

NIKOLAY TKACHENKO

Affiliation: Department of Chemistry and Biochemistry, Utah State University

Current program: Doctor of Philosophy

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EDUCATION

- | | |
|-----------------|---|
| 08/2018-Present | Ph.D., Physical Chemistry major, <i>Utah State University</i> , Logan, Utah, USA
GPA = 4.0 |
| 09/2013-07/2018 | Specialist degree, Fundamental and Applied Chemistry major, <i>Novosibirsk University</i> , Novosibirsk, Russia
GPA = 4.0 (<i>summa cum laude</i>) |
| 09/2011-05/2013 | High school diploma, <i>Educational and Scientific Center of Novosibirsk University</i> , Novosibirsk, Russia |

AWARDS AND GRANTS

Summer internship at Los Alamos National Laboratory (LANL) || June **2020**

Stephen Bialkowski Award in Environmental Chemistry, a support of a specific environmental chemistry research at the Department of Chemistry and Biochemistry, Utah State University || April **2020**

The Early Research Progress in Chemistry Award for outstanding research progress at Utah State University || April **2020**

Marjorie H. Gardner Teaching Award for outstanding work as a teaching assistant at Utah State University || March **2019**

British Petroleum Scholarship Award for High Academic Standing and Outstanding Leadership Qualities || **2017, 2016**

1st Degree Diploma of the “VII International Natural Sciences Tournament” – Individual Competition || November **2016**

1st Degree Diploma of the International Forum of Young Scientists “Science Game” – Team Competition || May **2016**

