

Nikita Fedik

Machine Learning | Computational Chemistry | Material Science

Director's Postdoc Fellow at Los Alamos National Laboratory

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	personal: nikitaFedik.github.io work: CNLS Nikita Fedik			LinkedIn: nfedik

EDUCATION

PhD **Utah State University, US** **2022**

Computational Chemistry; GPA=4.0 *summa cum laude*

Advisor: Prof. Alexander I. Boldyrev

B.Sc. **Southern Federal University, Russia** **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

machine learning interatomic potentials
data generation and visualization

Python
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
MS Office, Adobe Photoshop
Jupyter Notebook, VSCode

WORK EXPERIENCE

Director's Postdoc Fellow **2022 - present**

T-1 Division/Center for Non-Linear Studies (CNLS) at Los Alamos National Laboratory, US

GPU-enabled calculations of excited states + ML parametrization of Hamiltonians

Transition Path Sampling of molecules: data selection/generation for ML models

Graduate Research Assistant	2018 - 2022
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
Institute of Physical Organic Chemistry, Russia (Laboratory of Polyfunctional Materials Modeling)	summer 2018
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:	
<ul style="list-style-type: none"> - Mechanisms of organic reactions: computational study of methanal formation - Vibrational-Rotational Spectroscopy of HCl and DCl: a computational study 	

MANAGEMENT EXPERIENCE

Organizer of International Workshop “ <i>Machine Learning in Chemical and Materials Sciences 2024</i> ” Center for Nonlinear Studies, Los Alamos National Laboratory, USA	planned in 2024
Mentorship of summer graduate intern Los Alamos National laboratory, USA - Vitor Grizzi, University of Illinois at Urbana-Champaign	2023
Session Chair at <i>International Conference on Chemical Bonding 2023</i> session: Clusters and Spectroscopy, Lihue, USA	2023
Visit of Dr. James Stewart (Mr. Mopac) <i>host</i> , Los Alamos National Laboratory	2023
Session Chair at <i>Machine Learning and Informatics for Chemistry and Material</i> hands-on-workshop, Telluride, USA	
Session Chair at <i>International Conference on Chemical Bonding 2022</i> session: Bonding for Quantum Technology, Lihue, USA	2023
Assembly and administration of small computing cluster PRAGUE author of idea and administrator, Utah State University, USA <ul style="list-style-type: none"> - 15 nodes operated by Linux/Slurm - central NSF storage for software collection and user folders - used for departmental research and computational labs in PhysChem3090 	2019-2022

Computing time proposals for Boldyrev group and collaborators	2019-2022
<i>PI delegate, Utah State University, US</i>	
all my proposals were awarded maximum allocation time:	
<ul style="list-style-type: none"> - "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
Utah State University, US	
<ul style="list-style-type: none"> - Maksim Kulichenko, now PhD - Nikolay Tkachenko, now PhD 	

Mentorship of new undergraduate students	2015-2017
Southern Federal University, Russia	
<ul style="list-style-type: none"> - Oleg Demekhin, now PhD - Alexander Zagrebaev, now PhD 	

OUTREACH ACTIVITIES

Interactive Workshop on Machine Learning for Chemistry and Materials	2023
speaker/teacher, North Dakota State University	
Interactive museum project "Homo Creatus"	2013-2017
project links art and science and illustrates how life-changing inventions work	
<i>demonstrator, Southern Federal University, Russia</i>	
V Southern Festival of Science	2014
<i>presenter, Southern Federal University, Russia</i>	

EXTRA TRAINING

CS50: Intro to Computer Science, <i>Harvard University, online</i>	in progress
Introduction to Molecular Modeling in Drug Discovery, <i>Schrödinger</i>	2022
Machine Learning and Informatics for Chemistry and Materials, <i>Telluride Science Research Center</i>	2021
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	
The College of Science Doctoral Student Researcher of the Year	2022
Utah State University, USA	
Outstanding Graduate Student in Chemistry	2021
Utah State University, USA	
Early Research Progress in Chemistry	2019
Utah State University, USA	

Student of the Year in Natural Sciences Southern Federal University, Russia	2016
Commemorative medal for merits in science Rostov Area Government, Russia	2016
Superior Academic Achievement and Leadership Cargill, Inc., USA-Netherlands	2015

SCHOLARSHIPS


Teng Endowed Fellowship Utah State University, USA	2021
Summer Internship at Center for Nonlinear Studies (CNLS) Los Alamos National Laboratory, USA	2020
Cargill Global Scholars Program Cargill, Inc., USA-Russia	2014-2016
Science Merit Scholarship Southern Federal University, Russia)	2015-2017
Congress of Russian Americans Scholarship USA-Russia	2014-2016
Scholarship of private bank Center-Invest Southern Russia	2016, 2015, 2014
Scholarship of Rostov Area Governor Russia	2016, 2015
President's Scholarship Southern Federal University, Russia	2016

REVIEWING ACTIVITY

Reviewer for Journals: ChemPhysChem, Chemical Communications, Dalton Transactions, Physical Chemistry Chemical Physics, Chemical Physics, Canadian Journal of Chemistry, ChemistrySelect, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Computational and Theoretical Chemistry, RSC Advances, Molecules (MDPI), Chemistry (MDPI), Molecular Physics
22 reviews total

