NIKOLAY TKACHENKO

Affiliation: Department of Chemistry and Biochemistry, Utah State University;
Chemistry Division (C-IIAC), Los Alamos National Laboratory.
Current program: Doctor of Philosophy in Physical Chemistry
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EDUCATION

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

AWARDS AND GRANTS

Claude E. ZoBell Scholarship, a support for the graduate student pursuing degrees in biology, chemistry and biochemistry, geology, or physics. College of Science, Utah State University || June **2022**

Summer internship at Los Alamos National Laboratory (LANL) || May-August **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: 13

Total citations: 433 (**Google Scholar Profile**)

PUBLICATIONS

40) Tkachenko N.V., Rublev P., Dub P.A. "The Source of Proton in the Noyori−Ikariya Reaction", *ChemRxiv* **2022**, 10.26434/chemrxiv-2022-dbc0n. Under Review in *ACS Catalysis*. (IF = 13.08)

39) Getmanskii I.V., Koval V.V., Tkachenko N.V., Zaitsev S.A., Boldyrev A.I., Minyaev R.M. "Ultralight Supertetrahedral Aluminum: Stability at Various Temperatures", *MRS Bull.* **2022**, Accepted, DOI 10.1557/s43577-022-00383-6. (IF = 4.88)

38) Tkachenko N.V., Zhang Y., Cincio L., Boldyrev A.I., Tretiak S., Dub P.A. "Quantum Davidson Algorithm for Excited States", *ArXiv*, **2022**, 2204.10741. Under Review in *PRX Quantum*.

37) Tkachenko N.V., Chen W.X., Morgan H.W.T., Muñoz-Castro A., Boldyrev A.I., Sun Z.M. "Sn_{36}^{8-}: A 2.7 nm Naked Aromatic Tin Rod", *Chem. Commun.*, **2022**, *58*, 6223-6226. (IF = 6.22)

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**, *13*, 2149. (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 DOI: 10.1002/jcc.26854. (IF = 3.38)

34) Tkachenko N.V., Rublev P., Boldyrev A.I., Lehn J.M. "Superalkali Coated Rydberg Molecules", *Front. Chem.* **2022**, *10*, 880804. (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", *J. Chem. Inf. Model* **2022**, *62*, 2378-2386. (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 $[Ru_2Sn_{19}]^{4-}$ and $[Ru_2Sn_{20}]^{6-}$", Nano Res., **2022**, *15*, 5705–5711. (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 $[NO_3{\cdot}(H_2O)_n]^-$ (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 hypho species $[Sn_2Sb_5]^{3-}$", *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. "$[Sn_8]^{6-}$-bridged mixed-valence Zn(I)/Zn(II) in $\{[K_2ZnSn_8(ZnMes)]_2\}^{4-}$ Inverse Sandwich-Type Cluster Supported by Zn^I-Zn^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., Gavriliuk 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 $Ge@Pd_3$ 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 Be_2H_2, Mg_2H_2, Ca_2H_2, Sr_2H_2, and Ba_2H_2. 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 $[Zn_6Ge_{16}]^{4-}$ and $[Cd_6Ge_{16}]^{4-}$", *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 $\{[CuGe_9Mes]_2\}^{4-}$", *Chem. Commun.,* **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 phosphoborane", *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 $[Bi@In_8Bi_{12}]^{3-/5-}$ 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 $[Sb@In_8Sb_{12}]^{3-}$ and $[Sb@In_8Sb_{12}]^{5-}$", *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 HSO_3F–SbF_5–SO_2ClF", *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 H_2O_2 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 H_2O_2 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 AND INVITED TALKS

Invited seminar at Stanford University (T.J. Martinez group) "Exploring the Electronic-Structure Problem with Quantum Computers and Deciphering Exotic Chemical Bonding in Clusters and Solids" ‖ 8 Septebmer **2022**, Stanford, USA

International Conference on Chemical Bonding, *invited talk* "Simulating Electronic Structure on Quantum Computers with PermVQE and QDavidson Algorithms" ‖ 11-17 August **2022**, Kauai (Hawaii), USA

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 **Research Assistant, *Los Alamos National Laboratory*, USA**

Responsibilities:
Collecting and analyzing the data obtained during the computational research work; writing scientific papers; conceiving and designing of scientific projects.

08/2020-12/2020
01/2020-04/2020
01/2019-04/2019

Teaching Assistant, *Utah State University*, 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, *Utah State University*, USA

Responsibilities:
Collecting and analyzing the data obtained during the computational research work; writing scientific papers; conceiving and designing of scientific projects.

06/2016-07/2018

Research Assistant, *Boreskov Institute of Catalysis*, Russia

Responsibilities:
Collecting and analyzing the data obtained during the experimental research work; writing scientific papers.

06/2015-05/2016

Research Assistant, *Nikolaev Institute of Inorganic Chemistry*, 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

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;

LANGUAGE ABILITIES

First language: Russian

Second language: English

SCIENTIFIC INTERESTS

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