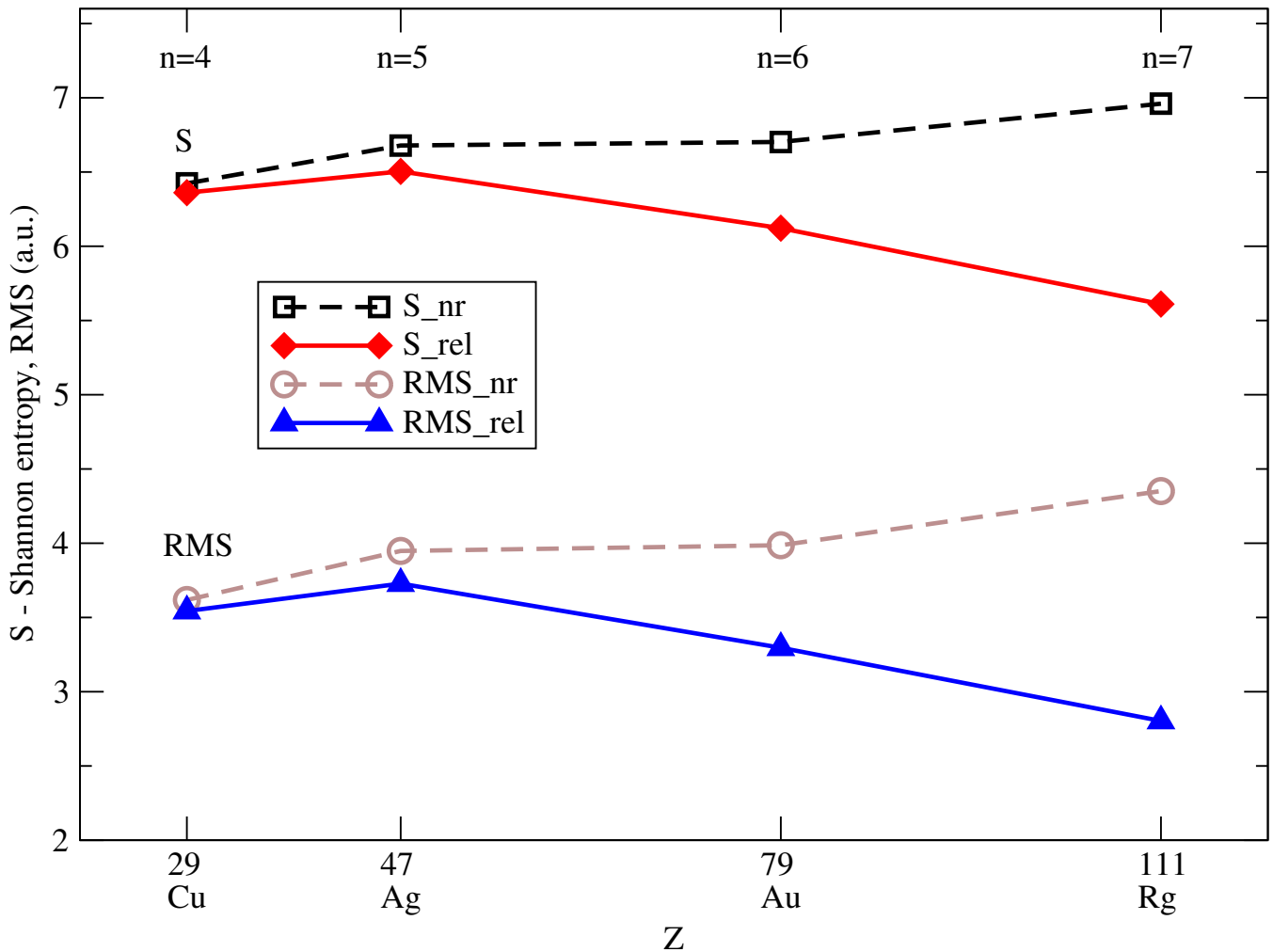
For continuous distribution

$$S = -\int d\boldsymbol{r} \, \ln(\rho(\boldsymbol{r}))\, \rho(\boldsymbol{r}) \, , \qquad \int d\boldsymbol{r} \, \rho(\boldsymbol{r}) = 1 \, . \tag{15}$$

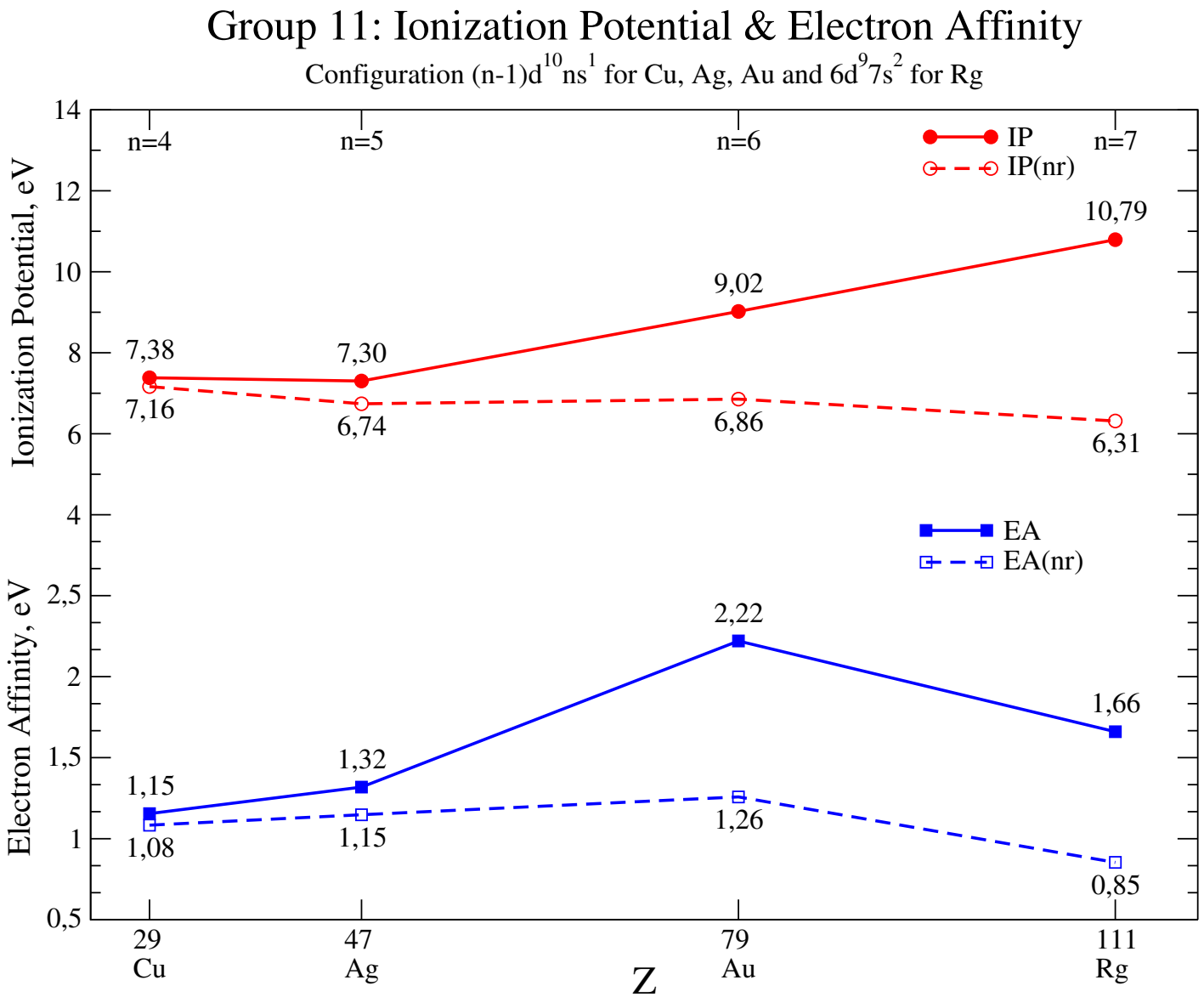
[1] *C.E. Shannon, Bell Syst. Tech. J. 27, 379; 623 (1948).*

Group 11. Shannon entropy (S). Atomic root mean square (RMS)

