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List of publications:

2023 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

arXiv:2310.09240 [cond-mat.mtrl-sci] (2023)

https://arxiv.org/abs/2310.09240

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. Prosnyak, M. L. Reitsma, L. V. Skripnikov, A. Vernon, A. Zaitsevskii

arXiv:2309.02037 [nucl-ex] (2023)

https://arxiv.org/abs/2309.02037

2023 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

arXiv:2308.05173 [physics.atom-ph] (2023)

doi: 10.48550/arXiv.2308.05173

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^+ 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 $\mathcal{CP}$-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. Rezynkina, 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