NIKOLAY TKACHENKO

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SUMMARY

I am a Postdoctoral Scholar at UC Berkeley and the Lawrence Berkeley National Laboratory. I hold a Ph.D. in Computational Chemistry with broad expertise in *computational materials design*, *quantum computing*, *catalysis*, *molecular simulations*, and *machine learning atomistic potentials*. I have been recognized with awards such as "J. R. Oppenheimer Distinguished Postdoctoral Fellow" appointment at Los Alamos National Laboratory and "ACS Utah Outstanding Graduate Student Award". My work covers a wide range of computational chemistry both on classical (*CPU/GPU*) as well as quantum gate-based platforms (*QPU*). Additionally, I am skilled in mentoring, communication, and collaboration, with a proven track record in successful scientific project management.

EDUCATION

2023 **Ph.D. in Computational Chemistry,** ***Utah State University***, Logan, Utah, USA

2018 **Specialist Degree** (Analog of M.S.) **in Fundamental and Applied Chemistry** (*summa cum laude*)
Novosibirsk State University, Novosibirsk, Russia

WORK EXPERIENCE

2023-now **Postdoctoral Scholar,** **University of California**, Berkeley, USA
Lawrence Berkeley National Laboratory, Berkeley, USA
(Martin Head-Gordon Group)
Research topic: Computational materials design for hydrogen storage and CO_2 capture; Development of modified BWs-CC2 method for accurate electronic structure calculations; Development of modified D3 and D4 schemes; Application of atomistic machine-learning potentials for accurate thermodynamical sampling of gas adsorption; Algorithms development for quantum chemistry on quantum computers;

2020-2023 **Graduate Student Contractor,** **Los Alamos National Laboratory**, Los Alamos, USA
(T1 Theoretical Division, Sergei Tretiak Supervision)
Research topics: Atomistic machine-learning potentials applications for configurational space sampling; Investigation of mechanisms of enantioselective catalytic hydrogenation reactions; Development of algorithms for ground and excited electronic state calculations on quantum computers;

2018-2023 **Graduate Research Assistant,** **Utah State University**, Logan, USA
(Alexander Boldyrev Group)
Research topic: Development of multicenter chemical bonding theory and investigation of its application in inorganic 3D-Zintl clusters and 2D materials;

2016-2018 **Undergraduate Research Assistant,** **Boreskov Institute of Catalysis**, Novosibirsk, Russia
(Konstantin Bryliakov Supervision)
Research topic: Experimental investigation of mechanisms of catalytic enantioselective aromatic C-H oxidation and oxidative coupling reactions with biomimetic non-heme iron complexes;

2015-2016 **Undergraduate Research Assistant,** **Nikolaev Institute of Inorganic Chemistry**, Novosibirsk, Russia
(Vladimir Fedin Group)
Research topic: Synthesis and characterization of zinc-containing metal-organic frameworks with unique fluorescence activity;

RESEARCH INTERESTS

Computational Materials Design; Electronic Structure Theory; Quantum Computing; Computational Catalysis; Adiabatic and Non-Adiabatic Molecular Dynamics Simulations; Monte Carlo Simulations; Chemical Bonding Theory.

TECHNICAL SKILLS

Programming languages: Python 3 (developer level); C++ (developer level);
Public software developed: *AdNDP 2.0* (DOI: 10.1039/C9CP00379G), *DFT-driven-PSO* (github.com/ntkachenko95), D3S/D4S/D4SL dispersion correction methods (implemented in Q-Chem code, github.com/ntkachenko95);
Molecular electronic structure codes: Gaussian, ORCA, Q-Chem, NEXMD (non-adiabatic MD);
Materials electronic structure codes: VASP, CP2K;
Wavefunction analysis: AdNDP, AdNDP 2.0, SSAdNDP, MultiWFN;
Quantum computing libraries: Qiskit, Openfermion;
Atomistic ML potentials: Atomic Simulation Environment, ANI family MLPs, MACE family MLPs.

