



NIKOLAY TKACHENKO

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Current program: Doctor of Philosophy

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AWARDS AND GRANTS

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: 6

Total citations: 94

PUBLICATIONS

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**, Accepted DOI: 10.1021/acs.inorgchem.0c01651 (IF=4.83)

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**, Accepted DOI: 10.1002/anie.202008276 (IF=12.26)

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=6.16, cited 1 time)

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 phosphoborane", *J. Comput. Chem.*, **2020**, Accepted DOI: 10.1002/jcc.26189. (IF=3.22)

14) Tkachenko N. V., X. W. Zhang, L. Qiao, C. C. Shu, D. Steglenko, A. Munoz-Castro, Z. M. Sun, A. I. Boldyrev "Spherical aromaticity of all-metal [Bi@In₈Bi₁₂]^{3-/5-} clusters", *Chem. Eur. J.*, **2020**, 26, 2073-2079. (IF=5.16, cited 2 times)

- 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=1.45, cited 1 time)
- 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=3.57, cited 11 times)
- 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=3.08, cited 2 times)
- 10) Tkachenko N. V. and Boldyrev A. I. "Multiple Local σ -Aromaticity of the Nonagermanide Clusters", *Chem. Sci.*, **2019**, 10, 5761-5765. (IF=9.56, cited 5 times)
- 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 $[\text{Sb@In}_8\text{Sb}_{12}]^{3-}$ and $[\text{Sb@In}_8\text{Sb}_{12}]^{5-}$ ", *Angew. Chem. Int. Ed.*, **2019**, 58, 8367-8371. (Featured on the Inside Cover Page) (IF=12.26, cited 10 times)
- 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=3.57, cited 13 times)
- 7) Tkachenko N. V. and Scheiner S. "Optical Stability of 1,1'-Binaphthyl Derivatives", *ACS Omega*, **2019**, 4, 6044-6049. (IF=2.58, cited 4 times)
- 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=1.12, cited 2 times)
- 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 $\text{HSO}_3\text{F}-\text{SbF}_5-\text{SO}_2\text{ClF}$ ", *Russ. J. Org. Chem.*, **2018**, 54, 792-794. (IF=0.75, cited 3 times)
- 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 H_2O_2 in the Presence of an Iron Aminopyridine Complex", *J. Organomet. Chem.*, **2018**, 871, 130-134. (IF=2.17, cited 2 times)
- 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 Catal.*, **2018**, 8, 5255-5260. (IF=12.22, cited 20 times)
- 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 H_2O_2 in the Presence of Iron Complexes of the PDP Family", *ChemCatChem*, **2018**, 10, 4052-4057. (IF=4.80, cited 8 times)
- 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=3.67, cited 9 times)

CONFERENCES

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 4th Conference-School for Young Researchers "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 || 19-21 April **2017**, Novosibirsk, Russia.

EDUCATION

08/2018-Present	Doctor of Philosophy, 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

EMPLOYMENT HISTORY

06/2020-present	Graduate Research Assistant, <i>Los Alamos National Laboratory</i> , USA
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.
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

Summer 2020	Participating in Los-Alamos National Laboratory Graduate Research Assistantship program. "Quantum Chemistry on Quantum Computers" project.
08/2018-12/2019	Participating in National Science Foundation grant CHE-1664379

CAREER OBJECTIVES

After the graduation from Utah State University I am planning to apply for a Post-Doctoral position in Los Alamos National Laboratory. I will continue to work on the Computational Chemistry topic. After 2-3 years of working as a postdoc, I plan to find a professorship and conduct an independent research.

LANGUAGE ABILITIES

First language: Russian

Second language: English

SKILLS

Programming using following programming languages: Python 3.7, C++;

Developing scientific software: AdNDP 2.0 (64 unique downloads, available through the link: <https://zenodo.org/record/2648092#.XLwJdpnQhPY>)

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

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.

HOBBIES

Playing the piano; wood carving; biking; chess.