

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

Vladimir Shabaev

St. Petersburg State University

18 December, 2022

## 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 (Og,  $Z = 118$ )

Ground-state configuration  $[\text{Rn}]7s^27p^6$  –  
“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

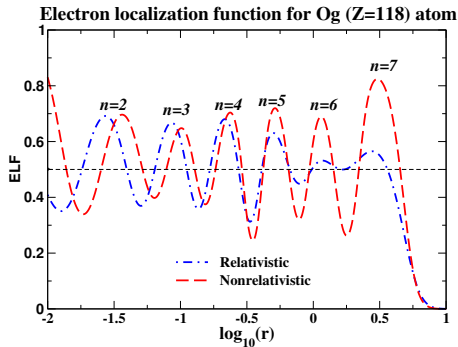
Rg,  $Z = 111$  Cn,  $Z = 112$

Nh,  $Z = 113$  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.

Periodic Table 1-172

1	2											13	14	15	16	17	18	
H	He											Al	Si	P	S	Cl	Ar	
3	4											5	6	7	8	9	10	
Li	Be											B	C	N	O	F	Ne	
11	12	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
Na	Mg											Al	Si	P	S	Cl	Ar	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cu	113	114	115	116	117	118	
119	120	121	156	157	158	159	160	161	162	163	164	139	140	169	170	171	172	
165	166											167	168					

57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
141	142	143	144	145	146	147	148	149	150	151	152	153	154	155

121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

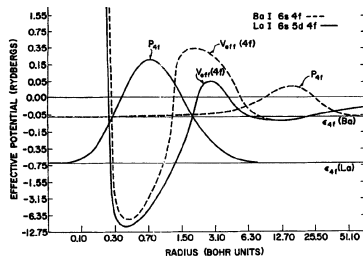
Image taken from P. Pyykkö, Chem. Rev. 112, 371 (2012).

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 (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 FIO

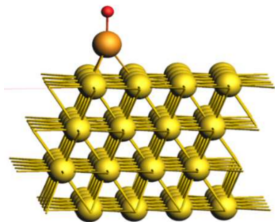
Currently investigated:

- Formation energy of oxides in the recoil chamber. Most probable ones are:
  - $\text{Hg} + \text{O} = \text{HgO}$  ( $E = -0.618$  eV)
  - $\text{Cn} + \text{O} = \text{CnO}$  ( $E = -0.733$  eV)
  - $\text{Fl} + \text{O} = \text{FIO}$  ( $E = -1.947$  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  $\text{HgO} > \text{FIO} > \text{CnO}$ .

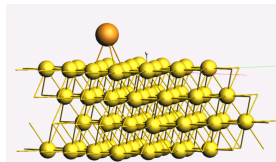
A. A. Kotov, Y. S. Kozhedub, D. A. Glazov, M. Ilias, V. Pershina, V. M. Shabaev, Chem. Phys. Chem., 16 November 2022.

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

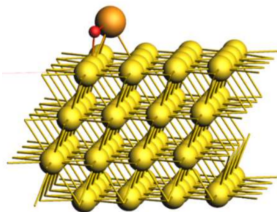
Talks at this meeting by Anton Ryzhkov and Dmitry Glazov:



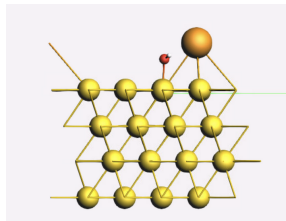
CnO



OgH



FIO



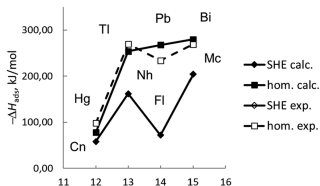
OgOH

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

Talks at this meeting by Anton Ryzhkov and Dmitry Glazov:

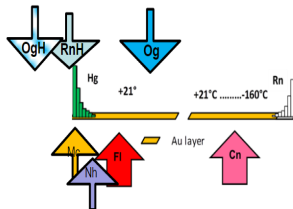
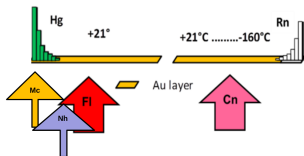
Previous study:

Hg/Cn, Tl/Nh, and Bi/Mc



Present work:

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



V. Pershina *et al.*, *Inorg. Chem.* **60**, 9796 (2021)

V. Pershina and M. Iliás, *Dalton Trans.* **51**, 7321 (2022)

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

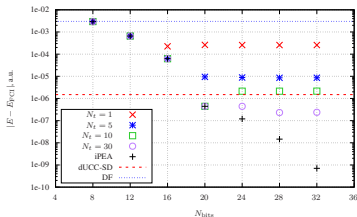
V. A. Zaytsev, M. E. Groshev, I. A. Maltsev *et al.*, arXiv:2209.00463.

## Details:

- 15 active electrons
- 26 orbitals
- $\sim 500\,000$  Sl. dets.

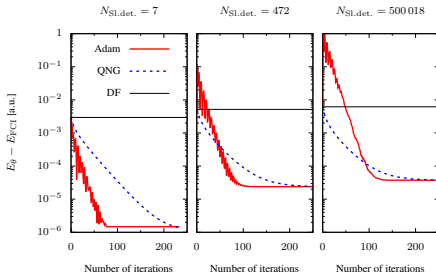
## iterative Phase Estimation

- Trotterization
- Number of bits
- Gates reduction strategies



## Variational Quantum Eigensolver

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





**Thank You for Your Attention**