The work of St. Petersburg's group on theory of superheavy elements

Vladimir Shabaev

St. Petersburg State University

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Principal topics

- Relativistic calculations of electronic structure of superheavy elements
- Chemical behavior of superheavy elements in gas-phase experiments: calculations and predictions
- Relativistic calculations of superheavy elements with quantum computers

Electronic structure of superheavy elements

Oganesson $(\mathrm{Og}, Z = 118)$
Ground-state configuration $[\mathrm{Rn}]7s^2 7p^6$ – "noble gas" group.

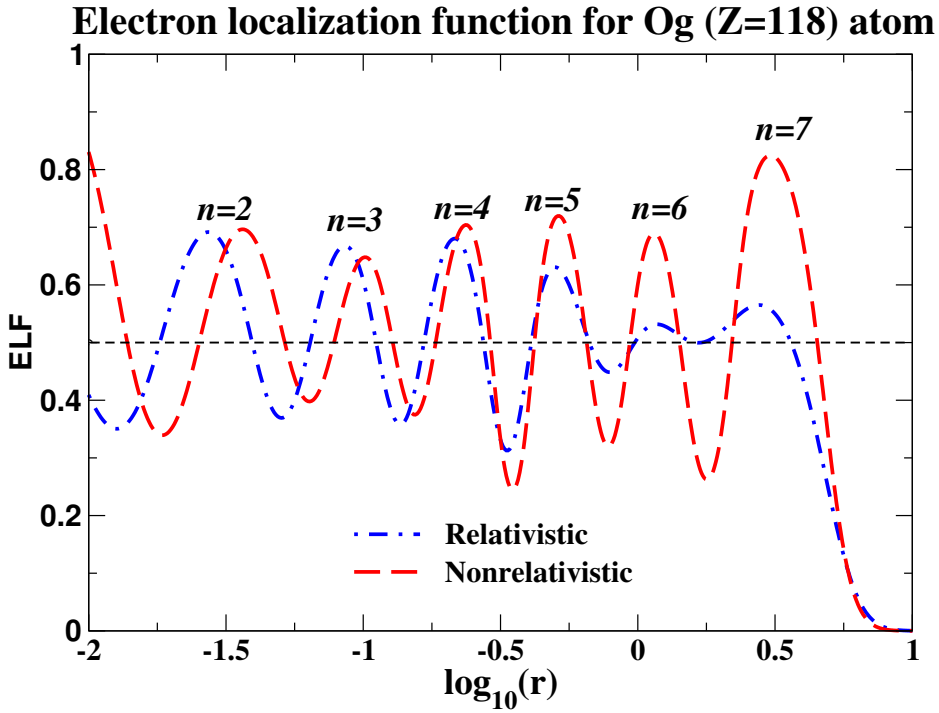
First element from the noble gases, which can form a weakly-bound negatively charged ion.
E. Eliav *et al.*, Phys. Rev. Lett. 77, 5350 (1996).

Bound-state energy of the additional electron is $0.076(10)$ eV.
M. Y. Kaygorodov *et al.*, Phys. Rev. A 104, 012819 (2021).

Calculations of the ionization potentials and electron affinities of elements
$\mathrm{Rg}, Z = 111 \quad \mathrm{Cn}, Z = 112$
$\mathrm{Nh}, Z = 113 \quad \mathrm{Fl}, Z = 114.$
M. Y. Kaygorodov *et al.*, Phys. Rev. A 106, 062805 (2022).

Study of the valence electronic density distribution using the electron localization function (ELF)

The value of ELF equal to 0.5 does not mean that the electron density is uniformly distributed.



I. I. Tupitsyn *et al.*, Opt. Spectr. 130, 1022 (2022).

Electronic structure of superheavy elements

Possible concepts of the extended Periodic Table, which include relativistic, correlation and QED effects.

