

Nikita Fedik

Director's Postdoc Fellow at Los Alamos National Laboratory
Machine Learning | Computational Chemistry | Materials Science



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EDUCATION

PhD Utah State University, US

2018-2022

Computational Chemistry; GPA=4.0 *summa cum laude*
Advisor: Prof. Alexander I. Boldyrev

B.Sc. Southern Federal University, Russia

2012-2017

Fundamental and Applied Chemistry; GPA = 4.0 *summa cum laude*

SKILLS

COMPUTATIONAL CHEMISTRY

thermodynamics, kinetics and spectroscopy
solid-state calculations, 2D/3D materials
multireference calculations
molecular dynamics, large-scale simulations
molecular design and chemical bonding

*Gaussian, ORCA, PSI4, VASP
AdNDP, AIMAll, MultiWFN
ASE, phonopy, aenet, hippynn, cclib*

MACHINE LEARNING

supervised learning, neural networks
hyperparameter search, model tuning
data generation, cleaning, and visualization

*Python, Jupyter Notebook, VSCode
numpy, sklearn, pytorch, skorch, matplotlib*

SYSTEM ADMINISTRATION/POWER USER

deployment of small HPC clusters
Windows and Linux machines
networks, remote access, NFS storage
schemes, illustrations, computer graphics

*Unix-shell, bash, ssh, Slurm
WinSCP, MobaXterm, TeamViewer
MS Office, Adobe Photoshop*

WORK EXPERIENCE

Director's Postdoc Fellow

2022 - present

T-1 Division/Center for Non-Linear Studies (CNLS) at Los Alamos National Laboratory, US
Development of machine learning parametrized reduced Hamiltonians for excited states

Graduate Research Subcontractor

2021 - 2022

Los Alamos National Laboratory, US (Dr. Sergei Tretiak group, T-1)
Organometallic potentials via transfer learning from organic models
Inclusion of long-range effects into ML-potentials

Graduate Research Assistant

2018 - 2021

Utah State University, US (Prof. Alexander I. Boldyrev group)
Design and study of novel chemical bonds in materials and atomic clusters
Advancement of computing infrastructure

Graduate Research Assistant

summer 2020

Los Alamos National Laboratory, US (Center for Non-linear Studies)
Generation of organometallics dataset for ML models

Graduate Research Assistant

summer 2019

summer 2018

Institute of Physical Organic Chemistry, Russia (Laboratory of Polyfunctional Materials Modeling)

Design of new polyfunctional 2D materials and new boron architectures

Undergraduate Research Assistant

2012 - 2017

Southern Federal University, Russia (Laboratory of Medicinal Chemistry)
Computational study of NO-donating mechanism in furoxans
Reactivity of biologically relevant heterocycles.

TEACHING EXPERIENCE

CHEM 1225 Chemical Principles in Lab II (Dr. Douglas Harris)

Fall 2018

CHEM 1225 Chemical Principles in Lab II (Dr. Robert Alumbaugh)

Fall 2019, 2020

Physical Chemistry Laboratory CHEM 3090 (Dr. Y. Rao and Prof. A. Boldyrev)

Spring 2021, 2022

Development of labs for Physical Chemistry Laboratory CHEM 3090:

- Mechanisms of organic reactions: computational study of methanal formation
- Vibrational-Rotational Spectroscopy of HCl and DCl: a computational study

OUTREACH ACTIVITIES

Assembly and administration of small computing cluster PRAGUE

2019-2022t

author of idea and administrator, Utah State University, US

- 15 nodes operated by Linux/Slurm
- central NSF storage for software collection and user folders
- used for departmental research and computational labs in PhysChem3090

Computing time proposals for Boldyrev group and collaborators

2019-2022

PI delegate, Utah State University, US

all my proposals were awarded maximum allocation time:

- "Improving Accuracy of Semiempirical Methods for Transition Metals with Machine Learning"
- "Capturing Relevant Properties of Clusters and Materials with Machine Learning"
- "Application of Artificial Intelligence in Clusters and 2D- and 3D-Materials"