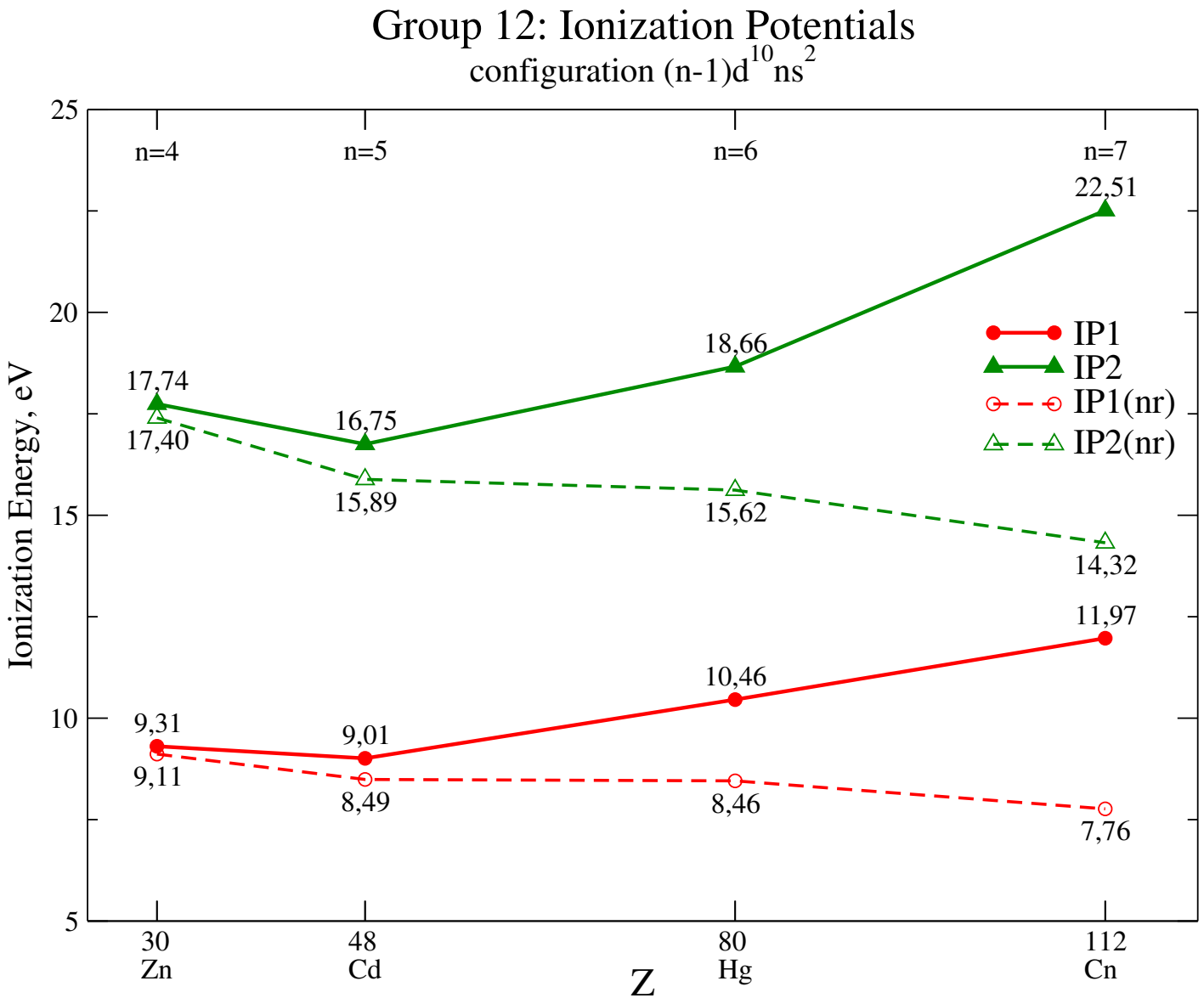
Configuration $(n-1)d^{10}ns^1$ for Cu, Ag, Au and $6d^97s^2$ for Rg