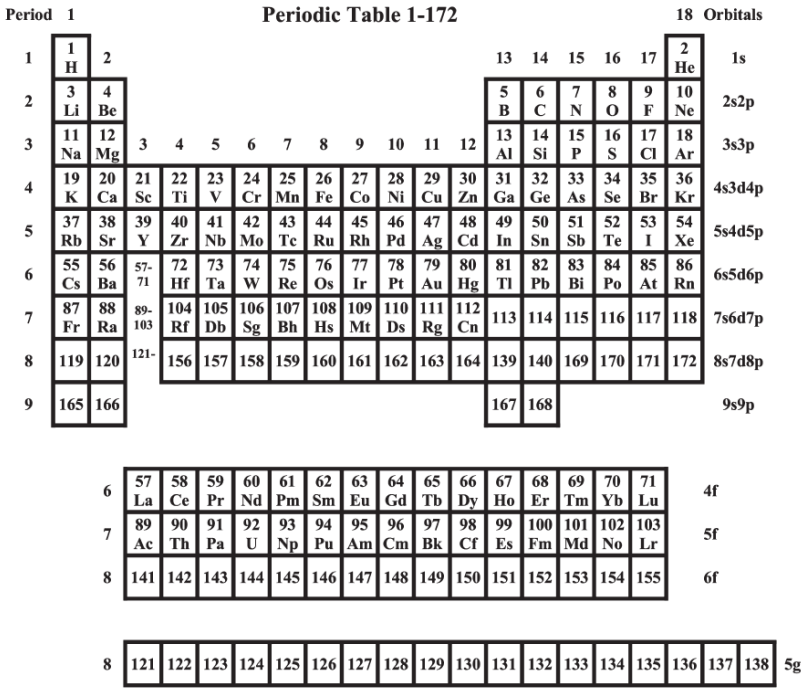


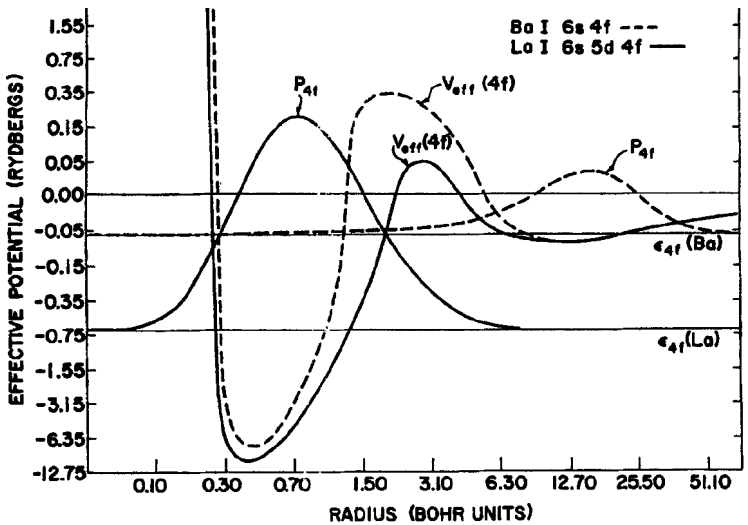
Image taken from P. Pyykkö, Chem. Rev. 112, 371 (2012).

QED effects in superheavy elements
A. V. Malyshev *et al.*, Phys. Rev. A 106, 012806 (2022).

Study of SHEs with Z=120-170
I. M. Savelyev, M. Y. Kaygorodov, Y. S. Kozhedub *et al.*, to be published.

Study of the properties of the $5g$-elements – superactinides

One of the features of the electronic structure of superheavy elements with $5g$-shell $(Z = 125 - 145)$ is that in these elements the so-called orbital collapse can take place, which is analogous to those of the case of rare earth elements.



Example of the orbital collapse for Barium $(\mathrm{Ba}, Z = 56)$.
Image taken from J.-R Connerade and R. C. Kamatak, *Handbook on the Physics and Chemistry of Rare Earths* 28, 1 (2000).

Chemical properties of HgO, CnO, and FlO

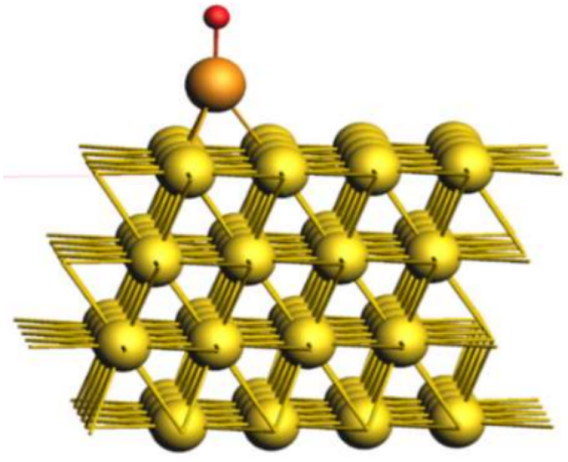
Currently investigated:

- Formation energy of oxides in the recoil chamber. Most probable ones are:
  - Hg + O = HgO (E = -0.618 eV)
  - Cn + O = CnO (E = -0.733 eV)
  - Fl + O = FlO (E = -1.947 eV)
- Molecular properties evaluated within *ab-initio* coupled-cluster approach with single, double and perturbative triple excitations:
  - Bond length
  - Ionization potential
  - Dipole moment
  - Electric dipole polarizability
- The calculated spectroscopic constants are indicative of the following trend in the reactivity of the oxides HgO > FlO > CnO.