CITATION METRICS

h-index: 12

Total citations: 330

PUBLICATIONS

- 36)** Xu H.L., Tkachenko N.V., Szczepanik D., Popov I.A., Muñoz-Castro A., Boldyrev A.I., Sun Z.M. "Symmetry Collapse due to the Presence of Multiple Local Aromaticity in Ge_{24}^{4-} ", *Nat. Commun.* **2022**, Accepted. (IF = 14.92)
- 35)** Rublev P., Tkachenko N.V., Boldyrev A.I. "Overlapping electron density and the global delocalization of π -aromatic fragments as the reason of conductivity of the biphenylene network", *J. Comput. Chem.* **2022**, Accepted. (IF = 3.38)
- 34)** Tkachenko N.V., Rublev P., Boldyrev A.I., Lehn J.M. "Superalkali Coated Rydberg Molecules", *Front. Chem.* **2022**, Accepted. (IF = 5.22)
- 33)** Yokelson D., Tkachenko N.V., Robey R., Li Y.W., Dub P.A. "Performance Analysis of CP2K Code for Ab Initio Molecular Dynamics", arXiv:2109.04536v1, under review in *J. Chem. Inf. Model.* (IF = 4.96)
- 32)** Chen W.X., Tkachenko N.V., Munoz-Castro A., Boldyrev A.I., Sun Z.M. "Ruthenium-mediated assembly and enhanced stability of heterometallic polystannides $[\text{Ru}_2\text{Sn}_{19}]^{4-}$ and $[\text{Ru}_2\text{Sn}_{20}]^{6-}$ ", *Nano Res.*, **2022**, Accepted, DOI: 10.1007/s12274-022-4178-9. (IF = 8.90)
- 31)** Minkin V.I., Ivakhnenko E.P., Knyazev P.A., Starikov A.G., Demidov O.P., Tkachenko N.V., Boldyrev A.I. "Electronic isomerism (electromerism) of 6,8-di-tert-butyl-3H-phenoxazin-3-one oxime radical", *Russ. Chem. Bull.*, **2022**, 1, 30-37. (IF = 1.22)
- 30)** Zhang W.Q., Tkachenko N.V., Qiao L., Boldyrev A.I., Sun Z.M. "Synthesis and structure of binary copper/silver–arsenic clusters derived from Zintl ion As_7^{3-} ", *Chin. J. Chem.*, **2022**, 40, 65-70. (IF = 6.00)
- 29)** Tkachenko N.V., Munoz-Castro A., Boldyrev A.I. "Occurrence of Double Bond in π -Aromatic Rings: An Easy Way to Design Doubly Aromatic Carbon-Metal Structures", *Molecules*, **2021**, 26, 7232. (IF = 4.41)
- 28)** Tkachenko N.V., Tkachenko A.A., Kulyukin V.A., and Boldyrev A.I. "DFT Study of Microsolvated $[\text{NO}_3 \cdot (\text{H}_2\text{O})_n]^-$ ($n = 1-12$) Clusters and Molecular Dynamics Simulation of Nitrate Solution", *J. Phys. Chem. A*, **2021**, 40, 8899–8906. (IF = 2.78)
- 27)** Tkachenko N.V., Popov I.A., Kulichenko M., Fedik N., Sun Z.M., Munoz-Castro A., and Boldyrev A.I., "Bridging Aromatic/Antiaromatic Units. Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-metal Clusters From Bonding and Magnetic Analyses", *Eur. J. Inorg. Chem.*, **2021**, 41, 4239-4250. (IF = 2.52)
- 26)** Xu Y.H., Tkachenko N.V., Popov I.A., Qiao L., Munoz-Castro A., Boldyrev A.I., and Sun Z.M. "Ternary aromatic and anti-aromatic clusters derived from the hypoh species $[\text{Sn}_2\text{Sb}_5]^{3-}$ ", *Nat. Commun.*, **2021**, 12, 4465. (IF = 14.92)
- 25)** Dub P.A., and Tkachenko N.V. "Mechanism of Potassium tert-Butoxide-Catalyzed Ketones Hydrogenation in the Solution Phase", *J. Phys. Chem. A*, **2021**, 125, 5726-5737. (IF = 2.78)
- 24)** Tkachenko N. V., Sud J., Zhang Y., Tretiak S., Anisimov P. M., Arrasmith A. T., Coles P. J., Cincio L., and Dub P. A. "Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in the Variational Quantum Eigensolver" *PRX Quantum*, **2021**, 2, 020337.
- 23)** Kulichenko M., Fedik N., Tkachenko N. V., Munoz-Castro A., Sun Z.-M., and Boldyrev A. I. "Spherical aromaticity in inorganic chemistry" In *Aromaticity: Modern Computational Methods and Applications*, **2021**, Ed. Israel Fernandez, Elsevier, ISBN: 9780128227237, pp. 447-488. (Invited Chapter)
- 22)** Dub P. A., Tkachenko N. V., Vyas V. K., Wills M., Smith J. S., and Tretiak S., "Enantioselectivity in the Noyori-Ikariya Asymmetric Transfer Hydrogenation of Ketones", *Organometallics*, **2021**, 40, 1402-1410. (IF = 3.88)
- 21)** Xu H. L., Tkachenko N. V., Munoz-Castro A., Boldyrev A. I., and Sun Z.-M. " $[\text{Sn}_8]^{6-}$ -bridged mixed-valence $\text{Zn(I)}/\text{Zn(II)}$ in $\{[\text{K}_2\text{ZnSn}_8(\text{ZnMes})_2]^{4-}$ Inverse Sandwich-Type Cluster Supported by $\text{Zn}^{\text{I}}\text{-Zn}^{\text{I}}$ Bond", *Angew. Chem. Int. Ed.*, **2021**, 60, 9990-9995. (IF = 15.34)
- 20)** Semenok D. V., Zhou D., Kvashnin A. G., Huang X., Galasso M., Kruglov I. A., Ivanova A. G., Gavriluk A. G., Chen W., Tkachenko N. V., Boldyrev A. I., Troyan I., Oganov A. R., and Cui T. "Novel Strongly Correlated Europium Superhydrides", *J. Phys. Chem. Lett.*, **2021**, 12, 32-40. (IF = 6.48)