Mentorship of new graduate students

2018

mentor, Utah State University, US

Mentorship of new undergraduate students

2015-2017

mentor, Southern Federal University, Russia

Interactive museum project "Homo Creatus"

2013-2017

project links art and science and illustrates how life-changing inventions work

demonstrator, Southern Federal University, Russia

V Southern Festival of Science

2014

presenter, Southern Federal University, Russia

EXTRA TRAINING

Deep Learning with IBM, Specialization, <i>edX</i>	in progress
UNIX Tools: Data, Software and Production Engineering, <i>edX</i>	2021
Python for Scientists and Engineers, <i>Enthought (live session)</i>	2021
Machine Learning Mastery Workshop, <i>Enthought (live session)</i>	2021
Tutorial Workshop: Machine Learning in Materials, <i>Data Science Institute, Columbia University</i>	2020

AWARDS

Director's Postdoc Fellowship	2022
Los Alamos National Laboratory (~30 fellowships per Laboratory per year)	
The College of Science Doctoral Student Researcher of the Year	2022
Utah State University, USA (rate: ~0.25%, 1 award per ~400 students)	
Outstanding Graduate Student in Chemistry	2021
Utah State University, USA (rate: ~3%, 1 award per 40 graduate students)	
Early Research Progress in Chemistry	2019
Utah State University, USA (rate: ~4%, 1-2 awards per 40 graduate students)	
Student of the Year in Natural Sciences	2016
Southern Federal University, Russia (rate: ~0.1%, 1 award per ~1000 students)	
Commemorative medal for merits in science	2016
Rostov Area Government, Russia (rate: ~0.01%, 1 award per ~8000 students)	
Superior Academic Achievement and Leadership	2015
Cargill, Inc., USA-Netherlands (10 awards per country)	

SCHOLARSHIPS

Teng Endowed Fellowship	2021
Utah State University, USA (rate: 1-2 awards per year)	
Summer Internship at Center for Nonlinear Studies (CNLS)	2020
Los Alamos National Laboratory, USA	
Cargill Global Scholars Program	2014-2016
Cargill, Inc., USA-Russia (rate: 10 awards per country)	
Science Merit Scholarship	2015-2017
Southern Federal University, Russia (rate: 10% of top students in College of Science)	
Congress of Russian Americans Scholarship	2014-2016
USA-Russia	
Scholarship of private bank Center-Invest	2016, 2015, 2014
Southern Russia (rate: ~20%: 250 awards per 1250 applicants)	
Scholarship of Rostov Area Governor	2016, 2015
Russia	
President's Scholarship	2016
Southern Federal University, Russia	

REVIEWING ACTIVITY

PUBLICATIONS

29 published articles + 1 in press (8 as a **first** author)

Citations: 304/370 (Web of Science/Google Scholar)