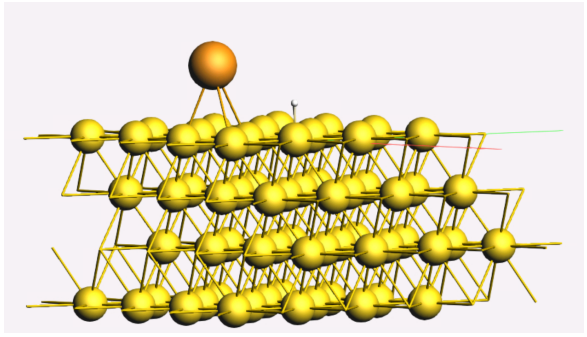
A. A. Kotov, Y. S. Kozhedub, D. A. Glazov, M. Ilias, V. Pershina, V. M. Shabaev, Chem. Phys. Chem., 16 November 2022.

Adsorption of SHEs and their compounds on Au(111) Surface

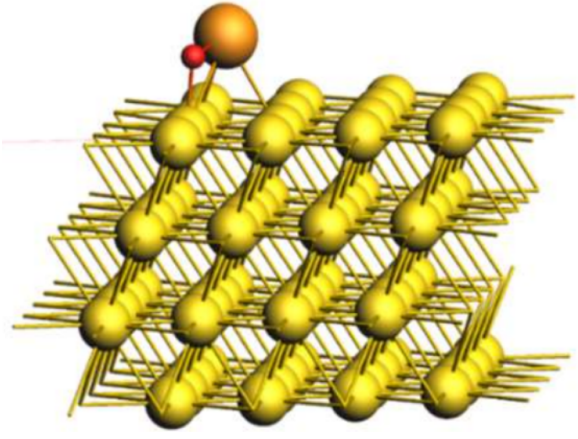
Talks at this meeting by Anton Ryzhkov and Dmitry Glazov:



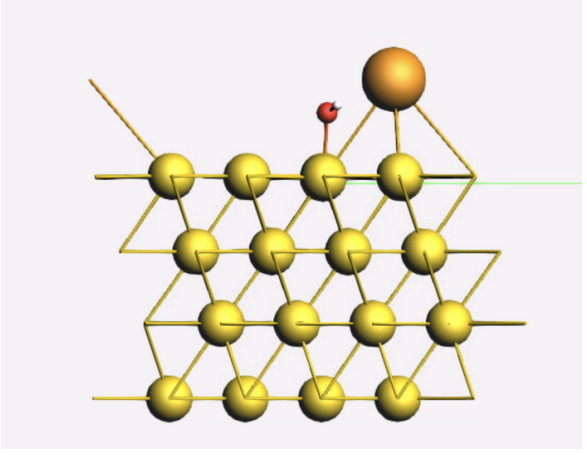
CnO



OgH



FlO

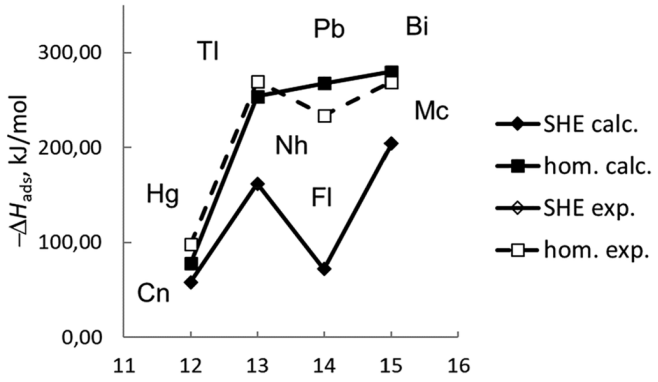


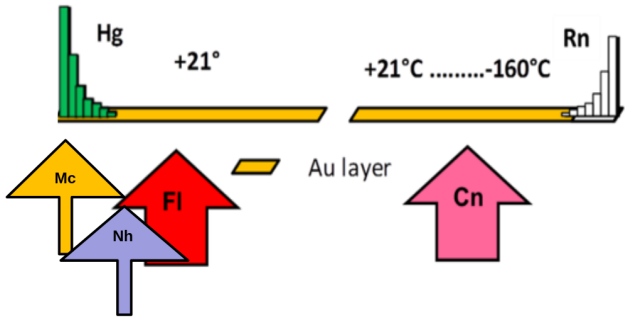
OgOH

Adsorption energy studies of SHEs and their compounds on Au(111) Surface

Talks at this meeting by Anton Ryzhkov and Dmitry Glazov:

Previous study:
Hg/Cn, Tl/Nh, and Bi/Mc

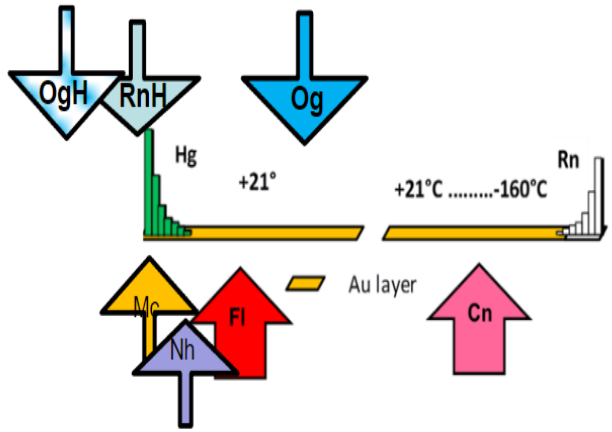




V. Pershina *et al.*, Inorg. Chem. **60**, 9796 (2021)
V. Pershina and M. Iliaś, Dalton Trans. **51**, 7321 (2022)

Present work:

- atoms: Hg/Cn, Tl/Nh, Pb/Fl, Bi/Mc, Po/Lv, At/Ts, and Rn/Og
- hydrids: BiH/McH, PoH/LvH, Ath/TsH, and RnH/OgH
- oxides: HgO/CnO and PbO/FlO
- hydroxides: AtOH/TsOH and RnOH/OgOH



Calculation of the moscovium ($Z = 115$) ground-state energy by quantum algorithms

V. A. Zaytsev, M. E. Groshev, I. A. Maltsev *et al.*, arXiv:2209.00463.

Details:

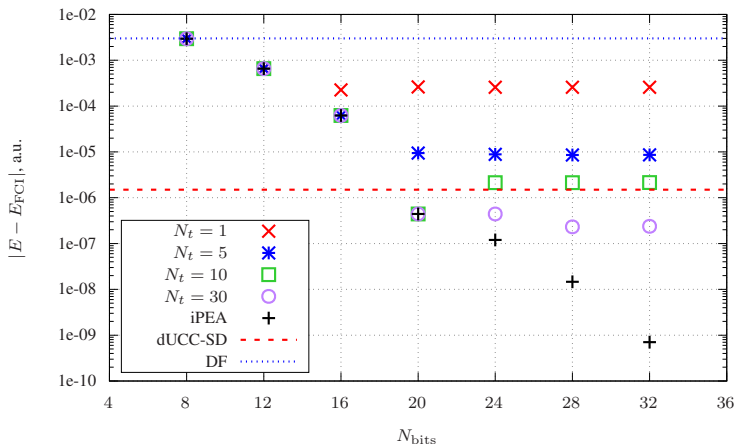
- 15 active electrons
- 26 orbitals
- ∼500 000 Sl. dets.

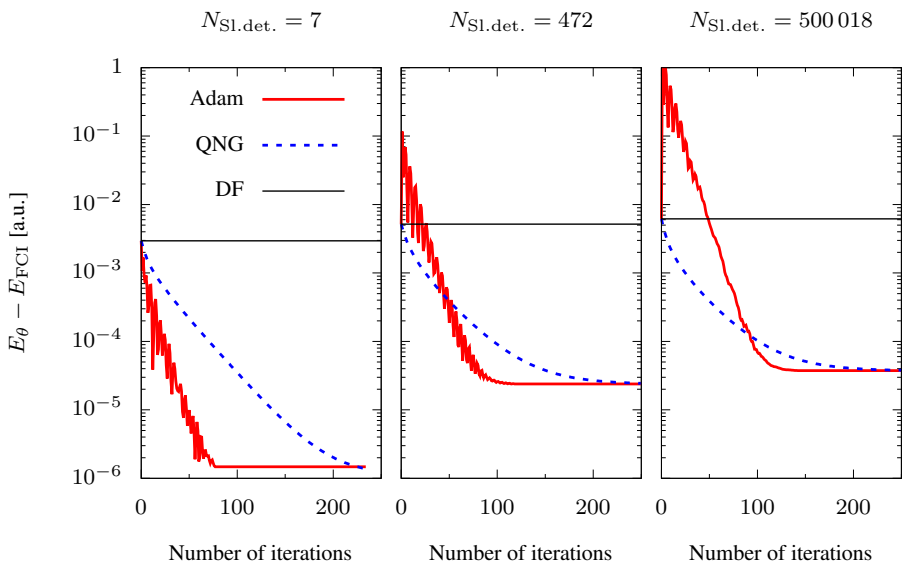
iterative Phase Estimation

- Trotterization
- Number of bits
- Gates reduction strategies

Variational Quantum Eigensolver

- Unitary Coupled Cluster ansatz
- Hardware Efficient ansatz
- Adam vs Quantum Natural Gradients





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