SCIENTIFIC PRODUCTION

Metrics:

Total citations: 874 (Google Scholar Profile); h-index: 18; i10-index: 28;
51 published research papers and 3 invited chapters (23 first, 9 equally contributing, and 4 corresponding author);
11 oral presentations at international conferences and other scientific meetings;

Publications

Topic abbreviations:
***MS**–computational materials science; **PC**–computational photochemistry; **QC**–quantum computing; **CAT**–computational catalysis; **MD**–method development; **CB**–chemical bonding; **ORG**–computational organic chemistry; **INC**–computational inorganic chemistry; **HPC**–high performance computing on CPU and GPU; **ML**–machine learning; **EXP**–experimental chemistry.*

55) Tkachenko N.V., Yabuuchi Y., Carsch K.M., Furukawa H., Long J.R., and Head-Gordon M. "Computational Optimization of Room Temperature Usable Capacity for Hydrogen Storage in MFU-4-Type Metal–Organic Frameworks via Pairwise Metal Substitutions." *ChemRxiv* **2024**, doi:10.26434/chemrxiv-2024-kw01p. Under review in *Chem. Sci.* (IF=7.6, citations=2) **(MS)**
54) Rohde R.C., Carsch K.M., Dods M.N., Jiang H.Z.H., McIsaac A.R., Klein R.A., Kwon H., Karstens S.L., Wang Y., Huang A.J., Taylor J.W., Yabuuchi Y., Tkachenko N.V., Meihaus K.R., Furukawa H., Yahne D.R., Bustillo K.C., Minor A.M., Reimer J.A., Head-Gordon M., Brown C.M., and Long J.R. "High-Temperature Carbon Dioxide Capture in a Porous Material with Terminal Zinc–Hydride Sites" *Science* **2024**, Accepted. (IF=44.7, citations=0) **(MS, EXP)**
53) Tkachenko N.V., Dittmer L.B., Tomann R., Head-Gordon M. "Smooth dispersion is physically appropriate: Assessing and amending the D4 dispersion model" *J. Phys. Chem. Lett.* **2024**, *15*, 10629–10637. (Featured on the Supplementary Cover Page) (IF=4.8, citations=1) **(MD)**
52) Tkachenko N.V., Head-Gordon M. "Smoother Semiclassical Dispersion for Density Functional Theory via D3S: Understanding and Addressing Unphysical Minima in the D3 Dispersion Correction Model" *J. Chem. Theory Comput.* **2024**, Accepted, doi: 10.1021/acs.jctc.4c01105. (IF=5.7, citations=1) **(MD)**
51) Lv X., Qian L., Tkachenko N.V., Zhang T., Qiu F., Aratani N., Ikeue T., Pan J., and Xue S. "Copper Complexation of Rosarin: Formation of a Bis-copper Rosarin and a Mono-copper Linear Tridipyrrin" *Dalton Trans.* **2024**, *53*, 16879–16884. (IF=3.5, citations=0) **(CB, INC, EXP)**
50) Melikyan G.G., Babayans N., Kalpakyan N., Herrera C., Rublev P., Tkachenko N.V., and Boldyrev A.I. "Cobalt-complexed acetylenic tetrads, a molecular scaffold for quadruple ionic functionalization reactions" *Organometalics* **2024**, Accepted, doi: 10.1021/acs.organomet.4c00088. (IF=2.5, citations=0) **(ORG, EXP)**
49) Yabuuchi Y., Furukawa H., Carsch K.M., Klein R.A., Tkachenko N.V., Huang A.J., Cheng Y., Taddei K.M., Novak E., Brown C.M., Head-Gordon M., and Long J.R. "Geometric Tuning of Coordinatively Unsaturated Copper (I) Sites in Metal–Organic Frameworks for Ambient-Temperature Hydrogen Storage", *J. Am. Chem. Soc.* **2024**, *146*, 22759–22776. (IF=14.4, citations=2) **(MS, EXP)**
48) Huang-Fu Z.-C., Tkachenko N.V., Qian Y., Zhang T., Brown J., Harutyunyan A., Chen G., and Rao Y. "Conical Intersections at Interfaces Revealed by Phase-Cycling Interface-Specific Two-Dimensional Electronic Spectroscopy (i2D-ES)", *J. Am. Chem. Soc.* **2024**, *146*, 20996–21007. (IF=14.4, citations=1) **(PC, EXP)**
47) Xue S., Tkachenko N.V., Wu F., Lv X., Liu N., Muñoz-Castro A., Ueno S., Matsuo K., Kuzuhara D., Aratani N., Shen Z., Yamada H., Boldyrev A.I., and Qiu F. "Conflicting Aromaticity in Trirhodium(I) Rosarin", *Inorg. Chem.*, **2024**, *63*, 11494–11500. (IF=4.3, citations=0) **(CB, INC, EXP)**