h-index: 11/12

IF = impact factor

30. Machine Learning for Molecular Properties: Going Beyond Interatomic Potentials IF = 41.4
N. Fedik, R. Zubatyuk, M. Kulichenko, N. Lubbers, J. S. Smith, B. Nebgen, R. Messerly, Y. W. Li, A. I. Boldyrev, K. Barros, O. Isayev, S. Tretiak
Nature Reviews Chemistry, **2022** (in press)
29. Mechanisms of Nitric Oxide Generation in Living Systems IF = 4.4
O. Burov, M. Kletskii, S. Kurbatov, A. Lisovin, **N. Fedik**
Nitric Oxide, **2021**, 118, 1-16.
28. The Rise of Neural Networks for Materials and Chemical Dynamics IF = 6.5
M. Kulichenko, J. Smith, B. Nebgen, Y. W. Li, **N. Fedik**, A. I. Boldyrev, N. Lubbers, K. Barros, S. Tretiak
The Journal of Physical Chemistry Letters, **2021**, 12(26), 6227-6243 (inside cover, invited review).
27. Band Gap Engineering and 14 Electron Superatoms in 2D Superoctahedral Boranes B₄X₂ (B, N, P, As, Sb) IF = 4.1
N. Fedik, D. Steglenko, A. Muñoz-Castro, R. M. Minyaev, V. I. Minkin
The Journal of Physical Chemistry C, **2021**, 125(31), 17280-17290.
26. Spherical Aromaticity in Inorganic Chemistry IF = N/A
M. Kulichenko, **N. Fedik**, N. V. Tkachenko, A. Muñoz-Castro, Z-M. Sun, A. I. Boldyrev
Aromaticity (**Book Chapter**), edited by Israel Fernandez, Elsevier, **2021**, 447-489.
25. Bridging Aromatic/Antiaromatic Units: Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-Metal Clusters from Bonding and Magnetic Analyses IF = 2.5
N. V. Tkachenko, I. A. Popov, M. Kulichenko, **N. Fedik**, Z-M. Sun, A. Muñoz-Castro, A. I. Boldyrev
European Journal of Inorganic Chemistry, **2021**, 41, 4239-4250.
24. "Bottled" Spiro-Doubly Aromatic Trinuclear [Pd₂Ru]⁺ Complexes IF = 9.8
M. Kulichenko, **N. Fedik**, A. Monfredini, A. Muñoz-Castro, D. Balestri, A. I. Boldyrev, G. Maestri
Chemical Science, **2020**, 12(1), 477-486.
23. Boron-made N₂: Realization of a B≡B Triple Bond in the B₂Al₃⁻ Cluster IF = 5.2
N. Fedik, C. Mu, I. A. Popov, W. Wang, H. Wang, K. H. Bowen, A. I. Boldyrev, X. Zhang
Chemistry – A European Journal, **2020**, 26(36), 8017-8021.
22. Reply to the Comment on "Realization of Lewis Basic Sodium Anion in the NaBH₃⁻ Cluster" IF = 15.3
G. Liu, **N. Fedik**, C. Martinez-Martinez, S. Ciborowski, X. Zhang, A. I. Boldyrev, K. Bowen
Angewandte Chemie International Edition, **2020**, 59(23), 8760-8764.
21. Can Aromaticity be a Kinetic Trap? Example of Mechanically Interlocked Aromatic Polycatenanes Built of Cyclo[18]carbon IF = 6.2
N. Fedik, M. Kulichenko, D. Steglenko, A. I. Boldyrev
Chemical Communications, **2020**, 56(18), 2711-2714.
20. Periodic F-defects on the MgO Surface as Potential Single-Defect Catalysts with Non-Linear Optical properties IF = 2.3
M. Kulichenko, **N. Fedik**, D. Steglenko, R. M. Minyaev, V. I. Minkin, A. I. Boldyrev
Chemical Physics, **2020**, 532, 110680.

