

Alexander Oleynichenko

10 November 2024

e-mail oleynichenko_av@pnpi.nrcki.ru

Web page <http://www.qchem.pnpi.spb.ru/Oleynichenko>
GitHub <https://github.com/aoleynichenko>
MSU ISTINA <https://istina.msu.ru/profile/aoleynichenko>
ResearchGate https://www.researchgate.net/profile/Alexander_Oleynichenko
Google Scholar <https://scholar.google.com/citations?user=BiyTcakAAAAJ&hl=en>

ORCID 0000-0002-8722-0705
ScopusID 57194777245
ResearcherID D-8821-2019
elibrary SPIN 2394-9953

List of publications:

2024 Recent advancements in atomic many-body methods for high-precision studies of isotope shifts

B. K. Sahoo, S. Blundell, A. V. Oleynichenko, R. F. Garcia Ruiz, L. V. Skripnikov, B. Ohayon
arXiv:2408.09959 [physics.atom-ph] (2024)
doi: 10.48550/arXiv.2408.09959

2024 Finite-order method to calculate approximate density matrices in the Fock-space multireference coupled cluster theory

A. V. Oleynichenko, A. Zaitsevskii, L. V. Skripnikov, E. Eliav
Mol. Phys., Alexander Nemukhin Special Issue, e2413416 (2024)
doi: 10.1080/00268976.2024.2413416

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

Yu. A. Demidov, A. A. Shalaevsky, A. V. Oleynichenko, A. A. Rusakov
Phys. Chem. Chem. Phys. 26, 23823 (2024)
doi: 10.1039/D4CP01868K

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. Berball, 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
Phys. Rev. A 110(1), L010802 (2024)
doi: 10.1103/PhysRevA.110.L010802

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}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_4

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. Kartheim, 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., REHE 2022 Special Issue, 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⁺ 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⁺ 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. Stryczyk, 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