46) Tkachenko N.V., Zhang Y., Cincio L., Boldyrev A.I., Tretiak S., and Dub P.A. "Quantum Davidson Algorithm for Excited States", *Quantum Sci. Technol.*, **2024**, 9, 035012. (IF=5.6, citations=18) **(QC, MD)**

45) Long D.B., Tkachenko N.V., Feng Q., Li X., Boldyrev A.I., Yang J., and Yang L.M. "Two-dimensional bimetal-embedded expanded phthalocyanine monolayers: a class of multifunctional materials with fascinating properties", *Adv. Funct. Mater.*, **2024**, *34*, 2313171. (IF=18.5, citations=2) **(MS)**

44) Tkachenko N.V., Tkachenko A.A., Nebjen B., Tretiak S., and Boldyrev, A.I. "Neural Network Atomistic Potentials for Global Energy Minima Search in Carbon Clusters", *Phys. Chem. Chem. Phys.*, **2023**, *25*, 21173-21182. (Featured on the Inside Cover Page; Highlighted as "2023 PCCP HOT Articles") (IF=2.9, citations=3) **(ML, MD)**

43) Rublev P., Tkachenko N.V., Dub P.A., and Boldyrev, A.I. "On the existence of CO_3^{2-} microsolvated clusters: a theoretical study", *Phys. Chem. Chem. Phys.*, **2023**, *25*, 14046-14055. (IF=2.9, citations=1) **(INC)**

42) Xu Y.H., Tkachenko N.V., Muñoz-Castro A., Boldyrev, A.I., and Sun Z.M. "A Branch of Zintl Chemistry: Metal Clusters of Group 15 Elements", In *Atomically Precise Nanochemistry*, **2023**, Wiley, pp. 395-422, DOI: 10.1002/9781119788676.ch13 (Invited Chapter, citations=0) **(INC)**

41) Rublev P., Tkachenko N.V., Pozdeev A.S., and Boldyrev A.I. "Tinning the Carbon: Hydrostannanes Strike Back", *Dalton Trans.*, **2023**, *52*, 29-36. (Featured on the Front Cover Page, highlighted as "Dalton Transactions HOT Articles") (IF=3.5, citations=5) **(INC)**

40) Tkachenko N.V., Sun Z.M., Boldyrev A.I., and Munoz-Castro A. "Advances in Cluster Bonding: Bridging Superatomic Building Blocks via Intercluster Bonds", In *Atomic Clusters with Unusual Structure, Bonding and Reactivity*, **2023**, Elsevier, pp. 321-332, DOI: 10.1016/B978-0-12-822943-9.00010-3. (Invited Chapter, citations=0) **(CB, INC)**

39) Getmanskii I.V., Koval V.V., Tkachenko N.V., Zaitsev S.A., Boldyrev A.I., and Minyaev R.M. "Ultralight Supertetrahedral Aluminum: Stability at Various Temperatures", *MRS Bull.* **2023**, *48*, 207-213. (IF=4.1, citations=0) **(MS)**

