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## List of publications:

### 2024 Uncovering Chemical Homology of Superheavy Elements: A Close Look at Astatine

Yu. A. Demidov, A. A. Shalaevsky, A. V. Oleynichenko, A. A. Rusakov

ChemRxiv (2024)

doi: 10.26434/chemrxiv-2024-6nl51

### 2024 Radiative lifetime of the $A^2\Pi_{1/2}$ state in RaF with relevance to laser cooling

M. Athanasakis-Kaklamanakis, S. G. Wilkins, P. Lassegues, L. Lalanne, J. R. Reilly, O. Ahmad, M. Au, S. W. Bai, J. Berbalk, C. Bernerd, A. Borschevsky, A. A. Breier, K. Chrysalidis, T. E. Cocolios, R. P. de Groote, C. M. Fajardo-Zambrano, K. T. Flanagan, S. Franchoo, R. F. Garcia Ruiz, D. Hanstorp, R. Heinke, P. Imgram, A. Koszorús, A. A. Kyuberis, J. Lim, Y. C. Liu, K. M. Lynch, A. McGlone, W. C. Mei, G. Neyens, L. Nies, A. V. Oleynichenko, A. Raggio, S. Rothe, L. V. Skripnikov, E. Smets, B. van den Borne, J. Warbinek, J. Wessolek, X. F. Yang, the ISOLDE Collaboration

arXiv:2403.09336 [physics.atom-ph] (2024)

doi: 10.48550/arXiv.2403.09336

### 2024 Optical cycling in charged complexes with Ra–N bonds

T. Isaev, A. V. Oleynichenko, D. A. Makinskii, A. Zaitsevskii

Chem. Phys. Lett. 845, 141301 (2024)

doi: 10.1016/j.cplett.2024.141301

### 2024 Excitation of the $^{229}\text{Th}$ nucleus by the hole in the inner electronic shells

M. G. Kozlov, A. V. Oleynichenko, D. Budker, D. A. Glazov, Y. V. Lomachuk, V. M. Shabaev, A. V. Titov, I. I. Tupitsyn, A. V. Volotka

Phys. Rev. A, 109(4), 042806 (2024)

doi: 10.1103/PhysRevA.109.042806

**2024** Compound-tunable embedding potential method to model local electronic excitations on *f*-element ions in solids: Pilot relativistic coupled cluster study of Ce and Th impurities in yttrium orthophosphate, YPO<sub>4</sub>

A. V. Oleynichenko, Y. V. Lomachuk, D. A. Maltsev, N. S. Mosyagin, V. M. Shakhova, A. Zaitsevskii, A. V. Titov

Phys. Rev. B, 109(12), 125106 (2024)

doi: 10.1103/PhysRevB.109.125106

**2023** Direct calculation of transition matrix elements in relativistic coupled cluster theory

A. V. Oleynichenko, A. V. Zaitsevskii, S. V. Kondratyev, E. Eliav

Opt. Spectrosc. 131(11), 1471 (2023)

doi: 10.61011/OS.2023.11.57024.5658-23

**2023** Nuclear charge radii of silicon isotopes

K. König, J. C. Berengut, A. Borschevsky, A. Brinson, B. A. Brown, A. Dockery, S. Elhatisari, E. Eliav, R. F. Garcia Ruiz, J. D. Holt, B.-S. Hu, J. Karthein, D. Lee, Y.-Zh. Ma, U.-G. Meissner, K. Minamisono, A. V. Oleynichenko, S. Pineda, S. D. Prosnjak, M. L. Reitsma, L. V. Skripnikov, A. Vernon, A. Zaitsevskii

Phys. Rev. Lett. 132(16), 162502 (2024)

doi: 10.1103/PhysRevLett.132.162502

**2023** *Ab initio* study of electronic states and radiative properties of the AcF molecule

L. V. Skripnikov, A. V. Oleynichenko, A. Zaitsevskii, N. S. Mosyagin, M. Athanasakis-Kaklamanakis, M. Au, G. Neyens

J. Chem. Phys. 159, 124301 (2023)

doi: 10.1063/5.0159888

**2023** Theoretical molecular spectroscopy of actinide compounds: the ThO molecule

A. Zaitsevskii, A. V. Oleynichenko, E. Eliav

Mol. Phys. e2236246 (2023)

doi: 10.1080/00268976.2023.2236246

**2023** LIBGRPP: a library for the evaluation of molecular integrals of the generalized relativistic pseudopotential operator over Gaussian functions

A. V. Oleynichenko, A. Zaitsevskii, N. S. Mosyagin, A. N. Petrov, E. Eliav, A. V. Titov

Symmetry, 15(1), 197 (2023)

doi: 10.3390/sym15010197

**2022** Relativistic Fock-space coupled cluster method: theory and recent applications

E. Eliav, A. Borschevsky, A. Zaitsevskii, A. V. Oleynichenko, U. Kaldor

Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, Elsevier (2022)

doi: 10.1016/B978-0-12-821978-2.00042-8

**2022** Generalized relativistic small-core pseudopotentials accounting for quantum electrodynamic effects: construction and pilot applications

A. Zaitsevskii, N. S. Mosyagin, A. V. Oleynichenko, E. Eliav  
Int. J. Quantum Chem., 123(8), e27077 (2022)  
doi: 10.1002/qua.27077

**2022 Ionization potentials and electron affinities of Rg, Cn, Nh, and Fl superheavy elements**

M. Y. Kaygorodov, D. P. Usov, E. Eliav, Y. S. Kozhedub, A. V. Malyshev, A. V. Oleynichenko, V. M. Shabaev,  
L. V. Skripnikov, A. V. Titov, I. I. Tupitsyn, A. V. Zaitsevskii  
Phys. Rev. A, 105(6), 062805 (2022)  
doi: 10.1103/PhysRevA.105.062805

**2022 The  $a^3\Sigma^+$  state of KCs revisited: hyperfine structure analysis and potential refinement**

V. Krumins, M. Tamanis, R. Ferber, A. V. Oleynichenko, L. V. Skripnikov, A. Zaitsevskii, E. A. Pazyuk,  
A. V. Stolyarov, A. Pashov  
J. Quant. Spectrosc. Radiat. Transf., 283, 108124 (2022)  
doi: 10.1016/j.jqsrt.2022.108124

**2022 Effect of the neutron quadrupole distribution in the TaO<sup>+</sup> cation**

G. Penyazkov, L. V. Skripnikov, A. V. Oleynichenko, A. V. Zaitsevskii  
Chem. Phys. Lett., 793, 139448 (2022)  
doi: 10.1016/j.cplett.2022.139448

**2022 Laser-coolable AcOH<sup>+</sup> ion for  $CP$ -violation searches**

A. V. Oleynichenko, L. V. Skripnikov, A. V. Zaitsevskii, V. V. Flambaum  
Phys. Rev. A, 105(2), 022825 (2022)  
doi: 10.1103/PhysRevA.105.022825

**2021 Large shape staggering in neutron-deficient Bi isotopes**

A. Barzakh, A. N. Andreyev, C. Raison, J. G. Cubiss, P. Van Duppen, S. Péru, S. Hilaire, S. Goriely,  
B. Andel, S. Antalic, Monthery M. Al, J. C. Berengut, J. Bieron, M. L. Bissell, A. Borschevsky, K. Chrysalidis,  
T. E. Cocolios, T. Day Goodacre, J. P. Dognon, M. Elantkowska, E. Eliav, G. J. Farooq-Smith, D. V. Fedorov,  
V. N. Fedosseev, L. P. Gaffney, R. F. Garcia Ruiz, M. Godefroid, C. Granados, R. D. Harding, R. Heinke,  
M. Huyse, J. Karls, P. Larmonier, G. Li J, K. M. Lynch, D. E. Maison, B. A. Marsh, P. Molkanov, P. Mosat,  
A. V. Oleynichenko, V. Panteleev, P. Pyykkö, M. L. Reitsma, K. Rezyunkina, R. E. Rossel, S. Rothe,  
J. Ruczkowski, S. Schiffmann, C. Seiffert, M. D. Seliverstov, S. Sels, L. V. Skripnikov, M. Stryjczyk, D. Studer,  
M. Verlinde, S. Wilman, A. V. Zaitsevskii  
Phys. Rev. Lett. 127(19), 192501 (2021)  
doi: 10.1103/PhysRevLett.127.192501

**2021 Relativistic Fock space coupled-cluster study of bismuth electronic structure to extract the Bi nuclear quadrupole moment**