- 19) Xu H.-L., Tkachenko N. V., Wang Z.-C., Chen W.-X., Qiao L., Munoz-Castro A., Boldyrev A. I., and Sun Z.-M. "A Sandwich-Type Cluster Containing Ge@Pd₃ Planar Fragment Flanked by Aromatic Nonagermanide Caps", *Nat. Commun.*, **2020**, *11*, 5286. (IF = 14.92)
- 18) Narendrapurapu B. S., Bowman M. C., Xie Y., Schaefer III H. F., Tkachenko N. V., Boldyrev A. I., and Li G. "Dibridged, Monobridged, Vinylidene-Like, and Linear Structures for the Alkaline Earth Dihydrides Be₂H₂, Mg₂H₂, Ca₂H₂, Sr₂H₂, and Ba₂H₂. Proposals for Observations", *Inorg. Chem.*, **2020**, *59*, 10404-10408. (IF = 5.17)
- 17) Xu H. L., Popov I. A., Tkachenko N. V., Wang Z. C., Munoz-Castro A., Boldyrev A. I., and Sun Z.-M. "σ-Aromaticity-Induced Stabilization of Heterometallic Supertetrahedral Clusters [Zn₆Ge₁₆]⁴⁻ and [Cd₆Ge₁₆]⁴⁻", *Angew. Chem. Int. Ed.* **2020**, *59*, 17286-17290. (IF = 15.34)
- 16) Wang Z. C., Tkachenko N. V., Qiao L., Matito E., Muñoz-Castro A., Boldyrev A. I., and Sun Z.-M. "All-Metal σ-Antiaromaticity in Dimeric Cluster Anion {[CuGe₉Mes]₂}⁴⁻", *ChemComm*, **2020**, *56*, 6583-6586. (IF = 6.22)
- 15) Steglenko D. V., Tkachenko N. V., Boldyrev A. I., Minyaev R. M., and Minkin V. I. "Stability, electronic and optical properties of two-dimensional phosphorane", *J. Comp. Chem.*, **2020**, *41*, 1456-1463. (IF = 3.38)
- 14) Tkachenko N. V., Zhang X. W., Qiao L., Shu C. C., Steglenko D., Munoz-Castro A., Sun Z.-M., and Boldyrev A. I. "Spherical aromaticity of all-metal [Bi@In₈Bi₁₂]^{3-/5-} clusters", *Chem. Eur. J.*, **2020**, *26*, 2073-2079. (IF = 5.24)
- 13) Tkachenko N. V., Song B., Steglenko D., Minyaev R. M., Yang L. M., and Boldyrev A. I. "Computational Prediction of the Low Temperature Ferromagnetic Semiconducting Two-Dimensional SiN Monolayer", *Phys. Status Solidi B*, **2019**, *257*, 1900619. (IF = 1.71)
- 12) Tkachenko N. V., Steglenko D., Fedik N., Boldyreva N. M., Minyaev R. M., Minkin V. I., and Boldyrev A. I. "Superoctahedral Two-Dimensional Metallic Boron with Peculiar Magnetic Properties", *Phys. Chem. Chem. Phys.*, **2019**, *21*, 19764-19771. (IF = 3.68)
- 11) Tkachenko N. V., Sun Z.-M., and Boldyrev A. I. "Record Low Ionization Potentials of Alkali Metal Complexes with Crown Ethers and Cryptands", *ChemPhysChem*, **2019**, *20*, 2060-2062. (Highlighted as Very Important Paper, featured on the Front Cover Page, highlighted in ChemViews Magazine) (IF = 3.10)
- 10) Tkachenko N. V., and Boldyrev A. I. "Multiple Local σ-Aromaticity of the Nonagermanide Clusters", *Chem. Sci.*, **2019**, *10*, 5761-5765. (IF=9.83)
- 9) Liu C., Tkachenko N. V., Popov I. A., Fedik N., Min X., Xu C. Q., Li J., McGrady J. E., Boldyrev A. I., and Sun Z.-M. "Structure and Bonding in [Sb@In₈Sb₁₂]³⁻ and [Sb@In₈Sb₁₂]⁵⁻", *Angew. Chem. Int. Ed.*, **2019**, *58*, 8367-8371. (Featured on the Inside Cover Page) (IF = 15.34)
- 8) Tkachenko N. V., and Boldyrev A. I. "Chemical bonding analysis of excited states using the adaptive natural density partitioning method", *Phys. Chem. Chem. Phys.*, **2019**, *21*, 9590-9596. (IF = 3.68)
- 7) Tkachenko N. V., and Scheiner S. "Optical Stability of 1,1'-Binaphthyl Derivatives", *ACS Omega*, **2019**, *4*, 6044-6049. (IF = 3.51)
- 6) Tkachenko N. V., and Bryliakov K. P. "Transition Metal Catalyzed Aerobic Asymmetric Coupling of 2-Naphthols", *Mini Rev. Org. Chem.*, **2019**, *16*, 392-398. (IF = 2.50)
- 5) Salnikov G. E., Genaev A. M., Shernyukov A. V., Zhu Z., Tkachenko N. V., and Koltunov K. Y. "Configurational Stability of 1,1'-Bi-2-naphthol in Superacid System HSO₃F-SbF₅-SO₂ClF", *Russ. J. Org. Chem.*, **2018**, *54*, 792-794. (IF=0.72)
- 4) Tkachenko N. V., Lyakin O. Y., Zima A. M., Talsi E. P., and Bryliakov K. P. "Effect of Different Carboxylic Acids on the Aromatic Hydroxylation with H₂O₂ in the Presence of an Iron Aminopyridine Complex", *J. Organomet. Chem.*, **2018**, *871*, 130-134. (IF=2.37)
- 3) Lyakin O. Y., Zima A. M., Tkachenko N. V., Bryliakov K. P., and Talsi E. P. "Direct Evaluation of the Reactivity of Nonheme Iron(V)-Oxo Intermediates toward Arenes", *ACS Catalysis*, **2018**, *8*, 5255-5260. (IF = 13.08)

2) Tkachenko N. V., Ottenbacher R. V., Lyakin O. Yu., Zima A. M., Samsonenko D. G., Talsi E. P., and Bryliakov K. P. "Highly Efficient Aromatic C-H Oxidation with H₂O₂ in the Presence of Iron Complexes of the PDP Family", *ChemCatChem*, **2018**, 10, 4052-4057. (IF=5.69)

1) Tkachenko N. V., Lyakin O. Y., Samsonenko D. G., Talsi E. P., and Bryliakov K. P. "Highly Efficient Asymmetric Aerobic Oxidative Coupling of 2-Naphthols in the Presence of Bioinspired Iron Aminopyridine Complexes", *Catal. Comm.*, **2018**, 104, 112-117. (IF=3.63)

CONFERENCES

ACS National Meeting & Expo, Oral Presentation, the symposium on "Synergy Between Quantum Computing and High-Performance Computing in Quantum Chemistry and Materials Science" || 5-16 April **2021**, USA.

ACS National Meeting & Expo, Physical Chemistry Poster Session, Sci-Mix Session || 25-29 August **2019**, San Diego (CA), USA.

27th International Chugaev Conference on Coordination Chemistry, Oral Presentation, "Physicochemical Methods in Coordination Chemistry" || 2-6 October **2017**, Nizhny Novgorod, Russia.

IV Scientific Conference Boreskov Readings dedicated to the 110th anniversary of Academician Georgii K. Boreskov, Poster Session || 19-21 April **2017**, Novosibirsk, Russia.

EMPLOYMENT HISTORY

06/2020-08/2020	Graduate Research Assistant, <i>Los Alamos National Laboratory</i> , USA Responsibilities: Collecting and analyzing the data obtained during the computational research work; writing scientific papers.
08/2020-12/2020 01/2020-04/2020 01/2019-04/2019	Teaching Assistant, <i>Utah State University</i> , USA Responsibilities: Conducting General Chemistry Recitations and Chemical Principles Laboratories; Grading students' works.
01/2021-Present 05/2019-12/2019 08/2018-12/2018	Research Assistant, <i>Utah State University</i> , USA Responsibilities: Collecting and analyzing the data obtained during the computational research work; writing scientific papers.
06/2016-07/2018	Research Assistant, <i>Boreskov Institute of Catalysis</i> , Russia Responsibilities: Collecting and analyzing the data obtained during the experimental research work; writing scientific papers.
06/2015-05/2016	Research Assistant, <i>Nikolaev Institute of Inorganic Chemistry</i> , Russia Responsibilities: Collecting and analyzing the data obtained during the experimental research work.

RECENT PROJECTS AND SPECIAL ACTIVITIES

Spring 2021 - Present	Participating in Los-Alamos National Laboratory sub-contract with Utah State University on the topic "Quantum Chemistry on Quantum Computers"
Summer 2020	Participating in Los-Alamos National Laboratory Graduate Research Assistantship program. "Quantum Chemistry on Quantum Computers", DR project.
08/2018-12/2019	Participating in National Science Foundation grant CHE-1664379

LANGUAGE ABILITIES

First language: Russian

Second language: English

SKILLS

Programming using following programming languages: Python 3, C++;

Developing scientific software:

AdNDP 2.0 (195 unique downloads, available through the links:
<https://zenodo.org/record/2648092#.XLwJdpnQhPY>,
<https://zenodo.org/record/3252298#.YNCrwOHPxPZ>)

DFT-driven-PSO (<https://github.com/ntkachenko95/DFT-driven-PSO>)

Performing quantum chemical calculations using following programs:
Gaussian, ORCA, VASP, CP2K;

Performing chemical bonding analysis using following programs: AdNDP,
AdNDP 2.0, SSAdNDP, MultiWFN;

Group website administration;

SCIENTIFIC INTERESTS

Quantum chemistry; Computational materials design; Computational catalysis; Chemical bonding of clusters and solids; Quantum computing; Application of artificial intelligence to materials design; Computational chemistry.