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List of publications:

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)

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)

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., e27077 (2022)

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)

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)

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)

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)

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. Rezynkina, 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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

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)

2017 Projection population analysis for molecules with heavy and superheavy atoms

A. Oleynichenko, A. Zaitsevskii
Nonlinear Phenomena in Complex Systems, 20(2), 177 (2017)

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)

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