38) Rublev P., Tkachenko N.V., and Boldyrev A.I. "Overlapping electron density and the global delocalization of π-aromatic fragments as the reason of conductivity of the biphenylene network", *J. Comp. Chem.* **2023**, *44*, 168-178. (IF=3.4, citations=9) **(MS)**

37) Tkachenko N.V., Rublev P., and Dub P.A. "The Source of Proton in the Noyori–Ikariya Catalytic Cycle", *ACS Catal.,* **2022**, *12*, 13149-13157. (IF=11.3, citations=9) **(CAT)**

36) Tkachenko N.V., Chen W.X., Morgan H.W.T., Muñoz-Castro A., Boldyrev A.I., and Sun Z.M. "Sn_{36}^{8-}: A 2.7 nm Naked Aromatic Tin Rod", *Chem. Commun.*, **2022**, *58*, 6223-6226. (IF = 4.9, citations=12) **(CB, MS, EXP)**

35) Xu H.L., Tkachenko N.V., Szczepanik D., Popov I.A., Muñoz-Castro A., Boldyrev A.I., and Sun Z.M. "Symmetry Collapse due to the Presence of Multiple Local Aromaticity in Ge_{24}^{4-}", *Nat. Commun.* **2022**, *13*, 2149. (IF=14.7, citations=15) **(CB, INC, EXP)**

34) Tkachenko N.V., Rublev P., Boldyrev A.I., and Lehn J.M. "Superalkali Coated Rydberg Molecules", *Front. Chem.* **2022**, *10*, 880804. (IF=3.8, citations=1) **(INC, ORG)**

33) Yokelson D., Tkachenko N.V., Robey R., Li Y.W., and Dub P.A. "Performance Analysis of CP2K Code for Ab Initio Molecular Dynamics", *J. Chem. Inf. Model* **2022**, *62*, 2378-2386. (Featured on the Inside Cover Page) (IF=5.6, citations=12) **(HPC)**

32) Chen W.X., Tkachenko N.V., Munoz-Castro A., Boldyrev A.I., and 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=9.9, citations=1) **(CB, INC, EXP)**

31) Minkin V.I., Ivakhnenko E.P., Knyazev P.A., Starikov A.G., Demidov O.P., Tkachenko N.V., and 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=1.7, citations=4) **(ORG, EXP)**

30) Zhang W.Q., Tkachenko N.V., Qiao L., Boldyrev A.I., and 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=5.5, citations=7) **(CB, INC, EXP)**

29) Tkachenko N.V., Munoz-Castro A., and 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=4.2, citations=7) **(CB, INC, ORG)**

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=2.7, citations=7) **(MD)**

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=2.2, citations=16) **(CB, INC)**

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=14.7, citations=13) **(CB, INC, EXP)**

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. (Featured on the Inside Cover Page) (IF=2.7, citations=13) **(CAT)**

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. (IF=9.3, citations=75) **(QC, MD)**

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, citations=3) **(CB, INC)**

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=2.5, citations=36) **(CAT, EXP)**

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=16.1, citations=10) **(CB, INC, EXP)**

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=4.8, citations=51) **(MS, EXP)**

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=14.7, citations=19) **(CB, INC, EXP)**

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=4.3, citations=4) **(INC)**

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=16.1, citations=34) **(CB, INC, EXP)**

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=4.9, citations=23) **(CB, INC, EXP)**

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=3.4, citations=30) **(MS)**

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=3.9, citations=25) **(CB, INC, EXP)**

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 2D SiN Monolayer", *Phys. Status Solidi B*, **2020**, *257*, 1900619. (IF=1.6, citations=17) **(MS)**

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. (Highlighted as "2023 PCCP HOT Articles")(IF=2.9, citations=44) **(MS)**

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) (IF=2.3, citations=26) **(INC, ORG)**

10) Tkachenko N. V., and Boldyrev A. I. "Multiple Local σ-Aromaticity of the Nonagermanide Clusters", *Chem. Sci.*, **2019**, *10*, 5761-5765. (IF=7.6, citations=39) **(CB, INC)**