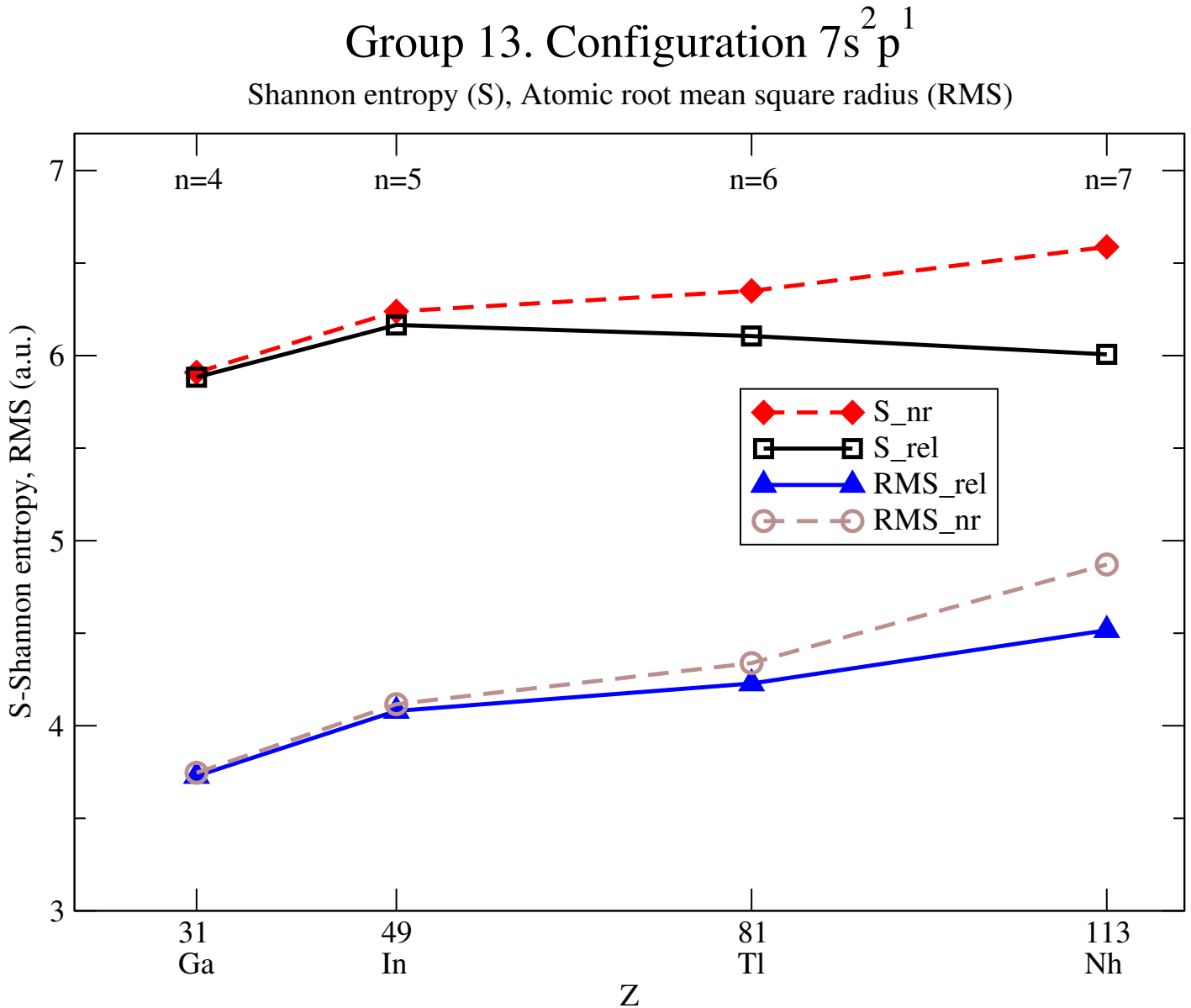


11th group of elements

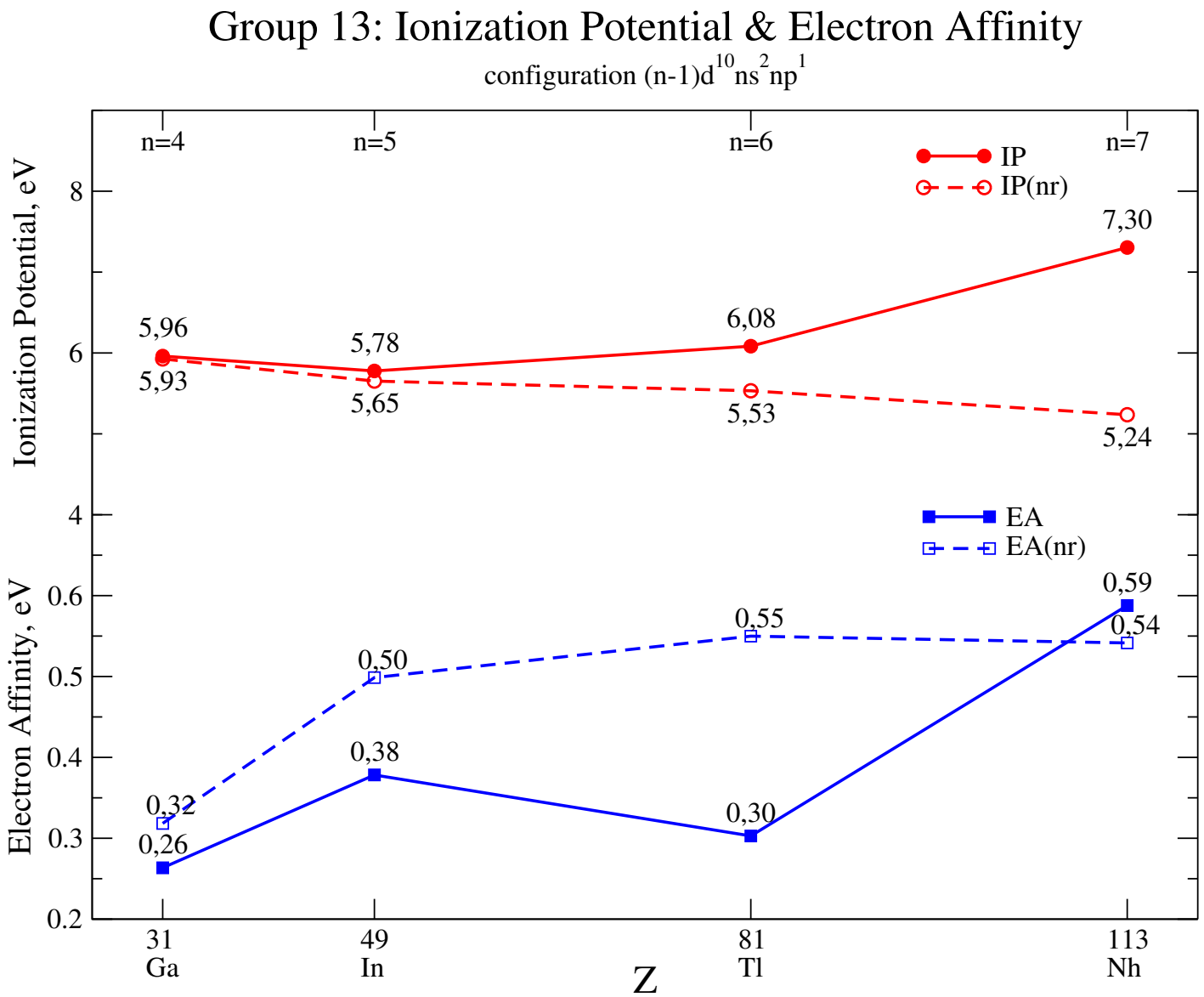


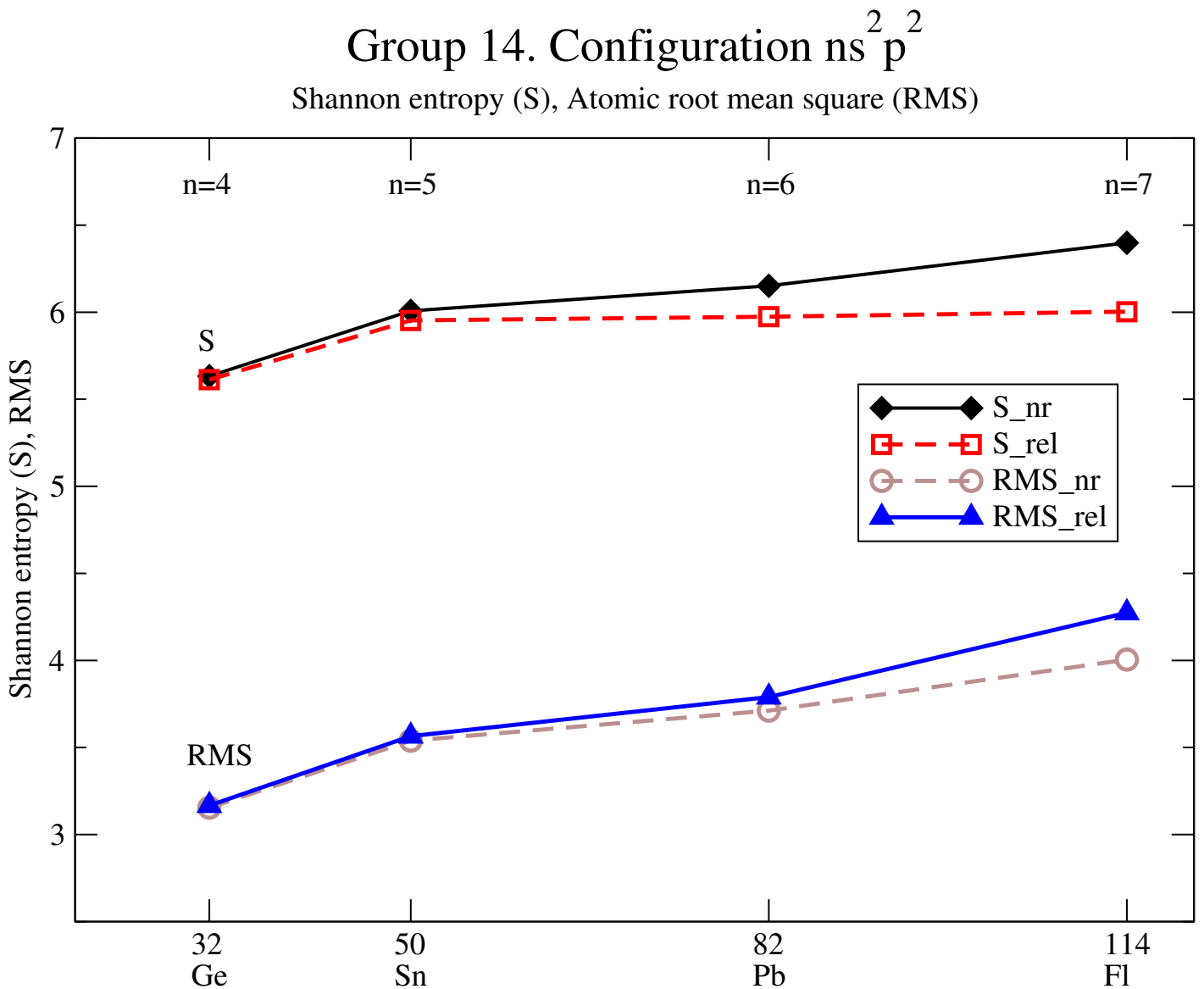
12th group of elements

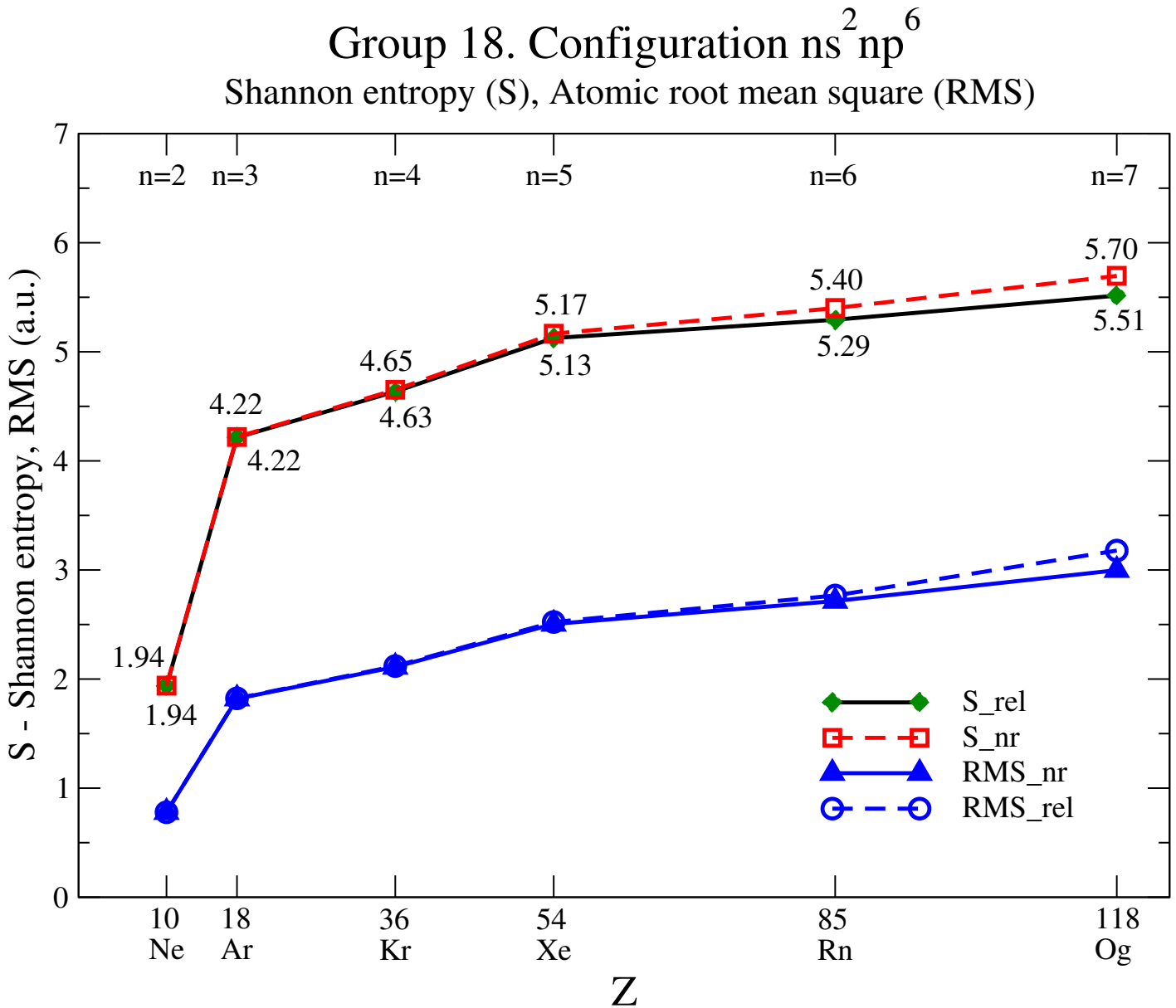



Group 13. Configuration 7s2p1
Shannon entropy (S), Atomic root mean square radius (RMS)
n=4
n=5
n=6
n=7
S_nr
S_rel
RMS_rel
RMS_nr
S-Shannon entropy, RMS (a.u.)
7
6
5
4
3
31
Ga
49
In
81
Tl
113
Nh
Z

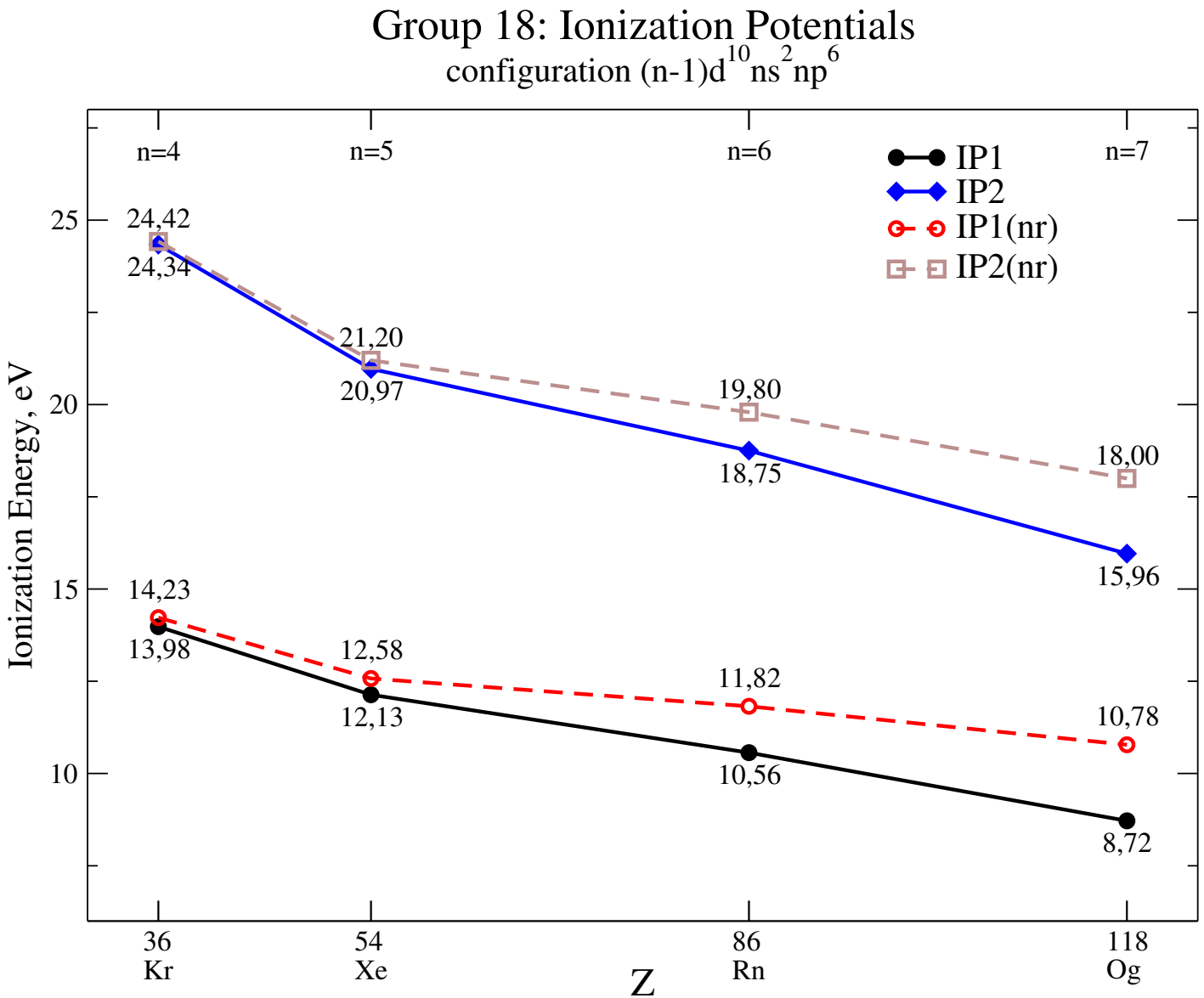
13th group of elements




Group 14. Configuration ns2 p2
Shannon entropy (S), Atomic root mean square (RMS)
Shannon entropy (S), RMS
7
6
5
4
3
n=4
n=5
n=6
n=7
S
RMS
S_nr
S_rel
RMS_nr
RMS_rel
32
Ge
50
Sn
82
Pb
114
Fl


Group 18. Configuration ns2np6
Shannon entropy (S), Atomic root mean square (RMS)
S - Shannon entropy, RMS (a.u.)
Z
n=2
n=3
n=4
n=5
n=6
n=7
1.94
1.94
4.22
4.22
4.65
4.63
5.17
5.13
5.40
5.29
5.70
5.51
S_rel
S_nr
RMS_nr
RMS_rel
10 Ne
18 Ar
36 Kr
54 Xe
85 Rn
118 Og