L. V. Skripnikov, A. V. Oleynichenko, A. V. Zaitsevskii, D. E. Maison, A. E. Barzakh  
Phys. Rev. C 104(3), 034316 (2021)  
doi: 10.1103/PhysRevC.104.034316

**2021 Electron affinity of oganesson**

M. Y. Kaygorodov, L. V. Skripnikov, I. I. Tupitsyn, E. Eliav, Y. S. Kozhedub, A. V. Malyshev, A. V. Oleynichenko, V. M. Shabaev, A. V. Titov, A. V. Zaitsevskii  
Phys. Rev. A 104(1), 012819 (2021)  
doi: 10.1103/PhysRevA.104.012819

**2021 Fourier-transform spectroscopy and relativistic electronic structure calculation on the  $c^3\Sigma^+$  state of KCs**

A. Kruzins, V. Krumins, M. Tamanis, R. Ferber, A. V. Oleynichenko, A. Zaitsevskii, E. A. Pazyuk, A. V. Stolyarov  
J. Quant. Spectrosc. Radiat. Transf. 276, 107902 (2021)  
doi: 10.1016/j.jqsrt.2021.107902

**2021 Ab initio relativistic treatment of the  $a^3\Pi - X^1\Sigma^+$ ,  $a'^3\Sigma^+ - X^1\Sigma^+$  and  $A^1\Pi - X^1\Sigma^+$  systems of the CO molecule**

N. S. Mosyagin, A. V. Oleynichenko, A. Zaitsevskii, A. V. Kudrin, E. A. Pazyuk, A. V. Stolyarov  
J. Quant. Spectrosc. Radiat. Transf. 263, 107532 (2021)  
doi: 10.1016/j.jqsrt.2021.107532

**2021 Ab initio study and assignment of electronic states in molecular RaCl**

T. A. Isaev, A. V. Zaitsevskii, A. Oleynichenko, E. Eliav, A. A. Breier, T. F. Giesen, R. F. Garcia Ruiz, R. Berger  
J. Quant. Spectrosc. Radiat. Transf. 269, 107649 (2021)  
doi: 10.1016/j.jqsrt.2021.107649

**2021 Axion-mediated electron-electron interaction in ytterbium monohydroxide molecule**

D. E. Maison, L. V. Skripnikov, A. V. Oleynichenko, A. Zaitsevskii  
J. Chem. Phys. 154, 224303 (2021)  
doi: 10.1063/5.0051590

**2020 Diagonal and off-diagonal hyperfine structure matrix elements in KCs within the relativistic Fock space coupled cluster theory**

A. V. Oleynichenko, L. V. Skripnikov, A. Zaitsevskii, E. Eliav, V. M. Shabaev  
Chem. Phys. Lett. 756, 137825 (2020)  
doi: 10.1016/j.cplett.2020.137825

**2020 Finite-field calculations of transition properties by the Fock space relativistic coupled cluster method: transitions between different Fock space sectors**

A. Zaitsevskii, A. Oleynichenko, E. Eliav  
Symmetry, 12(11), 1845 (2020)  
doi: 10.3390/sym12111845

**2020 Relativistic Fock space coupled cluster method for many-electron systems: non-perturbative account for connected triple excitations**

A. V. Oleynichenko, A. Zaitsevskii, L. V. Skripnikov, E. Eliav  
Symmetry, 12(7), 1101 (2020)  
doi: 10.3390/sym12071101

**2020** Towards high performance relativistic electronic structure modelling: the EXP-T program package  
A. Oleynichenko, A. Zaitsevskii, E. Eliav  
Commun. Comp. Inf. Sci. 1331, 375 (2020)  
doi: 10.1007/978-3-030-64616-5\_33

**2020** The branching ratio of intercombination  $A^1\Sigma^+ \sim b^3\Pi \rightarrow a^3\Sigma^+/X^1\Sigma^+$  transitions in the RbCs molecule: measurements and calculations  
V. Krumins, A. Kruzins, M. Tamanis, R. Ferber, A. Pashov, A. V. Oleynichenko, A. Zaitsevskii, E. A. Pazyuk, A. V. Stolyarov  
J. Quant. Spectrosc. Radiat. Transf. 256, 107291 (2020)  
doi: 10.1016/j.jqsrt.2020.107291

**2018** Electronic transition dipole moments in relativistic coupled-cluster theory: the finite-field method  
A. V. Zaitsevskii, L. V. Skripnikov, A. V. Kudrin, A. V. Oleinichenko, E. Eliav, A. V. Stolyarov  
Opt. Spectrosc. 124(4), 451 (2018)  
doi: 10.1134/S0030400X18040215

**2018** Global and local approaches to population analysis: bonding patterns in superheavy element compounds  
A. Oleynichenko, A. Zaitsevskii, S. Romanov, L. V. Skripnikov, A. V. Titov  
Chem. Phys. Lett. 695, 63 (2018)  
doi: 10.1016/j.cplett.2018.01.058

**2018** Test of computational approaches for gold-thiolate clusters calculation using Lomonosov supercomputer  
N. N. Nikitina, D. A. Pichugina, A. V. Oleynichenko, O. N. Ryzhova, K. E. Kopylov, V. V. Krotov, N. E. Kuzmenko  
Supercomputing Frontiers and Innovations, 5(4), 83 (2018)  
doi: 10.14529/jsfi180409

**2017** Projection population analysis for molecules with heavy and superheavy atoms  
A. Oleynichenko, A. Zaitsevskii  
Nonlinear Phenomena in Complex Systems, 20(2), 177 (2017)  
doi: 10.48550/arXiv.2112.05187

**2017** Quantum-chemical study of the effect of ligands on the structure and properties of gold clusters  
M. N. Golosnaya, D. A. Pichugina, A. V. Oleinichenko, N. E. Kuz'menko  
Russ. J. Phys. Chem. A, 91(2), 346 (2017)  
doi: 10.1134/S0036024417020108

## Conference talks:

### **2022** Analytic density matrices in relativistic coupled cluster theory

A. V. Oleynichenko, L. V. Skripnikov, A. Zaitsevskii

28 June 2022, Irkutsk State University, Russia

### **2021** Hyperfine structure parameters in alkali diatomics as functions of the internuclear separation

A. V. Oleynichenko, L. V. Skripnikov, A. Zaitsevskii, E. Eliav, V. M. Shabaev

5–10 September 2021, Brasov, Romania

### **2020** Relativistic Fock Space Coupled Cluster beyond CCSD: Theory and Implementation

A. Oleynichenko, A. Zaitsevskii, E. Eliav

23rd DIRAC Working Group Meeting 2020, 3–6 June 2020, Odense, Denmark

### **2020** Towards High Performance Relativistic Electronic Structure Modelling: The EXP-T Program Package

A. V. Oleynichenko, A. Zaitsevskii, E. Eliav

International conference “Russian Supercomputing Days – 2020”, 21–22 September 2020, Moscow, Russia

### **2019** Towards the Experimental Accuracy of Relativistic Coupled Cluster Calculations on Excited States of Alkali Diatomics

A. Oleynichenko, A. V. Stolyarov, E. Eliav, A. Zaitsevskii

13th European Conference on Atoms, Molecules, and Photons (ECAMP13), 8–12 April 2019, Florence, Italy

### **2019** A Relativistic Fock-Space Coupled Cluster Method: Towards Efficient Execution on GPUs

A. Oleynichenko, S. Kozlov, A. Zaitsevskii, E. Eliav

International conference “Russian Supercomputing Days – 2019”, 23–24 September 2019, Moscow, Russia

### **2016** Application of projection population analysis to molecules with heavy and superheavy atoms

A. Zaitsevskii, A. Oleynichenko

Hans Hellmann Prosymposium «Quantum Chemistry of Materials», 15–18 November 2016, Saint Petersburg

### **2016** Effective states of actinide and transactinide atoms in compounds

A. Zaitsevskii, A. Oleynichenko, A. V. Titov, L. V. Skripnikov, S. Romanov

Hans Hellmann Prosymposium «Quantum Chemistry of Materials», 15–18 November 2016, Saint Petersburg, Russia

### **2016** DFT Study of the Active Sites of Gold Clusters Anchored by Thiolate, Selenolate and Tellurolate Ligands

N. A. Nikitina, A. V. Oleynichenko, N. E. Kuz'menko, A. G. Majouga, D. A. Pichugina

Mechanisms of catalytic reactions: X International Conference (MCR-X), 2–6 October 2016, Svetlogorsk, Russia