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=16.1, citations=26) **(INC, EXP)**

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=3.3, citations=105) **(MD, CB, PC)**

7) Tkachenko N. V., and Scheiner S. "Optical Stability of 1,1'-Binaphthyl Derivatives", *ACS Omega*, **2019**, *4*, 6044-6049. (IF=3.7, citations=15) **(ORG)**

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=1.9, citations=18) **(EXP)**

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=0.8, citations=6) **(EXP)**

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=2.3, citations=12) **(EXP)**

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=11.3, citations=44) **(EXP)**

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=3.8, citations=28) **(EXP)**

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=3.4, citations=22) **(EXP)**

Awards:

15) *Best Flash Presentation Award* at the ACS Meetings Global Virtual Symposia Fall 2024 - Materials for Energy Storage ‖ Oct. **2024** (International competition, success rate < 6.0 % or 3 Awardee out of ~50 speakers)

14) *Molecules 2023 Best PhD Thesis Award*, goes to recently qualified PhD who have produced a highly anticipated thesis with great academic potential ‖ Jan. **2024** (International competition)

13) *Dr. William Moore Scholarship* for outstanding research progress in Physical Chemistry ‖ Apr. **2023** (Departmental Competition, success rate: < 15% or 1 Awardee out of ~7 students)

12) *Teng Outstanding Graduate Student in Chemistry* for outstanding research progress at Utah State University ‖ Apr. **2023** (Departmental Competition, success rate: < 15% or 1 Awardee out of ~7 students)

11) *Utah State University Robins Award: The Doctoral Student Researcher of the Year 2023,* goes to the doctoral student researcher at Utah State University who has shown superior research capability and academic excellence. ‖ Apr. **2023** (University Competition, success rate: < 0.15% or 1 Awardee out of ~800 students)

10) *College of Science PhD Student Researcher of the Year Award 2023*, given to a student, who has demonstrated outstanding research and academic achievements. Utah State University ‖ Feb. **2023** (USU College of Science Competition, success rate: < 1% or 1 Awardee out of ~150 students)

9) *J. R. Oppenheimer Distinguished Postdoctoral Fellow* appointment at Los Alamos National Laboratory; recognizes outstanding individuals whose research aligns with the Laboratory's mission - *declined* ‖ Dec. **2022** (International Competition, success rate < 0.25% or 1 Awardee out of ~400 postdocs)

8) *ACS Utah Outstanding Graduate Student Award 2022*, recognizes the research, mentorship, leadership, and public outreach of an outstanding chemistry graduate student in Utah ‖ Oct. **2022** (State Competition, success rate < 0.5% or 1 Awardee out of ~250 Ph.D. students)

7) *Claude E. ZoBell Scholarship*, a support for the graduate student pursuing degrees in biology, chemistry and biochemistry, geology, or physics. Utah State University ‖ Jun. **2022** (USU College of Science Competition, success rate: < 1% or 1 Awardee out of ~150 students)

6) *Stephen Bialkowski Award in Environmental Chemistry*, a support of a specific environmental chemistry research at the Department of Chemistry and Biochemistry, Utah State University ‖ Apr. **2020** (Departmental Competition, success rate: < 3% or 1 Awardee out of ~35 Ph.D. students)

5) *The Early Research Progress in Chemistry Award* for outstanding research progress at Utah State University ‖ Apr. **2020** (Departmental Competition, success rate: < 15% or 1 Awardee out of ~7 Ph.D. students)

4) *Marjorie H. Gardner Teaching Award* for outstanding work as a teaching assistant at Utah State University ‖ Mar. **2019** (Departmental Competition, success rate: < 10% or 3 Awardees out of ~35 Ph.D. students)

3) *British Petroleum Scholarship Award* for High Academic Standing and Outstanding Leadership Qualities ‖ **2017, 2016** (University Competition, success rate: < 5% or 10 Awardees out of ~250 students)

2) *1st Degree Diploma* of the "VII International Natural Sciences Tournament" – Individual Competition ‖ Nov. **2016** (International Competition, success rate: < 7% or 7 Awardees out of ~100 students)