19. Expansion Of Aromaticity Magnetic Criteria on Multi-Layer Structures. Magnetic Response and Spherical Aromaticity Of Matryoshka-Like $[\text{Sn}@\text{Cu}_{12}@\text{Sn}_{20}]^{12-}$ Cluster IF = 5.2
M. Kulichenko, **N. Fedik**, A. Muñoz-Castro, A. I. Boldyrev
Chemistry – A European Journal, **2019**, 26(10), 2263-2268.
18. Realization of Lewis Basic Sodium Anion in the NaBH_3^- Cluster IF = 15.3
G. Liu, **Fedik N.**, C. Martinez-Martinez, S. Ciborowski, X. Zhang, A. I. Boldyrev, K. Bowen
Angewandte Chemie International Edition, **2019**, 58, 13789-13793 (VIP article)
17. Structure and Bonding in $[\text{Sb}@\text{In}_8\text{Sb}_{12}]^{3-}$ IF = 15.3
C. Liu, N. V. Tkachenko, I. A. Popov, **N. Fedik**, X. Min, A. I. Boldyrev, Z.-M. Sun
Angewandte Chemie International Edition, **2019**, 58(25), 8367-8371. (inside cover)
16. Hydrated Sulfate Clusters $\text{SO}_4^{2-}(\text{H}_2\text{O})_n$ ($n=1-40$): Charge Distribution through Solvation Shells and Stabilization IF = 3.0
M. Kulichenko, **N. Fedik**, K. Bozhenko, A. I. Boldyrev
The Journal of Physical Chemistry B, **2019**, 123(18), 4065-4069.
15. Two Names of Stability: Spherical Aromatic or Superatomic Intermetalloid Cluster IF = 2.3
 $[\text{Pd}_3\text{Sn}_8\text{Bi}_6]^{4-}$
N. Fedik, M. Kulichenko, A. I. Boldyrev
Chemical Physics, **2019**, 522, 134-137 (Front cover).
14. Inorganic Molecular Electride Mg_4O_3 : Structure, Bonding and Nonlinear Optical Properties IF = 5.2
M. Kulichenko, **N. Fedik**, K. V. Bozhenko, A. I. Boldyrev
Chemistry – A European Journal, **2019**, 25(20), 5311-5315.
13. Aromatic character of $[\text{Au}_{13}]^{5+}$ and $[\text{MAu}_{12}]^{4+/6+}$ ($\text{M} = \text{Pd}, \text{Pt}$) cores in ligand protected gold nanoclusters—interplay between spherical and planar σ -aromatics IF = 3.7
N. Fedik, A. I. Boldyrev, A. Muñoz-Castro
Physical Chemistry Chemical Physics, **2019**, 21(45), 25215-25219.
12. Superoctahedral Two-dimensional Metallic Boron with Peculiar Magnetic Properties IF = 3.7
N. V. Tkachenko, D. Steglenko, **N. Fedik**, N. M. Boldyreva, R. M. Minyaev, V. I. Minkin, A. I. Boldyrev
Physical Chemistry Chemical Physics, **2019**, 21(36), 19764-19771.
11. Comprehensive study of nitrofuroxanoquinolines. New perspective donors of NO molecules IF = 4.4
N. Fedik, M. E. Kletskii, O. N. Burov, A. V. Lisovin, S. V. Kurbatov, V. A. Chistyakov, P. G. Morozov
Nitric Oxide, **2019**, 93, 15-24.
10. Structure And Bonding of New Boron and Carbon Superpolyhedra IF = 1.9
O. A. Gapurenko, R. M. Minyaev, **N. Fedik**, V. V. Koval, A. I. Boldyrev, V. I. Minkin
Structural Chemistry, **2019**, 30(3), 805-814.
9. Insight into The Nature of Rim Bonds in Coronene IF = 2.8
N. Fedik, A. I. Boldyrev
The Journal of Physical Chemistry A, **2018**, 122(43), 8585-8590.
8. Thiol-Induced Nitric Oxide Donation Mechanisms in Substituted Nitrobenzofuroxans IF = 4.4
M. E. Kletskii, O. N. Burov, **N. Fedik**, S. V. Kurbatov
Nitric Oxide, **2017**, 62, 44-51.
7. 10-Dimethylamino Derivatives of Benzo[h]quinolone and Benzo[h]quinazolines: Fluorescent Proton Sponge Analogues with Opposed peri-NMe₂-N=Groups. How to Distinguish between Proton Sponges and Pseudo-Proton Sponges IF = 4.4
A. F. Pozharskii, V. A. Ozeryanski, V. I. Mikshiev, A. S. Antonov, A. V. Chernyshev, A. V. Metelitsa, G. S. Borodkin, **N. Fedik**, O.V. Dyablo
Journal of Organic Chemistry, **2016**, 81(13), 5574-5587.