18th group of elements



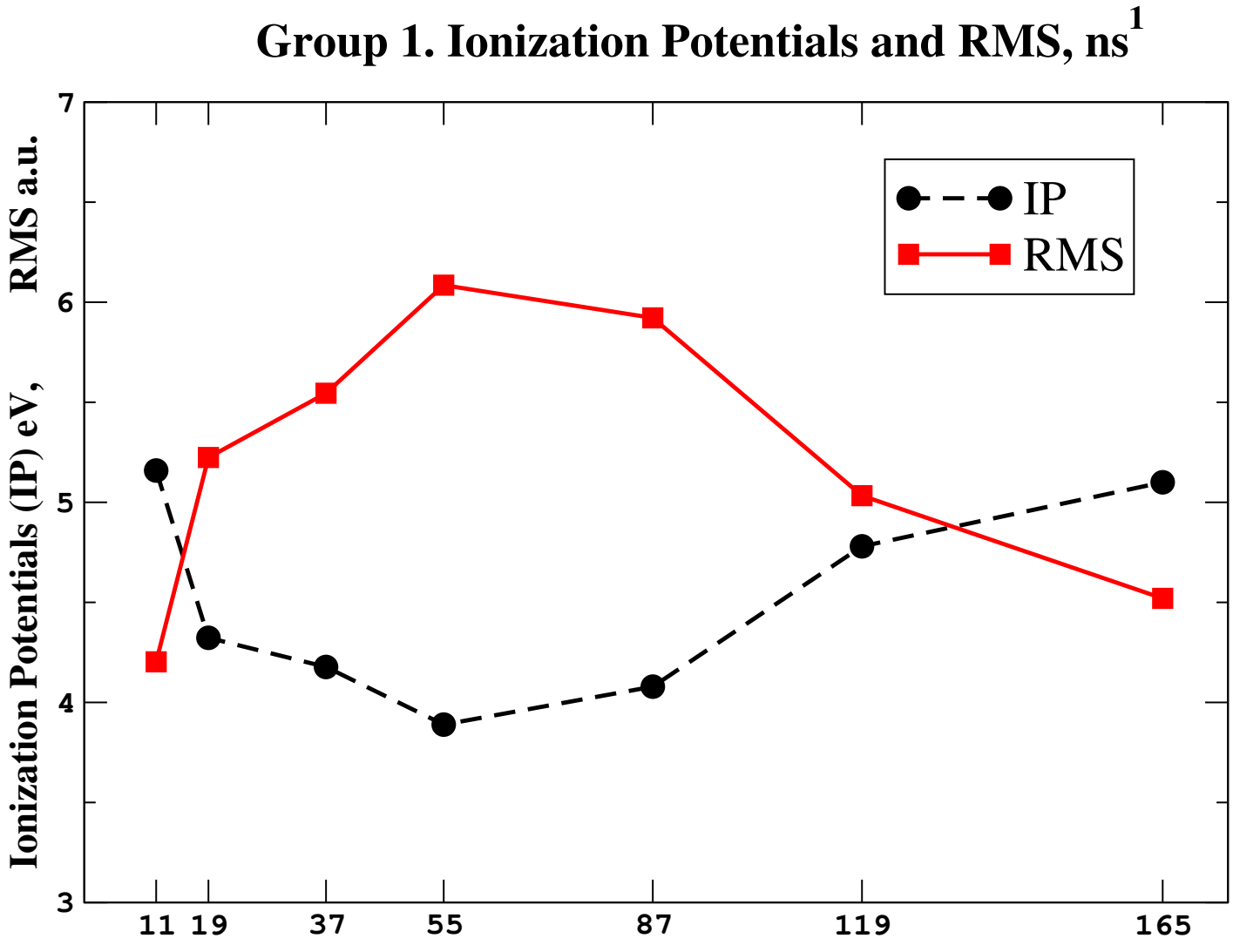

Group 1. Ionization Potentials and RMS, ns1
Ionization Potentials (IP) eV, RMS a.u.
7
6
5
4
3
11
19
37
55
87
119
165
IP
RMS

Таблица: One-electron energies and RMS valence shell radii of atoms with a serial number Z=163 and Z=164 and its homologous

n	Z	$\epsilon(d_{3/2})$	$\epsilon(d_{5/2})$	$\epsilon(ns)$	$\mathrm{RMS}(d_{5/2})$	$\mathrm{RMS}(d_{5/2})$	$\mathrm{RMS}(ns)$
4	29	-13.276	-12.906	-6.661	0.991	1.002	3.261
5	47	-14.312	-13.646	-6.453	1.371	1.396	3.451
6	79	-13.430	-11.667	-7.937	1.536	1.619	3.061
7	111	-14.082	-11.047	-11.593	1.708	1.868	2.588
8	163	-14.396	-6.310	-60.791	1.745	2.282	1.401
4	30	-20.977	-20.537	-8.126	0.875	0.883	2.848
5	48	-20.089	-19.290	-7.658	1.254	1.274	3.089
6	80	-17.689	-15.637	-8.926	1.431	1.499	2.843
7	112	-15.313	-12.030	-12.275	1.643	1.795	2.499
8	164	-15.875	-7.138	-65.815	1.680	2.161	1.359

For atom Z=164 RMS(5g) $\simeq 0.32$ a.u.

Dirac-Fock-Sturm method (DFS)

Within the DCB approximation, the many-electron wave function $\Psi(JM)$ can be obtained in the form of an expansion in terms of the configuration-state functions (CSF) $\Phi_I(JM)$:

$$\Psi(JM) = \sum_I C_I^{JM}\, \Phi_I(JM)\,. \tag{16}$$

Each function $\Phi_I(JM)$ is a an eigenfunction of the operators $\hat{J}^2$ и $\hat{J}_z$ and there is a linear combination of Slater determinants

$$\sum_K H_{KI}\, C_K^{JM} = E_I(J)\, C_I^{JM}\,, \tag{17}$$

where $H_{KI} = \langle \Phi_K \mid \hat{H}_{\rm DCB} \mid \Phi_I \rangle$.

The Slater determinants are constructed form the one-electron wave functions ψ_i obtained by the Dirac–Fock method in the basis of Dirac–Fock–Sturm (DFS) orbitals φ_k:

$$\psi_i = \sum_k u_{ki}\, \varphi_k\,. \tag{18}$$

The one-electron DFS functions, obtained by numerically solving the Dirac–Fock (DF) integro-differential equations for the occupied in the ground and low-lying excited states.

Dirac-Fock-Sturm method (DFS)

For virtual (high-lying vacant) one-electron states, the functions φ_k are obtained by numerically solving the Dirac–Fock–Sturm equations

$$\left[\hat{h}_{\mathrm{DF}} - \varepsilon_0\right] \varphi_k = \mu_k \, W(r) \, \varphi_k \, , \tag{19}$$

where $\hat{h}_{\mathrm{DF}}$ — is the Dirac–Fock operator, ε_0 — is the reference one-electron energy, and $W(r)$ is a positive weight function tending to zero at infinity.

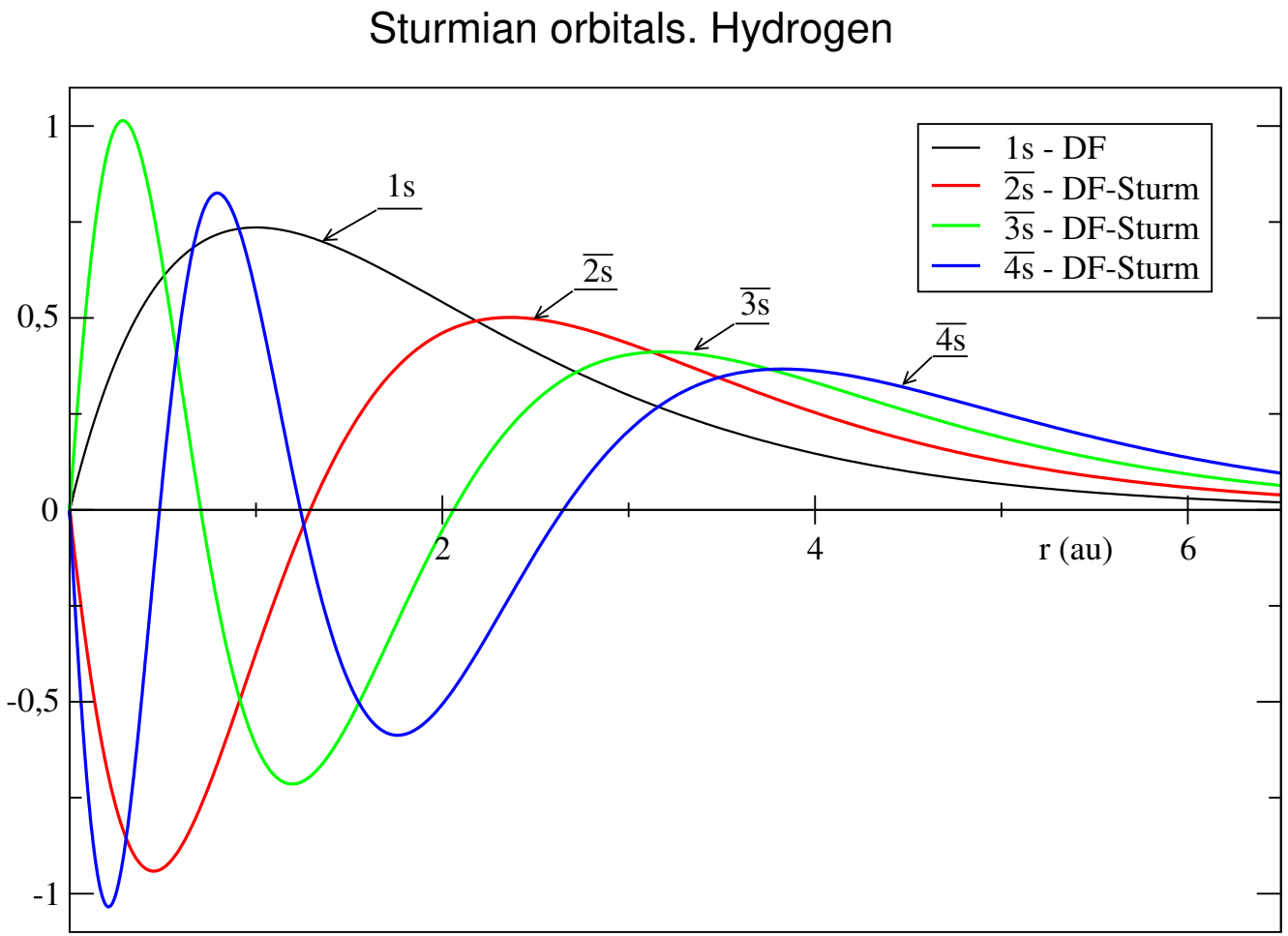
We note that all the DFS orbitals have approximately the same characteristic size and the same asymptotic at infinity, determined by the reference energy ε_0:

$$\varphi_k(r) \xrightarrow[r\to\infty]{} C_k \, \exp(-\sqrt{2\varepsilon_0}\, r) \, . \tag{20}$$

The function tending to a constant for $r \to 0$ was chosen as the weight function W (r):

$$W(r) = \frac{1 - \exp(-(\alpha r)^2)}{(\alpha r)^2} \, . \tag{21}$$

Hydrogen-like (Coulomb) Sturmians



One-electron model QED potential

The one-electron QED potential $V^{\rm QED}$ can be consider as the sum of *Vacuum Polarization* (VP) potential $V^{\rm VP}$ and *Self-Energy* (SE) potential $V^{\rm SE}$

$$V^{\rm QED} = V^{\rm VP} + V^{\rm SE} \tag{22}$$

With a good accuracy VP contribution can be presented as the sum of the local Uehling and Wichmann-Kroll potentials

$$V^{\rm VP} = V_{\rm Uehl} + V_{\rm WK} \tag{23}$$

The calculation of the self-energy is complicate and time-consuming part of the QED corrections.

We suppose that there exist one-electron self-energy (SE) operator $\hat{\Sigma}$ which can be directly included into the Dirac-Coulomb-Breit (DCB) many-electron calculations. The approximation to the self-energy operator $\hat{\Sigma}$ based on the expansion (1) is given by

$$V^{\rm SE} = \sum_{i,k=1}^{n} |\psi_i^{(0)}\rangle \Sigma_{ik} \langle \psi_k^{(0)}| \,, \quad \text{where} \quad \Sigma_{ij} = \langle \psi_i^{(0)}|\hat{\Sigma}|\psi_j^{(0)}\rangle \,. \tag{24}$$

The SE operator have to be localized in a small region whose size is on the order of Compton wavelength (1/137 a.u.)

One-electron model QED potential

The hydrogen-like wave functions should be replaced by the properly localized so-called projected functions ϕ_i. Then

$$V^{\rm SE} = \sum_{i,k=1}^{n} |\phi_i\rangle B_{ik} \langle\phi_k| \,, \tag{25}$$

The matrix elements B_{ik} are chosen so that the matrix elements of the model operator $V^{\rm SE}_{ik}$ calculated with hydrogen like wave functions $\psi^{(0)}_i$ have to be equal to matrix elements Q_{ik} of the symmetrized exact one-loop energy-dependent SE operator $\Sigma(\varepsilon)$

$$\langle i \mid V^{\rm SE} \mid k\rangle = Q_{ik} = \frac{1}{2}\,\left[\Sigma_{ik} + \Sigma_{ki}\right] \tag{26}$$

Then

$$B_{ik} = \sum_{j,l=1}^{n} (D^{-1})_{ji}\, Q_{jl}\, (D^{-1})_{lk} \,, \qquad D_{ik} = \langle\phi_i|\psi^{(0)}_k\rangle \tag{27}$$

This approximation to the SE operator is also not very successful. If any strongly localized function is orthogonal to the finite set of projection functions ϕ_i then the corresponding SE contribution will be equal to zero.

One-electron model QED potential

To overcome this problem we introduce the local potential $V_{\rm loc}^{\rm SE}$ in (4) by the following way

$$V^{\rm SE} = V_{\rm loc}^{\rm SE} + \sum_{i,k=1}^{n} |\phi_i\rangle \Delta B_{ik} \langle\phi_k| \,, \tag{28}$$

where

$$\Delta B_{ik} = \sum_{j,l=1}^{n} (D^{-1})_{ji}\, \Delta\Sigma_{jl}\, (D^{-1})_{lk} \,, \tag{29}$$

and $\Delta\Sigma_{ik} = \Sigma_{ik} - \langle\psi_i^{(0)}|V_{\rm loc}^{\rm SE}|\psi_k^{(0)}\rangle$.

At the present time, the matrix Σ is constructed in the interval $3 \le Z \le 125$. However, *A. Malyshev* is finishing work on expanding the region of Z up to Z=170.

This approximation to the SE operator was used in our papers [1-3]:

1. V.M. Shabaev, I.I. Tupitsyn, V.A. Yerokhin, Phys. Rev. A, 88, 012513 (2013)
2. V.M. Shabaev, I.I. Tupitsyn, V.A. Yerokhin, Computer Phys. Comm., 189, 175 (2015)
3. I.I. Tupitsyn, M.G. Kozlov, M.S. Safronova, V.M. Shabaev, and V.A. Dzuba, PRL, 117, 253001 (2016)

Таблица: Contributions to the first ionization potential I_1 and electron affinity EA of Rg (Z=111) atom (eV). Configuration: $6d^9 7s^2$

Contribution	I_1	EA
FSCC-SD	10.94(6)	1.92(6)
FSCC-T	−0.585	−0.076
Gaunt (FSCC)	0.026(1)	0.024(2)
Retard (CI)	−0.002(1)	−0.002(1)
Freq (CI)	−0.0006(3)	0.0001(3)
QED (CI)	0.021(3)	0.019(3)
Total	10.40(6)	1.89(6)
Eliav *et al.*	10.60	1.565
Lackenby *et al.*	11.175	
Hangele *et al.*	11.871	2.5077

1. E. Eliav et al., PRL, 73, 3203, (1994).
2. B. G. C. Lackenby et al., PRA, 101, 012514 (2020).
3. T. Hangele et al, J. Chem. Phys., 136, 214105 (2012).

Таблица: Contributions to the ionization potentials (IP) of Cn atom ($Z = 112$ element), in eV.

Contribution	$I_2^{J=0}$	$I_2^{J=2}$	$I_2^{J=3}$	$I_2^{J=4}$	I_1
FSCC-SD	23.32(4)	22.53(4)	22.69(4)	22.46(4)	11.93(4)
FSCC-T	−0.143(2)	−0.238(2)	−0.159(2)	−0.302(2)	−0.006(2)
Gaunt (FSCC)	−0.100(3)	−0.031(3)	−0.074(3)	0.025(2)	0.027(2)
Gaunt (CI)				0.029(2)	0.031(2)
Retard (CI)				−0.001(1)	−0.002(1)
Freq (CI)				−0.001(1)	−0.0006(2)
QED (CI)				0.025(3)	0.022(3)
Total	23.07(4)	22.26(4)	22.45(4)	22.20(4)	11.97(4)
Eliav *et al.*	23.28	22.54	22.68	22.49	11.97
Nash					11.675
Yu *et al.*				21.98	11.73
Lackenby *et al.*				22.84	12.14
Hangele *et al.*				21.989	11.353

1. E. Eliav et al., PRA, 52,2765, (1995).
2. T. Hangele et al, J. Chem. Phys., 136, 214105 (2012).
3. B. G. C. Lackenby et al., PRA, 101, 012514 (2020).
4. C. S. Nash et al., J. Phys. Chem. A, 109, 3493, (2005).
5. Y. J. Yu et al., EPJ D, 44, 51, (2007).

Таблица: Contributions to the ionization potentials (IP) and electron affinity (EA) of Nh atom ($Z = 113$ element), in eV.

Contribution	I_3	I_2	I_1	EA
FSCC-SD	33.42(3)	23.91(3)	7.38(1)	0.66(1)
FSCC-T	−0.060(24)	0.008(3)	0.049(19)	0.023(9)
Gaunt (CI)	−0.060(6)	−0.049(6)	−0.055(6)	−0.040(10)
Retard (CI)	0.004(1)	0.003(1)	0.004(1)	0.003(1)
Freq (CI)	−0.005(1)	−0.005(1)	−0.003(1)	−0.002(1)
QED (CI)	−0.088(6)	−0.078(8)	−0.001(1)	0.007(4)
Total	33.21(4)	23.79(3)	7.37(2)	0.65(1)
Dzuba *et al.*	33.5	23.6	7.37	
Eliav *et al.*	33.47	23.96	7.306	0.68(5)
Pershina *et al.*			7.420	
Hangele *et al.*		23.6271	7.2779	

1. V. A. Dzuba, PRA, 93, 032519 (2016).
2. E. Eliav et al., PRA, 53, (1996).
3. V. Pershina et al., J. Chem. Phys., 131, 084713, (2009).
4. T. Hangele et.al., J. Chem. Phys., 136, 214105, (2012).

Таблица: Contributions to the ionization potentials (IP) of Fl atom $Z = 114$ element, in eV.

Contribution	I_4	I_3	I_2	I_1
SD	46.19(4)	35.73(4)	16.92(4)	8.66(4)
T	−0.074(25)	−0.019(6)	0.054(18)	0.036(12)
Gaunt	−0.076(2)	−0.069(2)	−0.068(2)	−0.044(2)
Retard	0.006(2)	0.004(2)	0.006(2)	0.005(2)
Freq	−0.006(1)	−0.006(1)	−0.004(1)	−0.003(1)
QED	−0.105(5)	−0.093(5)	−0.004(2)	−0.003(3)
Total	45.94(5)	35.55(4)	16.90(4)	8.65(4)
Dzuba *et al.*			17.00	8.37
Landau *et al.*	46.272	35.739	16.871	8.539
Yu *et al.*	46.57	35.82	17.22	8.28
Nash				8.529
Hangele *et al.*		35.3826	16.1105	7.2601

1. *V. A. Dzuba, PRA, 93, 032519 (2016).*
2. *A. Landau et al., J.Chem. Phys., 114, (2001).*
3. *Y. J. Yu et al., J. Chem. Phys., 128, 124316, (2008).*
4. *C. S. Nash et al., J. Phys. Chem. A, 109, 3493, (2005).*
5. *T. Hangele, et al., J. Chem. Phys., 136, p. 214105, (2012)*

PERIODIC TABLE

Atomic Properties of the Elements

National Institute of Standards and Technology
U.S. Department of Commerce

Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS[§]

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum	c	299 792 458 m s^{-1}	(exact)
Planck constant	h	6.626 070 15 x 10^{-34} J Hz^{-1}	(exact)
elementary charge	e	1.602 176 634 x 10^{-19} C	(exact)
Avogadro constant	N_A	6.022 140 76 x 10^{23} mol^{-1}	(exact)
Boltzmann constant	k	1.380 649 x 10^{-23} J K^{-1}	(exact)
electron volt	eV	1.602 176 634 x 10^{-19} J	(exact)
electron mass	m_e	9.109 383 70 x 10^{-31} kg	
energy equivalent	$m_e c^2$	0.510 998 950 MeV	
proton mass	m_p	1.672 621 924 x 10^{-27} kg	
energy equivalent	$m_p c^2$	938.272 088 MeV	
fine-structure constant	α	1/137.035 999	
Rydberg energy	$R_\infty hc$	13.605 693 1230 eV	
Newtonian constant of gravitation	G	6.674 x 10^{-11} m^3 kg^{-1} s^{-2}	

[§]For the most accurate values of these and other constants, visit pml.nist.gov/constants.

Solids
Liquids
Gases
Artificially Prepared

Group	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIII	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
Period 1	1 $^2S_{1/2}$ **H** Hydrogen 1.008 1s 13.5984																	2 $^1S_0$ **He** Helium 4.0026 $1s^2$ 24.5874
2	3 $^2S_{1/2}$ **Li** Lithium 6.94 $[He]2s$ 5.3917	4 $^1S_0$ **Be** Beryllium 9.0122 $[He]2s^2$ 9.3227											5 $^2P^o_{1/2}$ **B** Boron 10.81 $[He]2s^22p$ 8.2980	6 $^3P_0$ **C** Carbon 12.011 $[He]2s^22p^2$ 11.2603	7 $^4S^o_{3/2}$ **N** Nitrogen 14.007 $[He]2s^22p^3$ 14.5341	8 $^3P_2$ **O** Oxygen 15.999 $[He]2s^22p^4$ 13.6181	9 $^2P^o_{3/2}$ **F** Fluorine 18.998 $[He]2s^22p^5$ 17.4228	10 $^1S_0$ **Ne** Neon 20.180 $[He]2s^22p^6$ 21.5645
3	11 $^2S_{1/2}$ **Na** Sodium 22.990 $[Ne]3s$ 5.1391	12 $^1S_0$ **Mg** Magnesium 24.305 $[Ne]3s^2$ 7.6462											13 $^2P^o_{1/2}$ **Al** Aluminum 26.982 $[Ne]3s^23p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.085 $[Ne]3s^23p^2$ 8.1517	15 $^4S^o_{3/2}$ **P** Phosphorus 30.974 $[Ne]3s^23p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.06 $[Ne]3s^23p^4$ 10.3600	17 $^2P^o_{3/2}$ **Cl** Chlorine 35.45 $[Ne]3s^23p^5$ 12.9676	18 $^1S_0$ **Ar** Argon 39.948 $[Ne]3s^23p^6$ 15.7596
4	19 $^2S_{1/2}$ **K** Potassium 39.098 $[Ar]4s$ 4.3407	20 $^1S_0$ **Ca** Calcium 40.078 $[Ar]4s^2$ 6.1132	21 $^2D_{3/2}$ **Sc** Scandium 44.956 $[Ar]3d4s^2$ 6.5615	22 $^3F_2$ **Ti** Titanium 47.867 $[Ar]3d^24s^2$ 6.8281	23 $^4F_{3/2}$ **V** Vanadium 50.942 $[Ar]3d^34s^2$ 6.7462	24 $^7S_3$ **Cr** Chromium 51.996 $[Ar]3d^54s$ 6.7665	25 $^6S_{5/2}$ **Mn** Manganese 54.938 $[Ar]3d^54s^2$ 7.4340	26 $^5D_4$ **Fe** Iron 55.845 $[Ar]3d^64s^2$ 7.9025	27 $^4F_{9/2}$ **Co** Cobalt 58.933 $[Ar]3d^74s^2$ 7.8810	28 $^3F_4$ **Ni** Nickel 58.693 $[Ar]3d^84s^2$ 7.6399	29 $^2S_{1/2}$ **Cu** Copper 63.546 $[Ar]3d^{10}4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.38 $[Ar]3d^{10}4s^2$ 9.3942	31 $^2P^o_{1/2}$ **Ga** Gallium 69.723 $[Ar]3d^{10}4s^24p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.630 $[Ar]3d^{10}4s^24p^2$ 7.8994	33 $^4S^o_{3/2}$ **As** Arsenic 74.922 $[Ar]3d^{10}4s^24p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.971 $[Ar]3d^{10}4s^24p^4$ 9.7524	35 $^2P^o_{3/2}$ **Br** Bromine 79.904 $[Ar]3d^{10}4s^24p^5$ 11.8138	36 $^1S_0$ **Kr** Krypton 83.798 $[Ar]3d^{10}4s^24p^6$ 13.9996
5	37 $^2S_{1/2}$ **Rb** Rubidium 85.468 $[Kr]5s$ 4.1771	38 $^1S_0$ **Sr** Strontium 87.62 $[Kr]5s^2$ 5.6949	39 $^2D_{3/2}$ **Y** Yttrium 88.906 $[Kr]4d5s^2$ 6.2173	40 $^3F_2$ **Zr** Zirconium 91.224 $[Kr]4d^25s^2$ 6.6341	41 $^6D_{1/2}$ **Nb** Niobium 92.906 $[Kr]4d^45s$ 6.7589	42 $^7S_3$ **Mo** Molybdenum 95.95 $[Kr]4d^55s$ 7.0924	43 $^6S_{5/2}$ **Tc** Technetium (97) $[Kr]4d^55s^2$ 7.1194	44 $^5F_5$ **Ru** Ruthenium 101.07 $[Kr]4d^75s$ 7.3605	45 $^4F_{9/2}$ **Rh** Rhodium 102.91 $[Kr]4d^85s$ 7.4589	46 $^1S_0$ **Pd** Palladium 106.42 $[Kr]4d^{10}$ 8.3369	47 $^2S_{1/2}$ **Ag** Silver 107.87 $[Kr]4d^{10}5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.41 $[Kr]4d^{10}5s^2$ 8.9938	49 $^2P^o_{1/2}$ **In** Indium 114.82 $[Kr]4d^{10}5s^25p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.71 $[Kr]4d^{10}5s^25p^2$ 7.3439	51 $^4S^o_{3/2}$ **Sb** Antimony 121.76 $[Kr]4d^{10}5s^25p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10}5s^25p^4$ 9.0097	53 $^2P^o_{3/2}$ **I** Iodine 126.90 $[Kr]4d^{10}5s^25p^5$ 10.4513	54 $^1S_0$ **Xe** Xenon 131.29 $[Kr]4d^{10}5s^25p^6$ 12.1298
6	55 $^2S_{1/2}$ **Cs** Cesium 132.91 $[Xe]6s$ 3.8939	56 $^1S_0$ **Ba** Barium 137.33 $[Xe]6s^2$ 5.2117		72 $^3F_2$ **Hf** Hafnium 178.49 $[Xe]4f^{14}5d^26s^2$ 6.8251	73 $^4F_{3/2}$ **Ta** Tantalum 180.95 $[Xe]4f^{14}5d^36s^2$ 7.5496	74 $^5D_0$ **W** Tungsten 183.84 $[Xe]4f^{14}5d^46s^2$ 7.8640	75 $^6S_{5/2}$ **Re** Rhenium 186.21 $[Xe]4f^{14}5d^56s^2$ 7.8335	76 $^5D_4$ **Os** Osmium 190.23 $[Xe]4f^{14}5d^66s^2$ 8.4382	77 $^4F_{9/2}$ **Ir** Iridium 192.22 $[Xe]4f^{14}5d^76s^2$ 8.9670	78 $^3D_3$ **Pt** Platinum 195.08 $[Xe]4f^{14}5d^96s$ 8.9588	79 $^2S_{1/2}$ **Au** Gold 196.97 $[Xe]4f^{14}5d^{10}6s$ 9.2256	80 $^1S_0$ **Hg** Mercury 200.59 $[Xe]4f^{14}5d^{10}6s^2$ 10.4375	81 $^2P^o_{1/2}$ **Tl** Thallium 204.38 $[Hg]6p$ 6.1083	82 $^3P_0$ **Pb** Lead 207.2 $[Hg]6p^2$ 7.4167	83 $^4S^o_{3/2}$ **Bi** Bismuth 208.98 $[Hg]6p^3$ 7.2855	84 $^3P_2$ **Po** Polonium (209) $[Hg]6p^4$ 8.414	85 $^2P^o_{3/2}$ **At** Astatine (210) $[Hg]6p^5$ 9.3175	86 $^1S_0$ **Rn** Radon (222) $[Hg]6p^6$ 10.7485
7	87 $^2S_{1/2}$ **Fr** Francium (223) $[Rn]7s$ 4.0727	88 $^1S_0$ **Ra** Radium (226) $[Rn]7s^2$ 5.2784		104 $^3F_2$ **Rf** Rutherfordium (267) $[Rn]5f^{14}6d^27s^2$ 6.02	105 $^4F_{3/2}$ **Db** Dubnium (268) $[Rn]5f^{14}6d^37s^2$ 6.8	106 ^{0} **Sg** Seaborgium (269) $[Rn]5f^{14}6d^47s^2$ 7.8	107 $^{5/2}$ **Bh** Bohrium (270) $[Rn]5f^{14}6d^57s^2$ 7.7	108 ^{4} **Hs** Hassium (269) $[Rn]5f^{14}6d^67s^2$ 7.6	109 **Mt** Meitnerium (278)	110 **Ds** Darmstadtium (281)	111 **Rg** Roentgenium (282)	112 **Cn** Copernicium (285)	113 **Nh** Nihonium (286)	114 **Fl** Flerovium (289)	115 **Mc** Moscovium (289)	116 **Lv** Livermorium (293)	117 **Ts** Tennessine (294)	118 **Og** Oganesson (294)