1) *1st Degree Diploma* of the International Forum of Young Scientists "Science Game" – Team Competition ‖ May **2016** (National Competition, success rate: < 5% or 1 Team Awardee out of ~20 teams)

Conferences and Invited Talks:

13) Invited keynote speaker at UC Davis annual Chemical Engineering and Materials Science (CHMS) Research Symposium "Tuning Hydrogen Binding Enthalpy in Metal-Organic Frameworks and Correcting Unphysical Potential Energy Surfaces in D3 and D4 Dispersion Models" ‖ 18 Oct. **2024**, Davis, USA

12) Oral presentation at ACS Fall 2024, "Global Virtual Symposium in Materials for Energy Storage" ‖ 18-22 Aug. **2024**, USA

11) Oral and poster presentations at Gordon Research Conference/ Gordon Research Seminar on Computational Chemistry, University of Southern Maine in Portland, Maine ‖ 20 Jul. **2024**, Portland, USA

10) Discussion Leader at NSF Challenge Institute for Quantum Computation Annual Meeting "Quantum chemistry and fermionic encoding" ‖ 17 Jun. **2024**, Berkeley, USA

9) Invited seminar at "Quantum Gathering" lecture series, University of California, Berkeley "Correlation-Informed Permutation of Qubits for Reducing Ansatz Depth in Electronic Structure Simulation on Quantum Computers" ‖ 18 Aug. **2023**, Berkeley, USA

8) Invited seminar at Computer Science Department, Utah State University "Quantum Computing and Its Applications in Quantum Chemistry" ‖ 30 Nov. **2022**, Logan, USA
7) Invited seminar at Stanford University "Exploring the Electronic-Structure Problem with Quantum Computers and Deciphering Exotic Chemical Bonding in Clusters and Solids" ‖ 8 Sep. **2022**, Stanford, USA
6) Invited talk at International Conference on Chemical Bonding, "Simulating Electronic Structure on Quantum Computers with PermVQE and QDavidson Algorithms" ‖ 11-17 Aug. **2022**, Kauai (Hawaii), USA
5) Oral presentation at ACS National Meeting & Expo, the symposium on "Synergy Between Quantum Computing and High-Performance Computing in Quantum Chemistry and Materials Science" ‖ 5-16 Apr. **2021**, USA
4) Invited talk at C-IIAC division, Los Alamos National Laboratory "Electronic Structure Simulation on Near-Term Quantum Computers with LANL-Developed PermVQE Algorithm" ‖ 17 Dec. **2020**, Los Alamos National Laboratory.
3) Poster presentation at ACS National Meeting & Expo, Physical Chemistry Session, Sci-Mix Session ‖ 25-29 Aug. **2019**, San Diego (CA), USA
2) Oral presentation at 27th International Chugaev Conference on Coordination Chemistry, "Physicochemical Methods in Coordination Chemistry" ‖ 2-6 Oct. **2017**, Nizhny Novgorod, Russia
1) Poster presentation IV Scientific Conference Boreskov Readings dedicated to the 110th anniversary of Academician Georgii K. Boreskov ‖ 19-21 Apr. **2017**, Novosibirsk, Russia

Teaching Experience

6) CHEM 6010 Quantum Chemistry, Lecturing a full course ‖ Jan.-May **2023**, Utah State University
5) CHEM 3060 Physical Chemistry I, Lecturing a part of the course ‖ Aug.-Dec. **2021**, **2022**, Utah State University
4) CHEM 1215 Chemical Principles Laboratory I, Labs ‖ Aug.-Dec. **2020**, Utah State University
3) CHEM 1225 Chemical Principles Laboratory II, Labs ‖ Jan.-May **2020**, Utah State University
2) CHEM 1220 Principles of Chemistry II, Recitations ‖ Jan.-May **2019**, Utah State University
1) Structure of Matter, Recitations ‖ **2016-2018**, Novosibirsk State University