6. Mechanisms For the Formation of Five-Membered Rings In Ethene Addition Reactions with Azomethine Ylide and Allyl Anion IF = 1.5
M. E. Kletsii, O. N. Burov, N. Fedik, S. V. Kurbatov
Chemistry of Heterocyclic Compounds, 2016, 52(09) «Percyclic reactions in organic chemistry», 700-710.
5. Synthesis and Study of Conformation of 8-Hydroxy-2-(2-(Pyridin-4-Yl)Vinyl)Quinoline By NMR Spectroscopy Correlation IF = N/A
D. A. Svetlichnyy, **N. Fedik**
St. Petersburg State University, 2016, 3(61), 171-179 (DOI: 10.21638/11701/spbu04.2016.205).
4. Molecular Structure and Protonation Trends In 6-Methoxy- And 8-Methoxy-2,4,5-Tris(Dimethylamino)-Quinolines IF = 3.2
O. V. Dyablo, A. F. Pozharskii, E. A. Shmoilova, V. A. Ozeryanski, N. Fedik, K. Yu. Suponitsky
Journal of Molecular Structure, 2015, 1107, 305-315.
3. Experimental and Quantum-Chemical Study Of Nucleophilic Substitution Mechanism in Berberine IF = 1.5
O.N. Burov, M.E. Kletsii, **N. Fedik**, A. N. Lisovin, S.V. Kurbatov
Chemistry of Heterocyclic Compounds, 2015, 51(11/12), 997-1007.
2. Mechanism of Thiol-Induced Nitrogen(II) Oxide Donation by Furoxans: a Quantum Chemical Study IF = 1.5
O. N. Burov, M. E. Kletsii, **N. Fedik**, A. N. Lisovin, S. V. Kurbatov
Chemistry of Heterocyclic Compounds, 2015, 51(11/12), 951-960.
1. Cycloaddition Of [3]Dendralene Derivatives To Dinitrobenzofuroxan and Nitrobenzodifuroxan IF = 1.5
P. G. Morozov, S. V. Kurbatov, Yu. P. Semenyuk, O. N. Burov, M. E. Kletsii, **N. Fedik**, K. F. Suzdalev
Chemistry of Heterocyclic Compounds, 2015, 51(10), 903-912.

PRESENTATIONS

16. Understanding and Designing Chemical Bonding: Synergy of Experiment and Computations 2022, seminar, Center for Nonlinear Studies, Los Alamos National Laboratory, USA
15. Accurate Machine Learned Semi-Empirical Hamiltonian for Titanium Complexes 2021, poster presentation, Laboratory Directed Research & Development, Los Alamos National Laboratory, USA
14. Dative or not Dative? How Tiny NaBH_3^- Cluster Triggered Big Debates. 2021, oral presentation, Utah State University, USA
13. Size Does not Matter: Machine Learning Potentials Trained on X_n Stoichiometries are Applicable for X_{n+m} Systems 2021, oral presentation, ACS Spring 2021 National Meeting, USA
12. From Data to Machine Learning Models: Design of Interatomic Potentials 2020, oral presentation, Utah State University, USA
11. Machine Learning Parametrization of Empirical and Semiempirical Methods for Improving Transition Metal Chemistry 2019, oral presentation, Los Alamos National Laboratory, USA
10. Artificial Intelligence Driven Exploration of Potential Energy Surfaces 2019, oral presentation, Utah State University, USA
9. Dualism of Electronically Enriched Boron Clusters: from Transmutation to Nitrogen to Formation of Inverse Lewis Pair 2019, poster presentation, ACS Fall 2019 National Meeting, USA, San Diego
8. Coronene's Conundrum in Organic Chemistry. Is It Finally Solved? 2018, oral presentation, Utah State University, USA

7. About Educational System in The USA And Graduate Study Experience at Utah State University
2018, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia
6. Search for New NO-Donors by Methods of Quantum Chemistry
2017, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia
5. Quantum Chemical Study of NO Donation Mechanisms
2017, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia
4. Furoxans as NO Donating Drugs: Theoretical Study
2016, *oral presentation*, Southern Federal University, Russia
3. Study of Reactivity of Alkaloid Berberine Derivatives
2016, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia
2. Mechanisms of Nucleophilic Substitution in Alkaloid Berberine as a Potential Drug
2015, *oral presentation*, Southern Federal University, Russia
1. Structure of 8-Hydroxyquinoline Derivatives as Ligands For Oleds
2014, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia