Study of the valence electronic density distribution in $112 \leq Z \leq 120$ atoms

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Saint-Petersburg State University, Russia

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Tihany, Hungary

Study of the valence electronic density distribution in ~~112≤Z≤120 atoms~~
Z=118 atom

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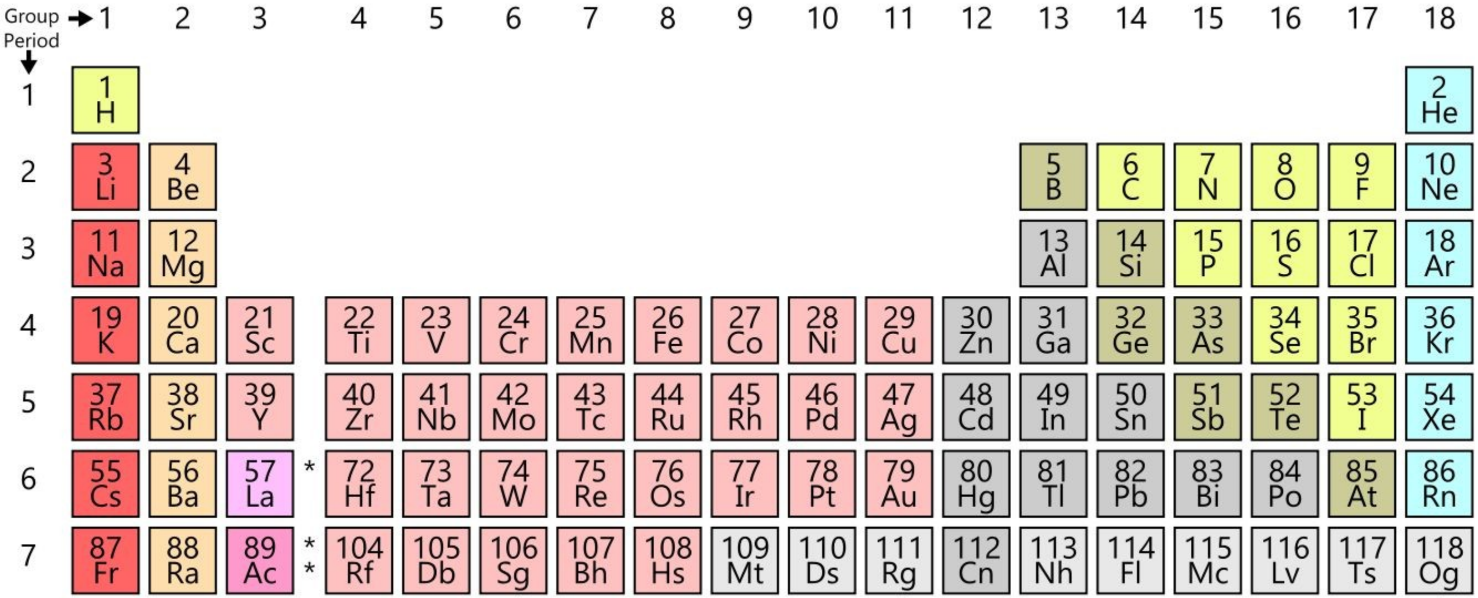
The Periodic Table



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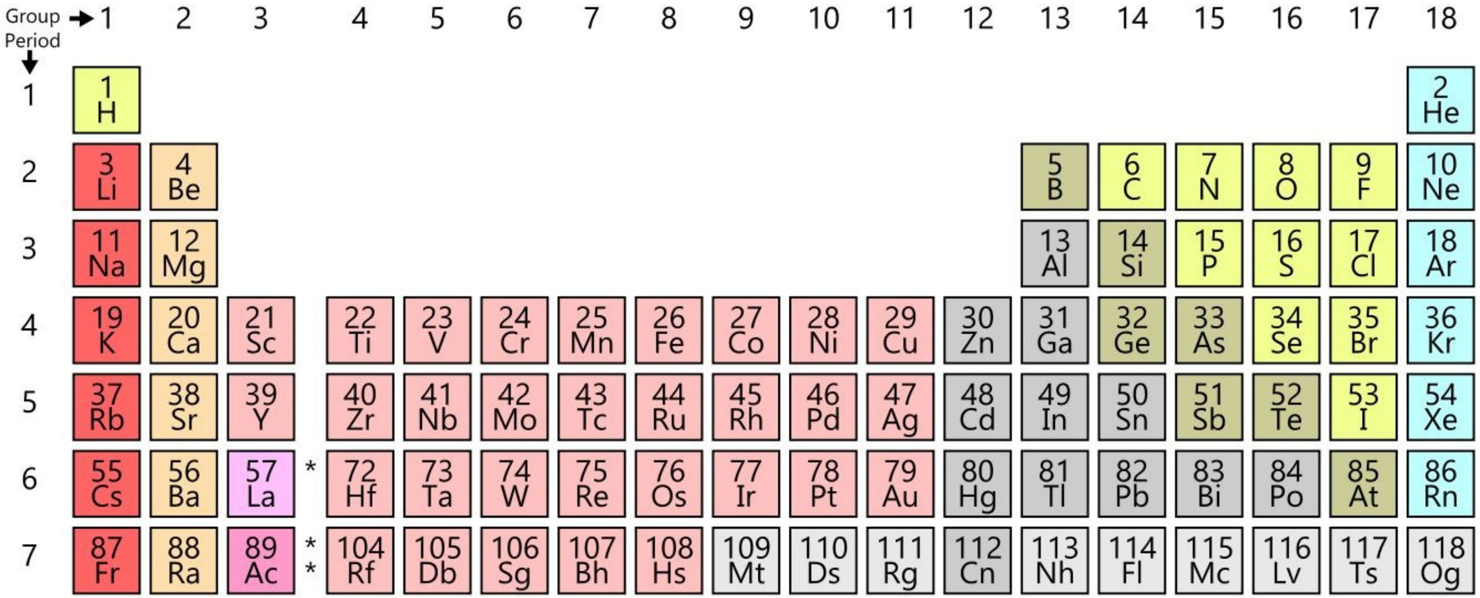
The Periodic Table (SHE Z≥103)



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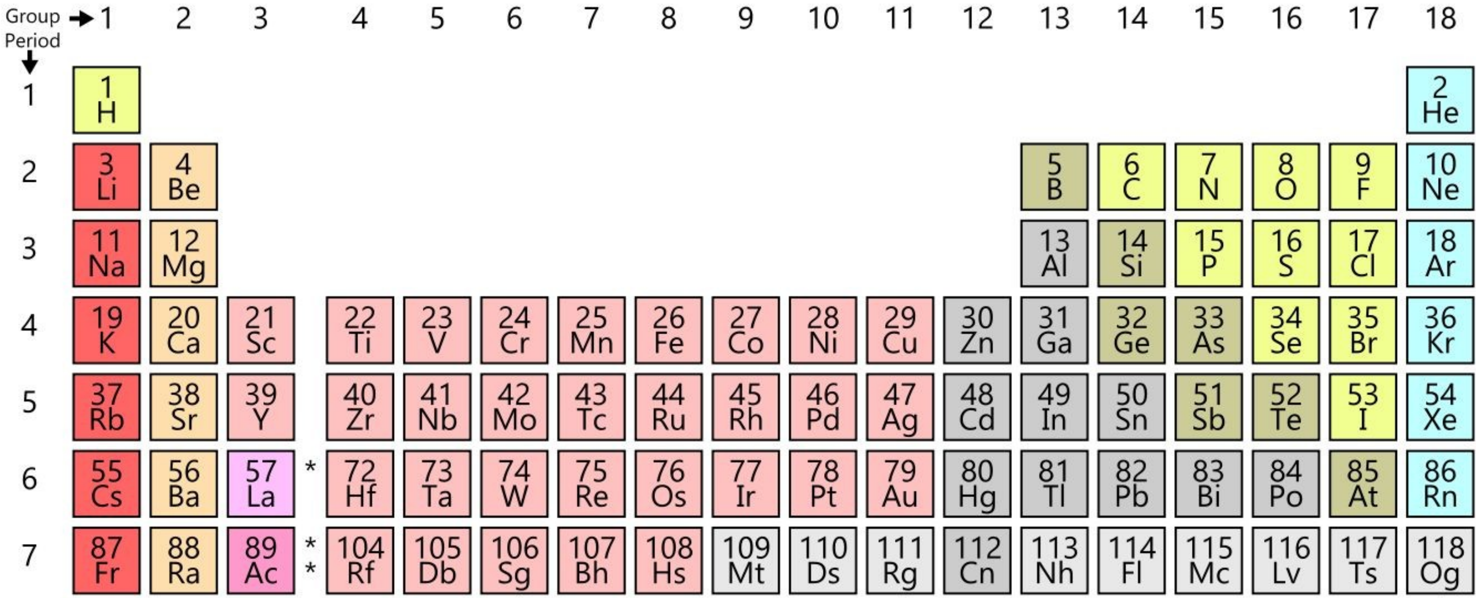

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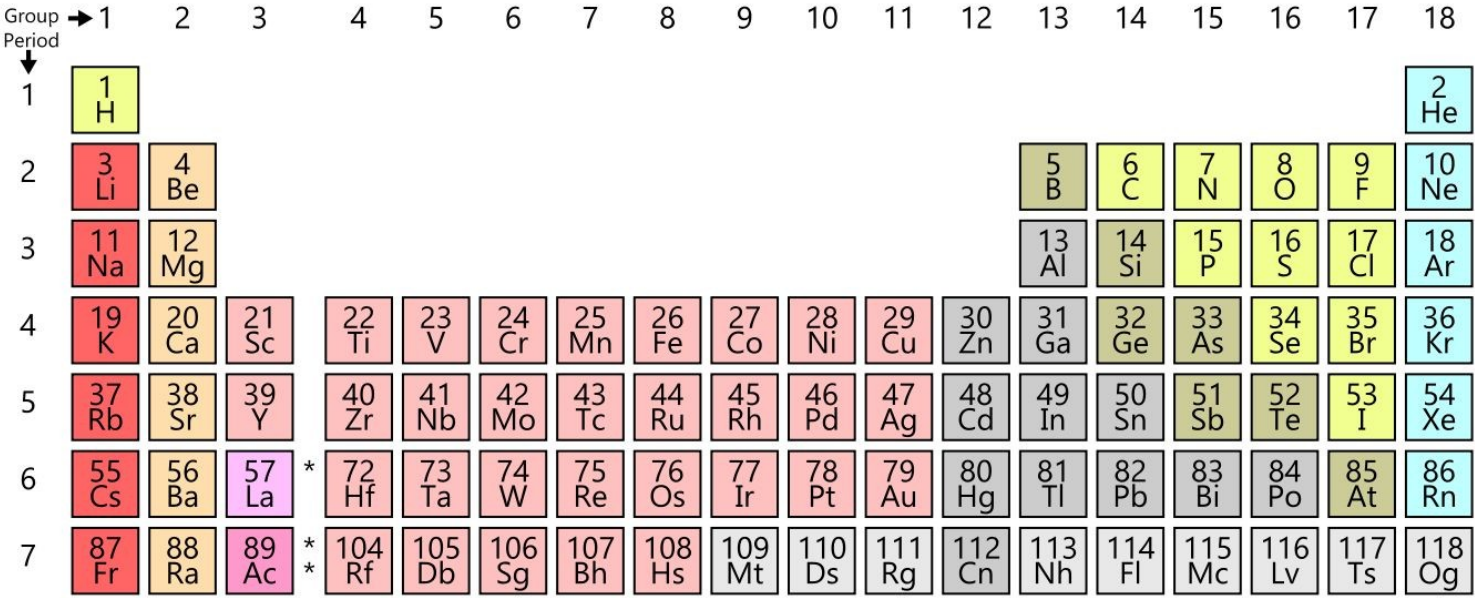

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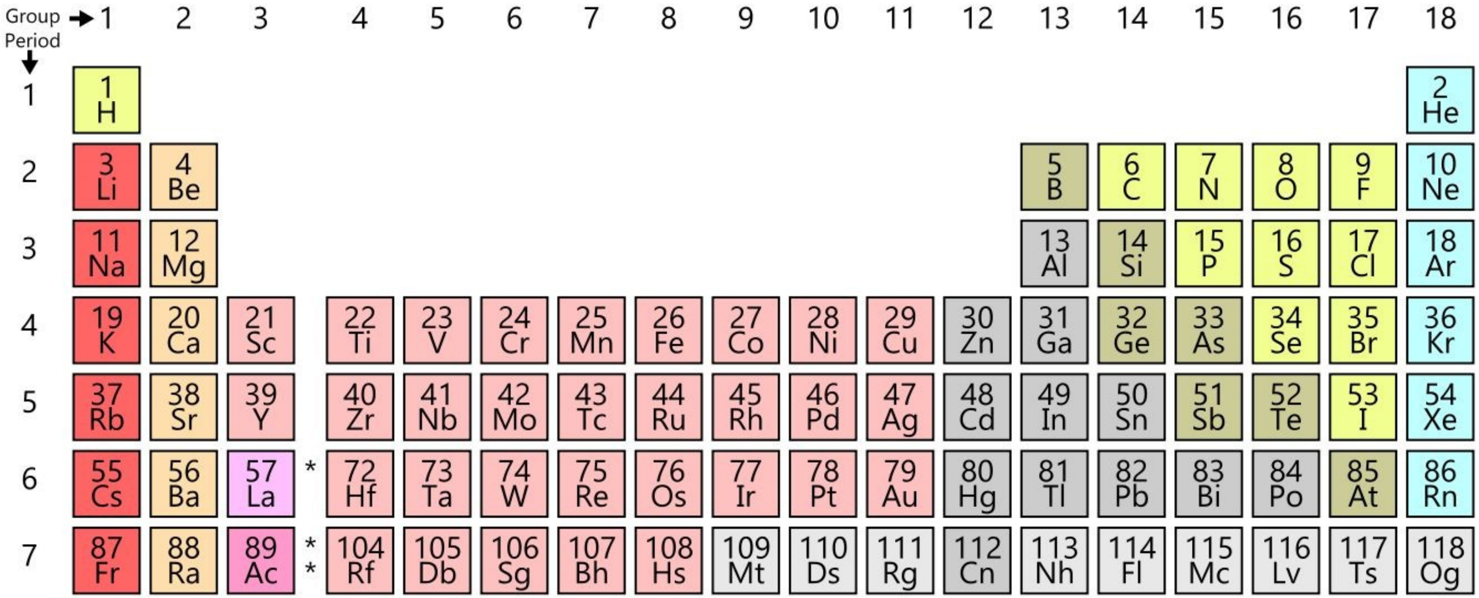

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Strong relativistic effects may influence SHE atomic shell structure resulting in exotic and anomalous properties.

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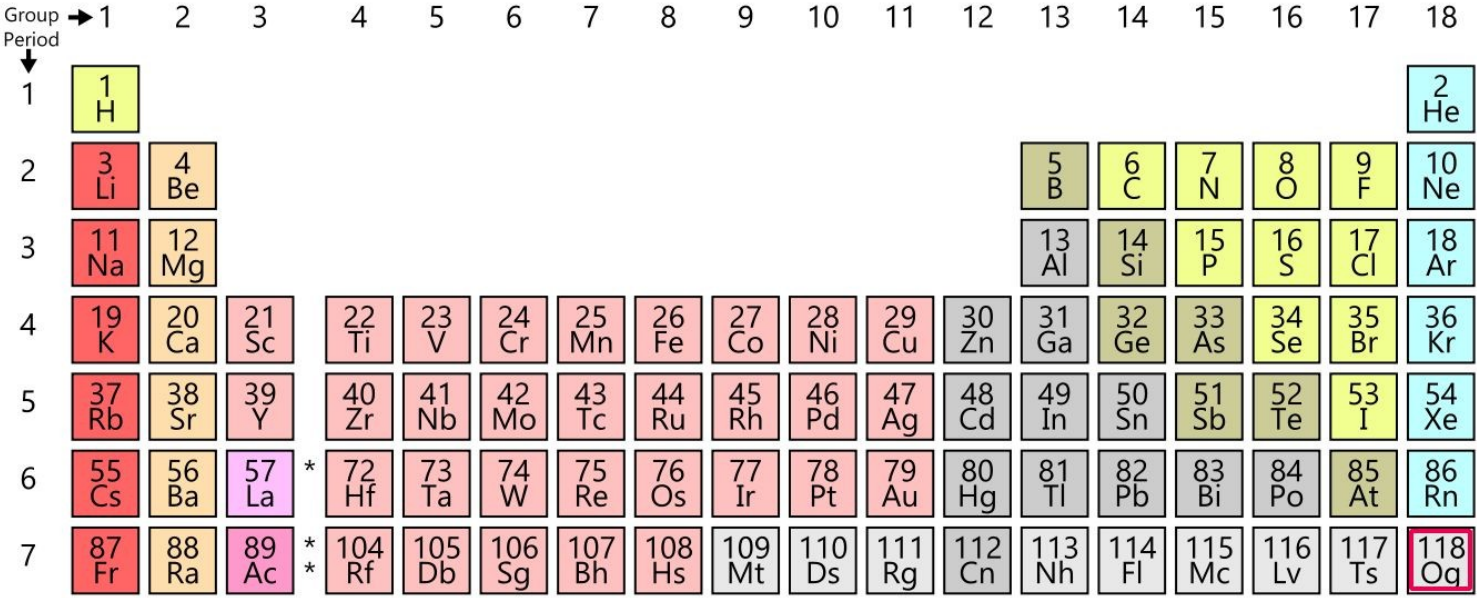

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With *special attention* paid to Og atom $[\mathrm{Rn}]5f^{14}6d^{10}7s^{2}7p^{6}$

Oganesson atom

Og is **not a typical** noble gas element. It is the first noble gas element with a **positive electron affinity** of 0.064 eV [1,2].

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The **conclusion** was deduced from analysis of the ***electron localization function*** (ELF) [4], which was firstly introduced in quantum chemistry to study the distribution of electron density in molecules.

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Electron localization function

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Where $D(r)$ is Dirac-Fock *conditional probability* of finding one spin-like electron in a vicinity of another one with the same spin

$$D(r) = \frac{1}{2}\left[\tau - \frac{1}{4}\frac{|\nabla\rho(r)|^2}{\rho(r)}\right],$$

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And $D_0(r)$ corresponds to *a uniform electron* (Thomas-Fermi) *gas* kinetic energy density

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

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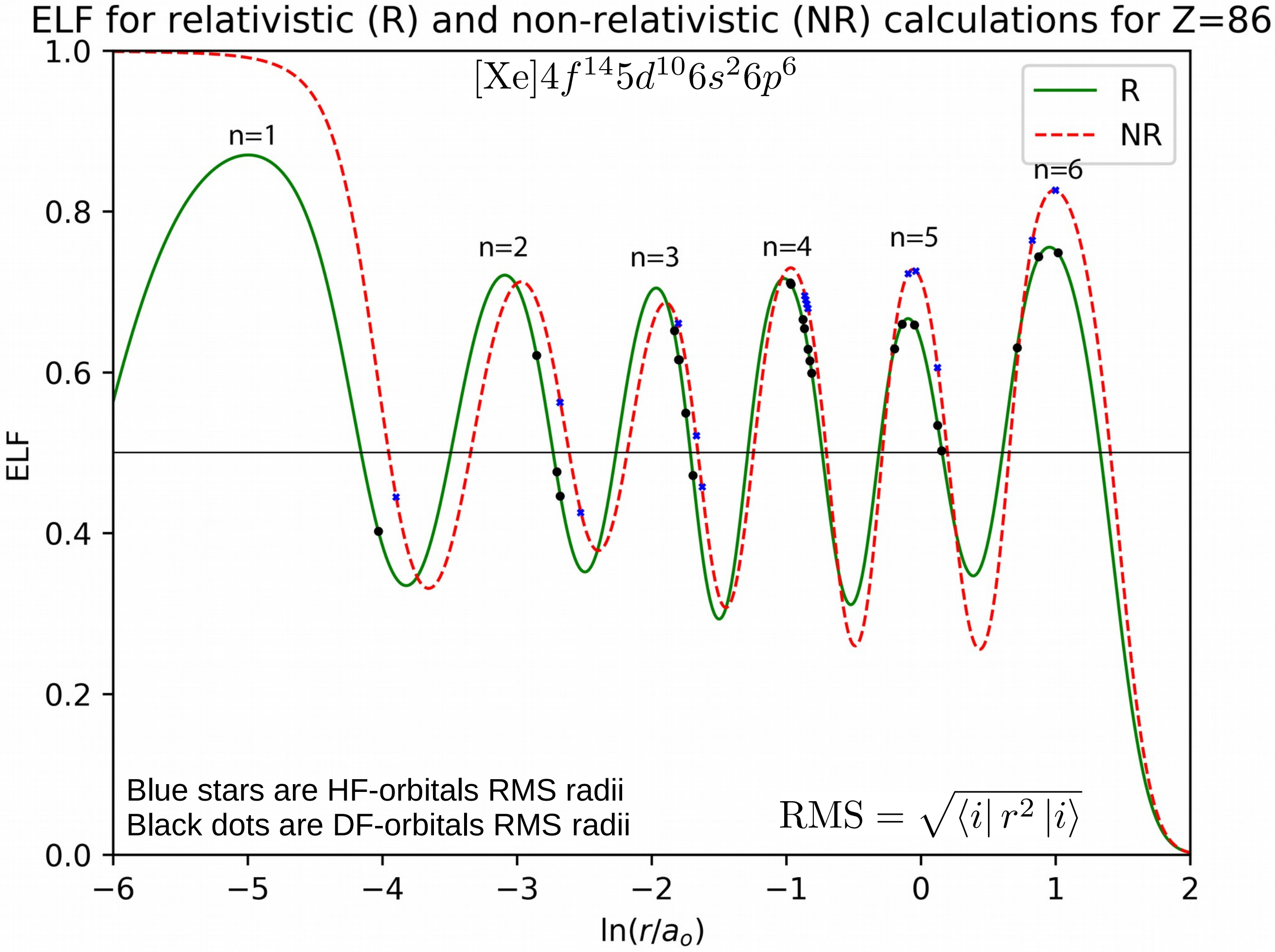
Atomic shells indicated by the ELF maxima and separated by the ELF minima.

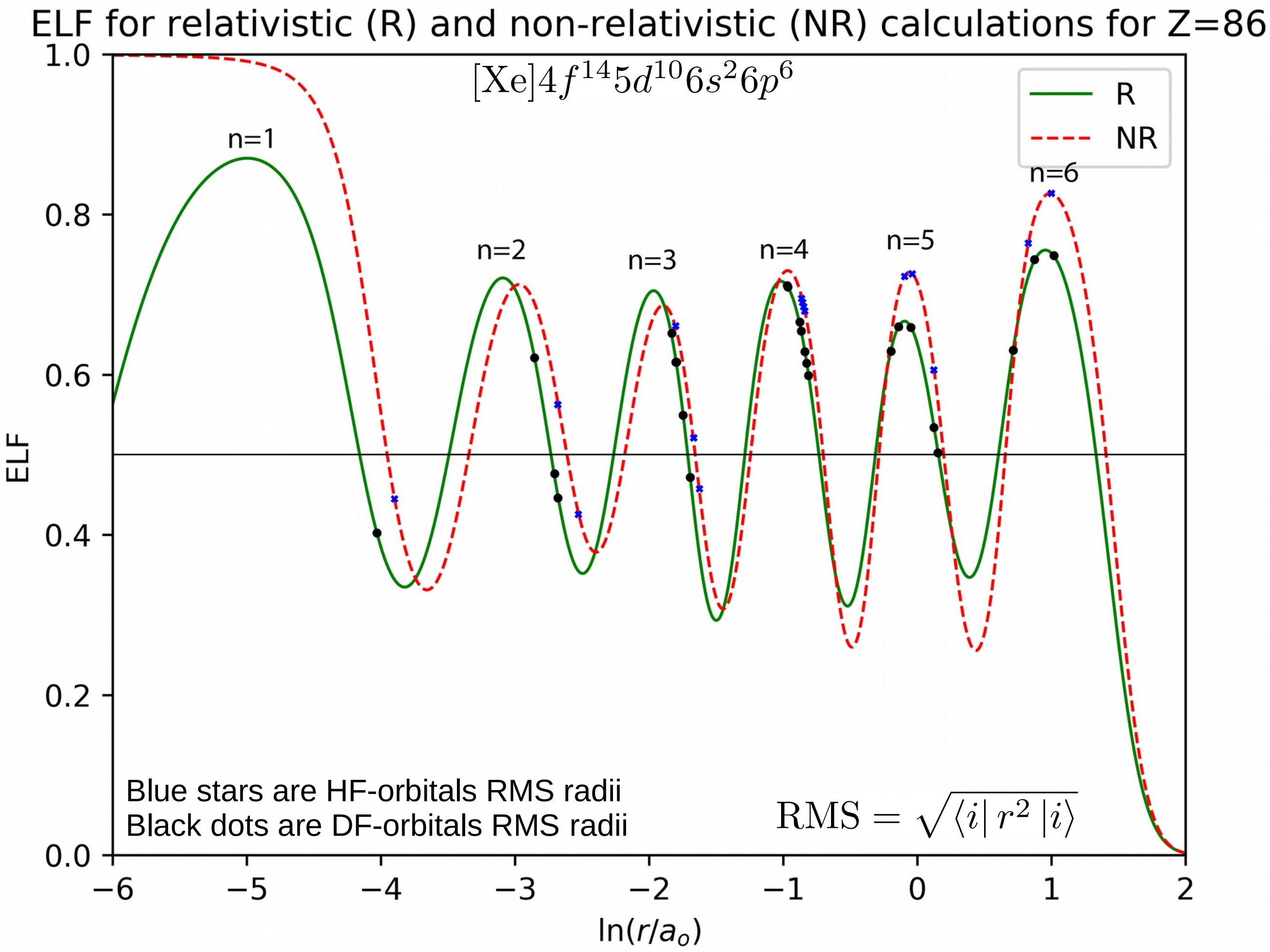
Electron localization function for Z=86



Blue stars are HF-orbitals RMS radii
Black dots are DF-orbitals RMS radii

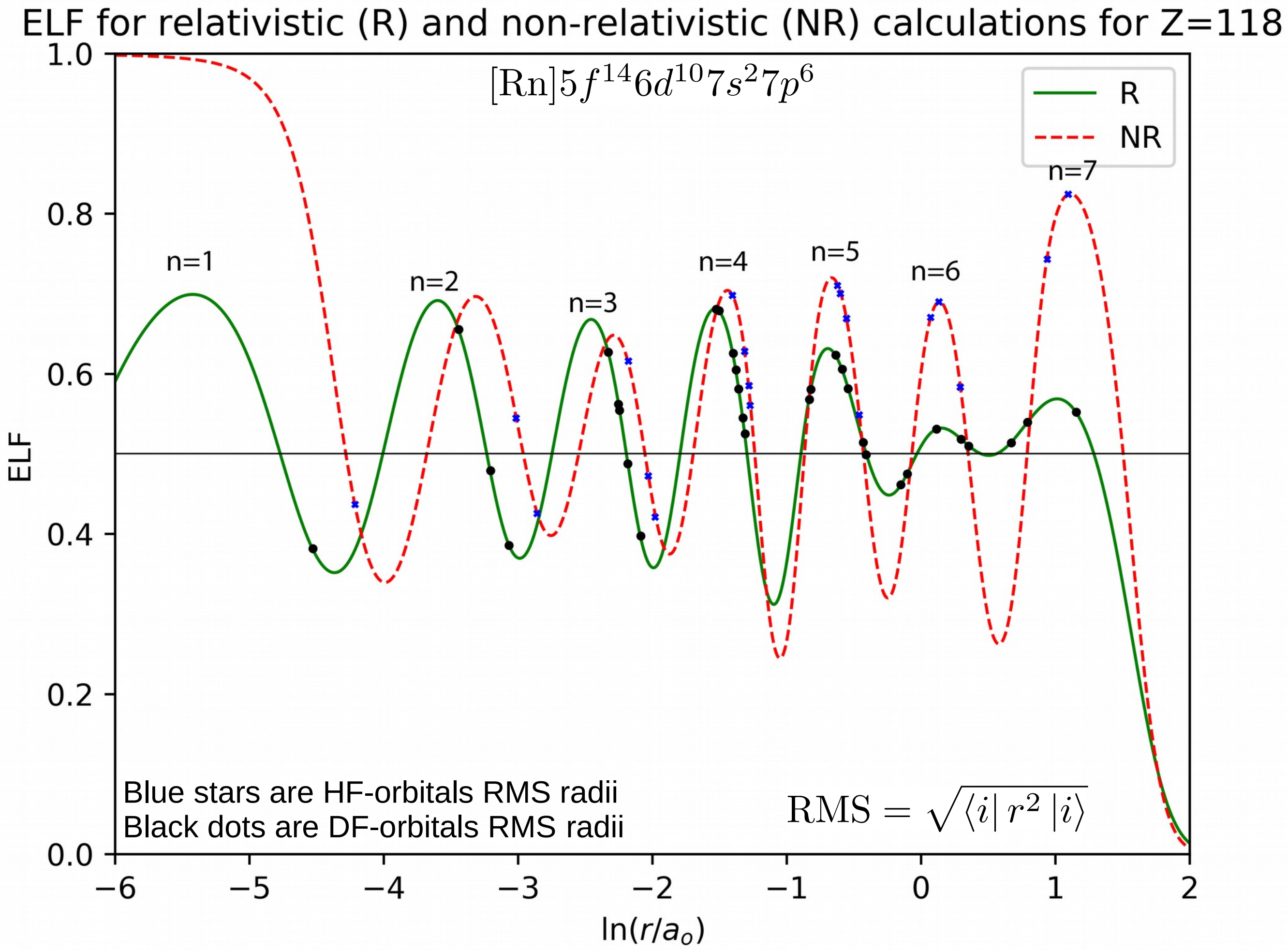
$$\mathrm{RMS} = \sqrt{\langle i|\, r^2 \,|i\rangle}$$

Electron localization function for Z=86



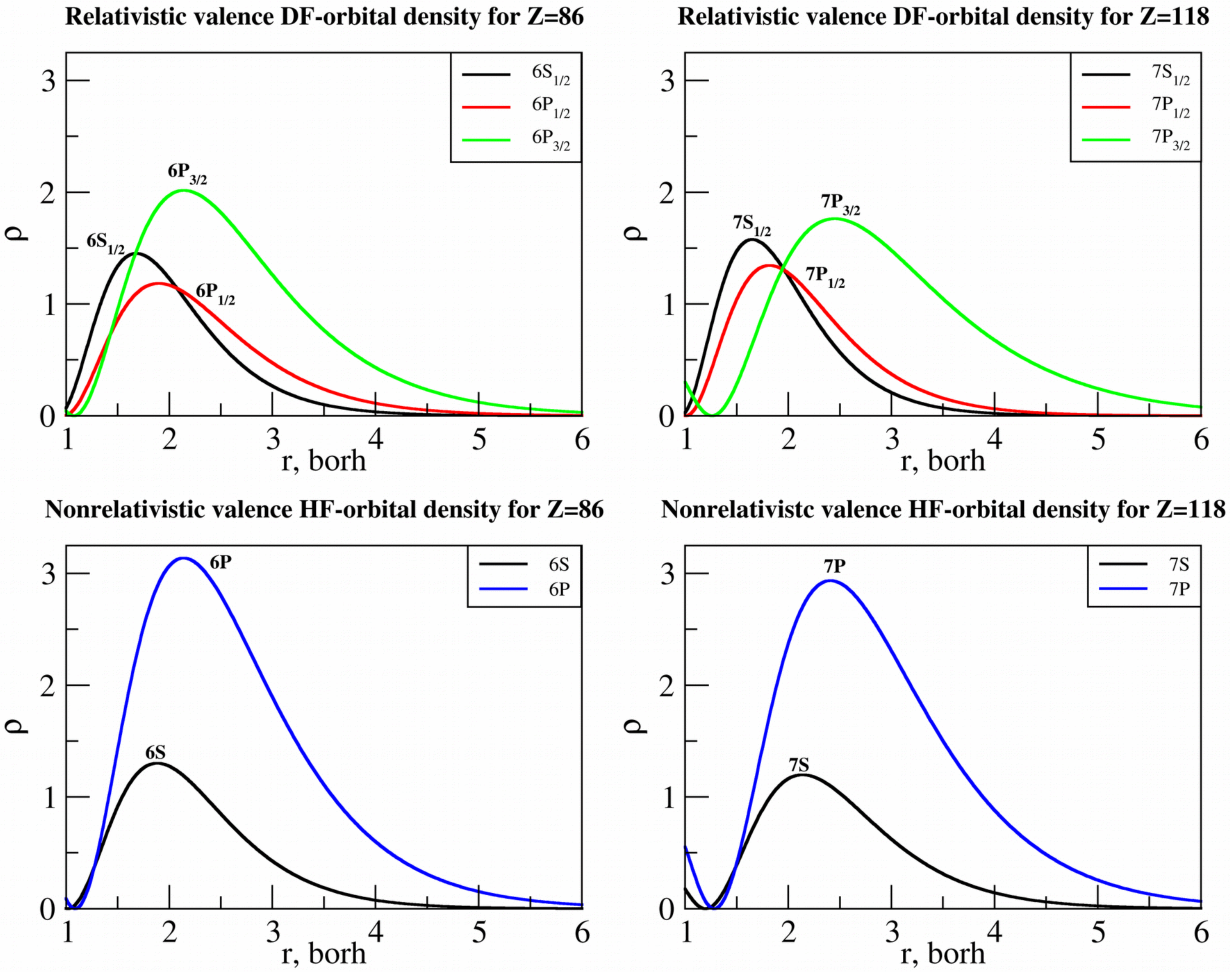
According to ELF results, one can see **clear shell structure** for Radon atom in **both relativistic** DF and **nonrelativistic** HF calculations

Electron localization function for Z=118



Based on ELF results, P. Jerabek, *et al.*, PRL **120**, 053001 (2018) deduced that Og exhibits like a uniform electron gas

Valence shell charge densities for Rn and Og atoms


Relativistic valence DF-orbital density for Z=86

Relativistic valence DF-orbital density for Z=118

Nonrelativistic valence HF-orbital density for Z=86

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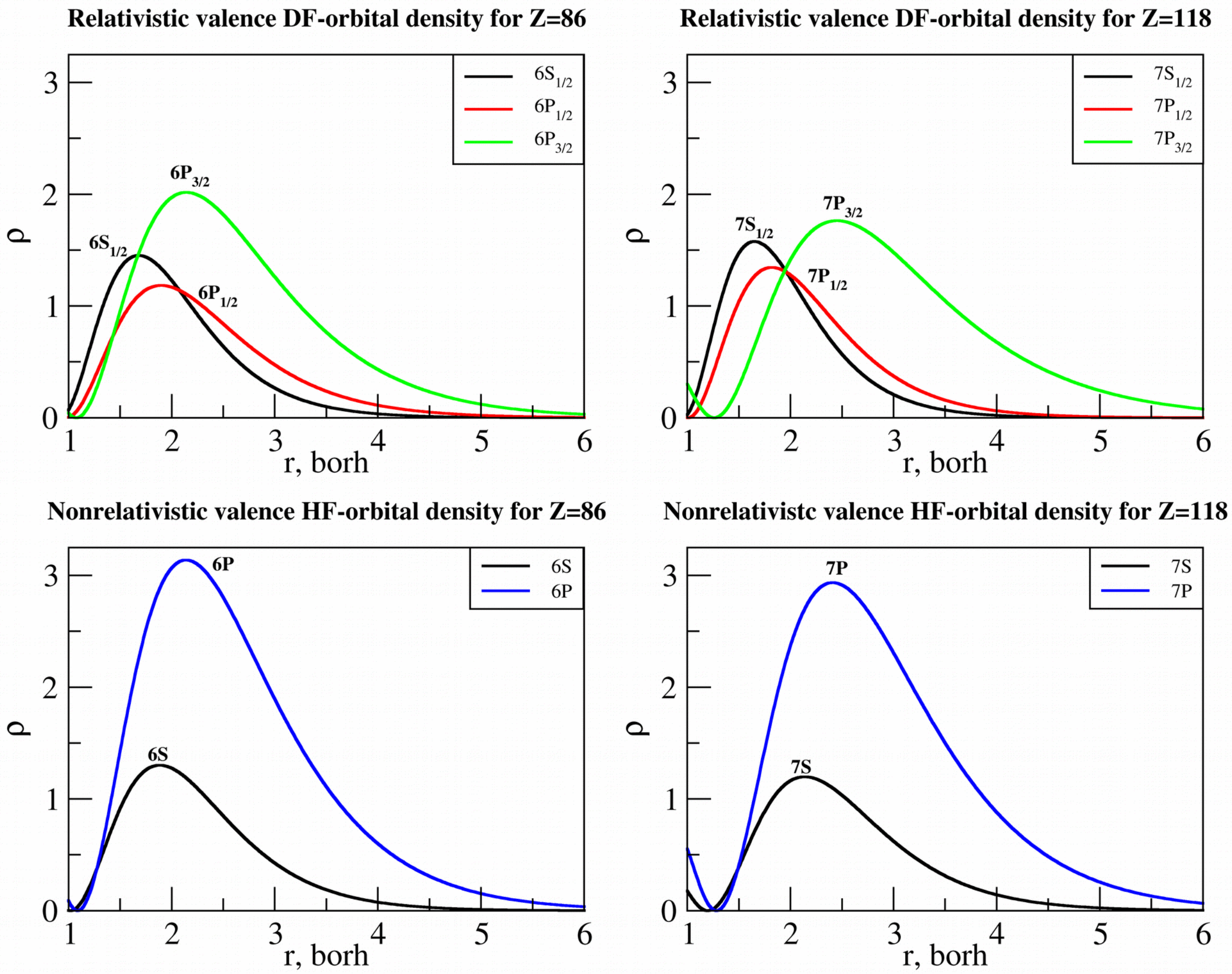
Valence shell charge densities for Rn and Og atoms



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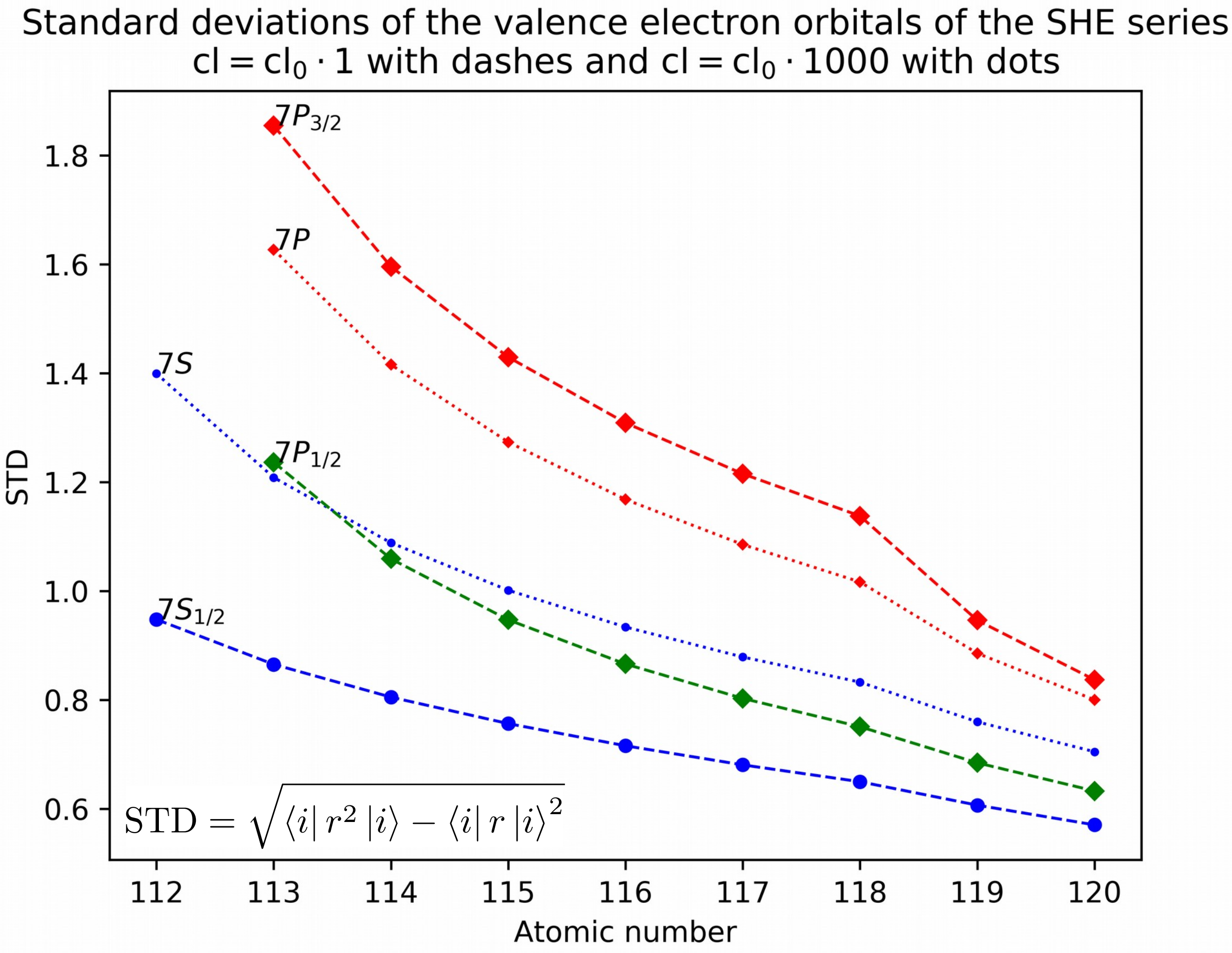
Nonrelativistic valence HF-orbital density for Z=86

Nonrelativistc valence HF-orbital density for Z=118

There is **nothing special** in valence shell charge density in Og atom compare with lighter Rn atom

Widths (STD) of the valence DF-orbitals



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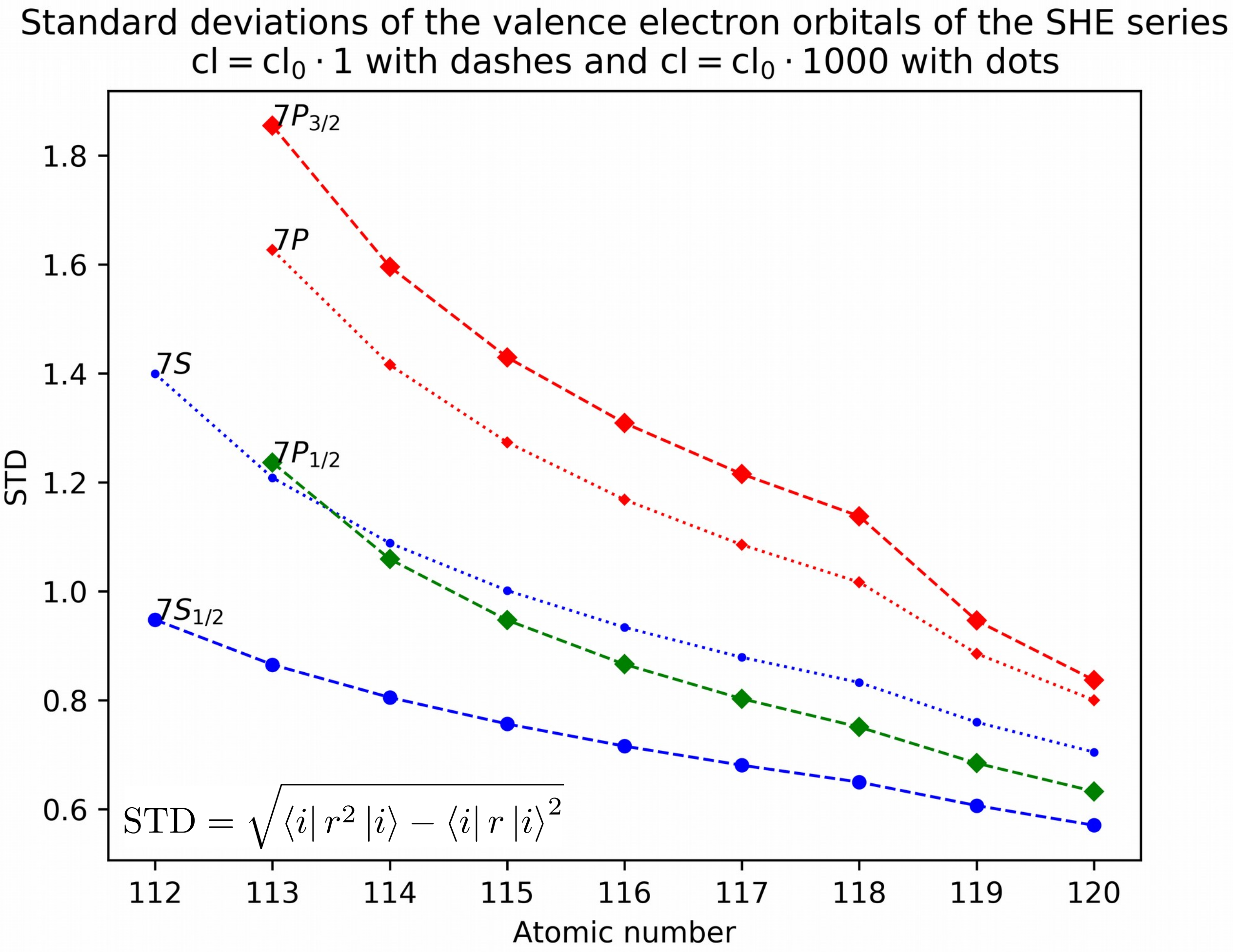


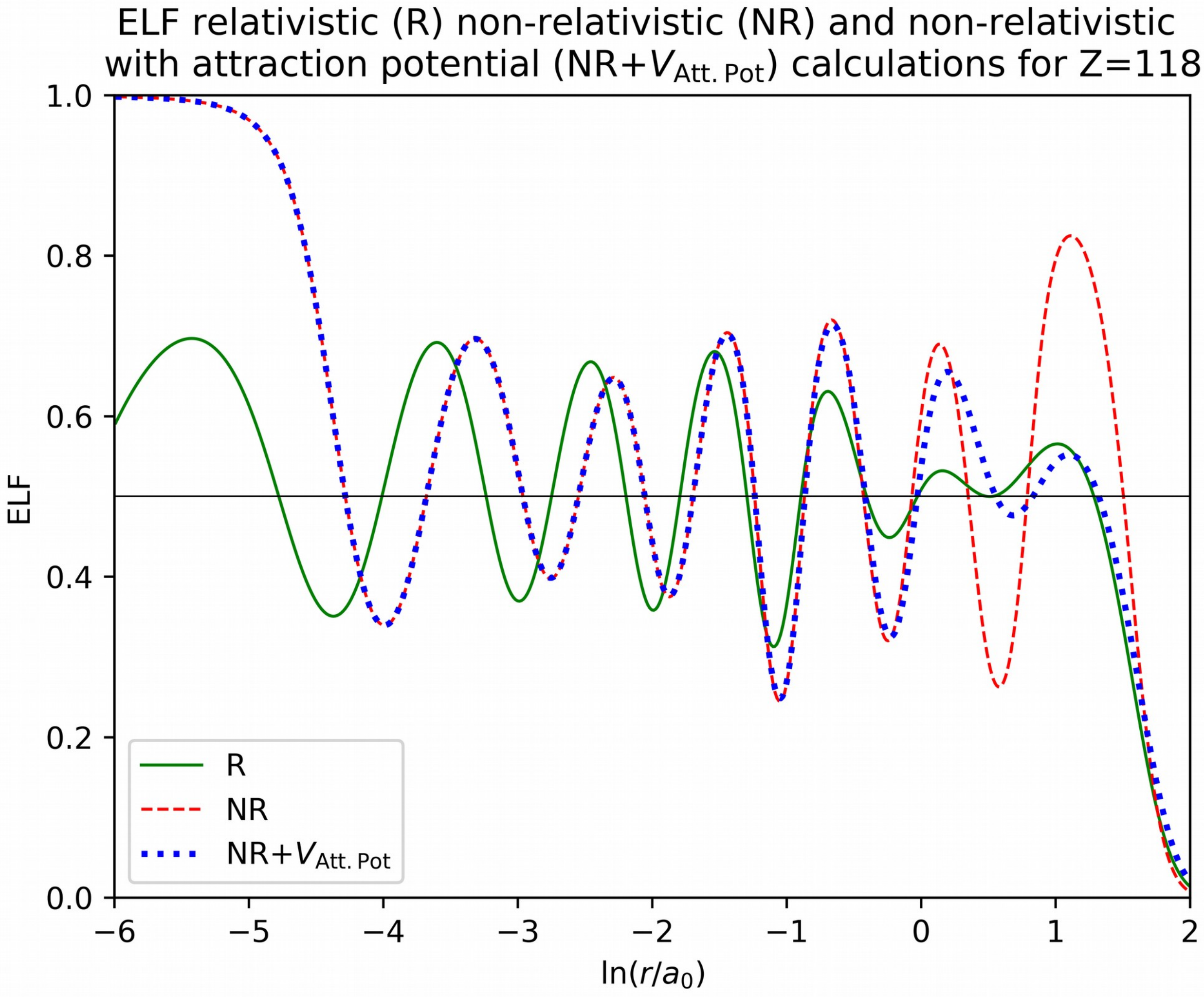
In SHE series **widths** valence orbitals tend to be **more compact** with increase of atomic number

Localized attraction potential

Localized attraction potential $V_{\mathrm{Att.loc.}}(r)$ was added to $7P_{1/2}$ and $7S_{1/2}$ orbitals in Dirac-Fock equations to simulate contraction of the orbitals in nonrelativistic calculations

$$V_{\mathrm{Att.loc.}}(r) = -22500 e^{-140r} \quad \text{[a.u.]}$$

Localized attraction potential



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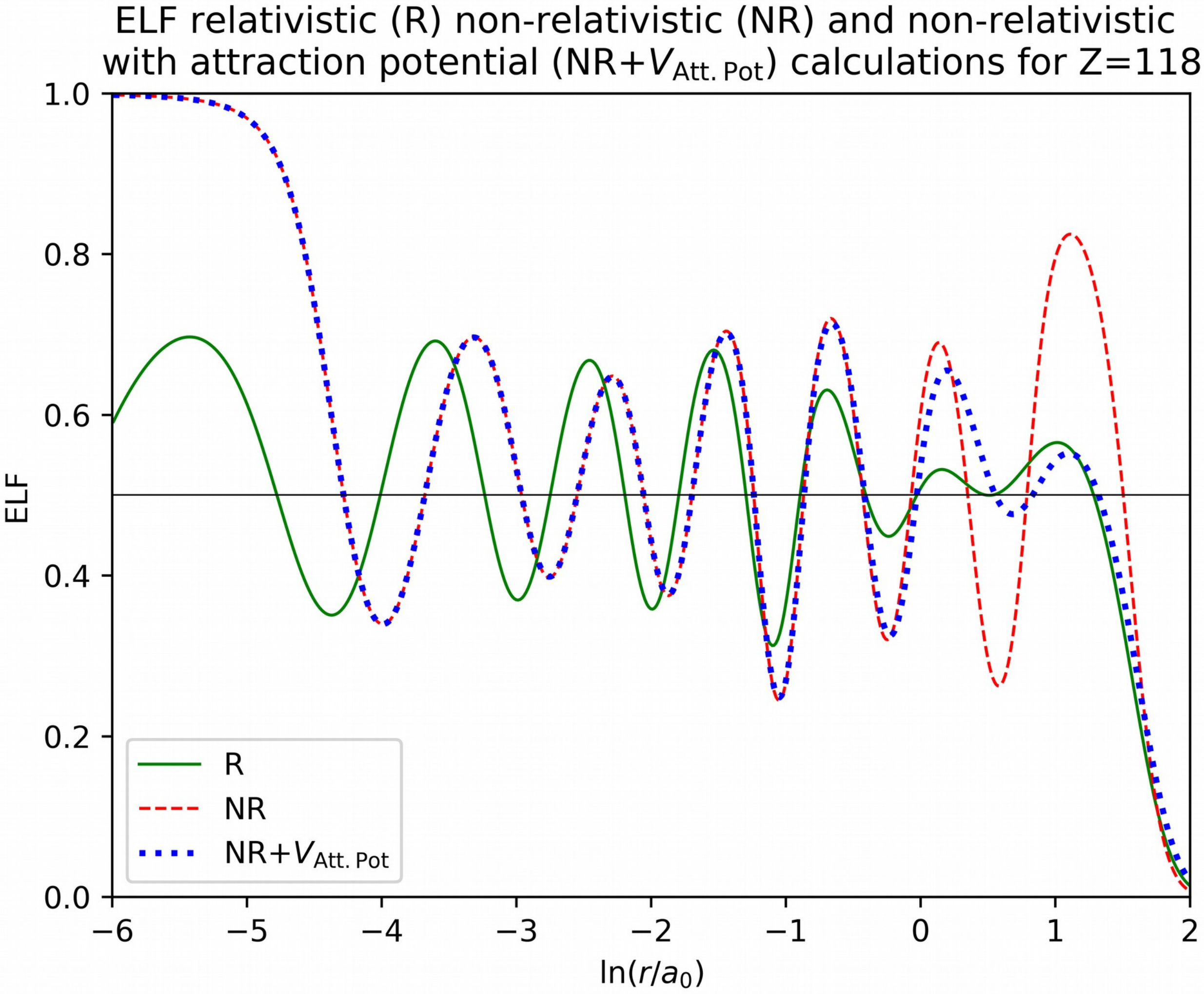

Smearing out which is shown by ELF is a **consequence of overlapping** the densities due to relativistic contraction

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Comparison of ELF for **Og** and **Rn** obtained in our relativistic and non-relativistic calculations **confirms** the **numerical results** of the paper [P. Jerabek, *et al.*, PRL **120**, 053001 (2018)]. Obtained **ELF** values in relativistic the case for n = 7 is close to **0.5**, as it **should be** for uniform electron gas.

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For a uniform electron gas $\mathrm{ELF}(r) = 0.5$, however if $\mathrm{ELF}(r) = 0.5$, it **does not ensure** that charge **density** is **distributed uniformly.**

Thank you!

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Backup

Conditional probability

The probability of finding two particles **simultaneously** at positions 1 and 2 in a multielectron system is given by the following expression:

$$P_2(r_1, r_2) = \sum_{\tau} \rho_2(r_1\tau, r_2\tau | r_1\tau, r_2\tau)$$

where

$$\rho_2(x_1, x_2 | x_1^{'}, x_2^{'}) = \sum_{ijkl} \Gamma_{ij,kl} \varphi_i^*(x_1)\varphi_j^*(x_2)\varphi_k(x_1^{'})\varphi_l(x_2^{'}), \quad x = (r, \tau)$$

Here $\Gamma_{ij,kl}$ is the second-order reduced density matrix in the basis $\varphi_i(x)$

$$\Gamma_{ij,kl} = \frac{1}{2} \langle\Psi| a_i^+ a_j^+ a_l a_k |\Psi\rangle$$

The $P_2(r_1, r_2)$ probability is equal to zero if $r_1 = r_2$

$$P_2(r, r) = 0$$

The definition of the conditional probability (CP) i.e., the probability density of finding electron 2 nearby, r_2 when electron 1 is at r_1 reads

$$P_x(r_1, r_2) = \frac{P_2(r_1, r_2)}{\rho_1(r_1)}, \quad P_x(r_1, r_1) = 0.$$

Electron localization measure

Consider the **exchange charge density** probability defined by

$$P_x(r, r+s) = \frac{P_2(r, r+s)}{\rho_1(r)}.$$

For **small deviations short-range behavior** may be obtained using Taylor expansion

$$P_x(r, r+s) = e^{s\cdot\nabla_2} P_x(r, r_2)\Big|_{r_2=r}.$$

The spherical average of the Taylor expansion is given by

$$\frac{1}{4\pi}\int e^{s\cdot\nabla} d\Omega = \frac{\sinh(s\delta)}{s\nabla} = 1 + \frac{1}{3!}s^2\Delta + \frac{1}{5!}s^4\Delta^2 + \ldots$$

Then

$$P_x(r, r+s) \sim \frac{1}{3!}s^2\Delta_2 P_x(r, r_2)\Big|_{r_2=r}, \quad as \quad s \to 0.$$

The smaller the probability of finding a second like-spin electron near the reference point, **the more highly localized** is the reference electron. Hence, *electron localization measure* is related to the smallness of the expression

$$D(r) = \frac{1}{2}\Delta_2 P_x(r, r_2)|_{r_2=r} = \frac{1}{2}\Delta_2 \frac{P_2(r, r_2)}{\rho_1(r)}\Bigg|_{r_2=r}.$$

Electron localization measure

Collecting altogether, one finds

$$D(r) = \frac{1}{2}\frac{1}{\rho_1(r)}\sum_{\tau}\sum_{ijkl}\Gamma_{ij,kl}\varphi_i^*(r,\tau)\varphi_k(r,\tau)\nabla\varphi_j^*(r,\tau)\nabla\varphi_l(r,\tau).$$

For **one-determinant wave-function**

$$D_{ij} = \delta_{ij}, \qquad \Gamma_{ij,kl} = \frac{1}{2}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk})$$

and

$$\rho_2(x_1x_2|x_1^{'}x_2^{'}) = \rho_1(x_1,x_1^{'})\rho_1(x_2,x_2^{'}) - \rho_1(x_1,x_2^{'})\rho_1(x_2,x_1^{'}),$$

Where

$$\rho_1(r) = \sum_{\tau}\sum_{i}|\varphi_i(r,\tau)|^2.$$

Therefore, in **Dirac-Fock approximation** electron localization measure is given by

$$D(r) = \frac{1}{2}\sum_{j,\tau}|\nabla\varphi_j(r,\tau)|^2 - \frac{1}{4}\frac{1}{\rho_1(r)}|\nabla\rho_1(r)|^2, \qquad D(r) > 0.$$

Thomas-Fermi theory

Consider **free electrons** confined to a box with volume *V.* The *number of states* available in a *momentum range* is given by

$$d^3N = 2\frac{V}{(2\pi)^3}d^3p.$$

Assume that all states up to the Fermi momentum are filled. Then the particle density is

$$\rho = \frac{N}{V} = \frac{1}{\pi^2}\int_0^{p_f} p^2 dp = \frac{1}{3\pi^2}p_f^3.$$

The kinetic energy density is given by

$$\varepsilon_k = \frac{E_k}{V} = \frac{1}{\pi^2}\int_0^{p_f} \frac{p^2}{2}p^2 dp = \frac{1}{10\pi^2}p_f^5.$$

Use this relation between the kinetic-energy density and the particle density to obtain

$$\varepsilon_k = \frac{3}{10}(3\pi^2)^{2/3}\rho^{5/3}.$$