Lanthanides	57 $^2D_{3/2}$ **La** Lanthanum 138.91 $[Xe]5d6s^2$ 5.5769	58 $^1G^o_4$ **Ce** Cerium 140.12 $[Xe]4f5d6s^2$ 5.5386	59 $^4I^o_{9/2}$ **Pr** Praseodymium 140.91 $[Xe]4f^36s^2$ 5.4702	60 $^5I_4$ **Nd** Neodymium 144.24 $[Xe]4f^46s^2$ 5.5250	61 $^6H^o_{5/2}$ **Pm** Promethium (145) $[Xe]4f^56s^2$ 5.577	62 $^7F_0$ **Sm** Samarium 150.36 $[Xe]4f^66s^2$ 5.6437	63 $^8S^o_{7/2}$ **Eu** Europium 151.96 $[Xe]4f^76s^2$ 5.6704	64 $^9D^o_2$ **Gd** Gadolinium 157.25 $[Xe]4f^75d6s^2$ 6.1498	65 $^6H^o_{15/2}$ **Tb** Terbium 158.93 $[Xe]4f^96s^2$ 5.8638	66 $^5I_8$ **Dy** Dysprosium 162.50 $[Xe]4f^{10}6s^2$ 5.9391	67 $^4I^o_{15/2}$ **Ho** Holmium 164.93 $[Xe]4f^{11}6s^2$ 6.0215	68 $^3H_6$ **Er** Erbium 167.26 $[Xe]4f^{12}6s^2$ 6.1077	69 $^2F^o_{7/2}$ **Tm** Thulium 168.93 $[Xe]4f^{13}6s^2$ 6.1843	70 $^1S_0$ **Yb** Ytterbium 173.05 $[Xe]4f^{14}6s^2$ 6.2542	71 $^2D_{3/2}$ **Lu** Lutetium 174.97 $[Xe]4f^{14}5d6s^2$ 5.4259
Actinides	89 $^2D_{3/2}$ **Ac** Actinium (227) $[Rn]6d7s^2$ 5.3802	90 $^3F_2$ **Th** Thorium 232.04 $[Rn]6d^27s^2$ 6.3067	91 $^4K_{11/2}$ **Pa** Protactinium 231.04 $[Rn]5f^26d7s^2$ 5.89	92 $^5L_6$ **U** Uranium 238.03 $[Rn]5f^36d7s^2$ 6.1941	93 $^6L_{11/2}$ **Np** Neptunium (237) $[Rn]5f^46d7s^2$ 6.2655	94 $^7F_0$ **Pu** Plutonium (244) $[Rn]5f^67s^2$ 6.0258	95 $^8S^o_{7/2}$ **Am** Americium (243) $[Rn]5f^77s^2$ 5.9738	96 $^9D^o_2$ **Cm** Curium (247) $[Rn]5f^76d7s^2$ 5.9914	97 $^6H^o_{15/2}$ **Bk** Berkelium (247) $[Rn]5f^97s^2$ 6.1978	98 $^5I_8$ **Cf** Californium (251) $[Rn]5f^{10}7s^2$ 6.2817	99 $^4I^o_{15/2}$ **Es** Einsteinium (252) $[Rn]5f^{11}7s^2$ 6.3676	100 $^3H_6$ **Fm** Fermium (257) $[Rn]5f^{12}7s^2$ 6.50	101 $^2F^o_{7/2}$ **Md** Mendelevium (258) $[Rn]5f^{13}7s^2$ 6.58	102 $^1S_0$ **No** Nobelium (259) $[Rn]5f^{14}7s^2$ 6.66	103 $^2P^o_{1/2}$ **Lr** Lawrencium (266) $[Rn]5f^{14}7s^27p$ 4.96

Atomic Number
Ground State
Symbol
Name
Standard Atomic Weight[†](u)
Ground-state Configuration
Ionization Energy (eV)

58 $^1G^o_4$ **Ce** Cerium 140.12 $[Xe]4f5d6s^2$ 5.5386

[†]Based upon ^{12}C. () indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciaaw.org and pml.nist.gov/data.

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