PUBLICATIONS

32 published articles (9 as a **first** author) + 1 chapter
Citations: 562 in Google Scholar
h-index: 16
IF = impact factor

32. Synergy of Semiempirical Models and Machine Learning in Computational Chemistry
N. Fedik, B. Nebgen, N. Lubbers, K. Barros, M. Kulichenko, Y. W. Li, R. Zubatyuk, R. Messerly, O. Isayev, S. Tretiak
The Journal of Chemical Physics, **2023**, 159, 110901.
 **front cover image, featured, invited review**

31. NEXMD v2.0 Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations IF = 5.5
V. M. Freixas, W. Malone, X. Li, H. Song, H. Negrin-Yuvero, R. Pérez-Castillo, A. White, T. R. Gibson, D. V. Makhov, D. V. Shalashilin, Y. Zhang, **N. Fedik**, M. Kulichenko, R. Messerly, L. N. Mohanam, S. Sharifzadeh, A. Bastida, S. Mukamel, S. Fernandez-Alberti, S. Tretiak
Journal of Chemical Theory and Computation, **2023**, 19, 5356-5368.
30. Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation IF = 5.5
M. Kulichenko, K. Barros, N. Lubbers, **N Fedik**, G. Zhou, S. Tretiak, B. Nebgen, A. M. N. Niklasson
Journal of Chemical Theory and Computation, **2023**, 19, 3209-3222.
29. Extending machine learning beyond interatomic potentials for predicting molecular properties 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**, 6, 653-672.
28. 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.
27. 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 image, invited review**
26. 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.
25. 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.
24. 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.
23. “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.
22. 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.
21. 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.
20. 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.

19. 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.
18. 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.
17. 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 – Editor’s pick of top 10%**
16. 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**)
15. 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.
14. Two Names of Stability: Spherical Aromatic or Superatomic Intermetalloid Cluster $[\text{Pd}_3\text{Sn}_8\text{Bi}_6]^{4-}$ IF = 2.3
N. Fedik, M. Kulichenko, A. I. Boldyrev
Chemical Physics, **2019**, 522, 134-137.
 **front cover image**
13. 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.
12. Aromatic character of $[\text{Au}_{13}]^{5+}$ and $[\text{MAu}_{12}]^{4+/6+}$ ($M = \text{Pd}, \text{Pt}$) 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.
11. 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.
10. Comprehensive study of nitrofuoroquinolines. 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.
9. 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.
8. 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.
7. 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.

6. 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
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. IF = 4.4
5. Mechanisms For the Formation of Five-Membered Rings In Ethene Addition Reactions with Azomethine Ylide and Allyl Anion
M. E. Kletskii, O. N. Burov, N. Fedik, S. V. Kurbatov
Chemistry of Heterocyclic Compounds, 2016, 52(09) «Peryclic reactions in organic chemistry», 700-710. IF = 1.5
4. Molecular Structure and Protonation Trends In 6-Methoxy- And 8-Methoxy-2,4,5-Tris(Dimethylamino)-Quinolines
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. IF = 3.2
3. Experimental and Quantum-Chemical Study Of Nucleophilic Substitution Mechanism in Berberine
O.N. Burov, M.E. Kletskii, **N. Fedik**, A. N. Lisovin, S.V. Kurbatov
Chemistry of Heterocyclic Compounds, **2015**, 51(11/12), 997-1007. IF = 1.5
2. Mechanism of Thiol-Induced Nitrogen(II) Oxide Donation by Furoxans: a Quantum Chemical Study
O. N. Burov, M. E. Kletskii, **N. Fedik**, A. N. Lisovin, S. V. Kurbatov
Chemistry of Heterocyclic Compounds, **2015**, 51(11/12), 951-960. IF = 1.5
1. Cycloaddition Of [3]Dendralene Derivatives To Dinitrobenzofuroxan and Nitrobenzodifuroxan
P. G. Morozov, S. V. Kurbatov, Yu. P. Semenyuk, O. N. Burov, M. E. Kletskii, **N. Fedik**, K. F. Suzdalev
Chemistry of Heterocyclic Compounds, **2015**, 51(10), 903-912. IF = 1.5

PRESENTATIONS

23. Journey to Differentiable Models: Chemical Bonding, Electronic Structure and Machine Learning
2023, invited seminar, North Dakota State University, USA
22. Synergy of Semiempirical Quantum Mechanics and Machine Learning
2023, poster presentation, Conference on Excited State Processes 2023, USA
21. Ground and Excited State Properties on Intersection of Machine Learning and Semiempirical Models
2023, invited talk, International Conference on Chemical Bonding (ICCB-23), USA
20. Bridging the Scales: Chemical Bonding, Machine Learning, and Differentiable Physics for Nanomaterials Exploration
2023, invited talk, Nanomaterials: Computation, Theory, Machine Learning and Experiment; Telluride Science Research Center, USA
19. Beyond Interatomic Potentials: Machine Learning Models for Practical Chemical Discovery
2022, seminar, Center for Nonlinear Studies, Los Alamos National Laboratory, USA
18. Machine Learnable Chemical Properties Along the Atomistic Scale
2022, invited talk, Machine Learning and Informatics for Chemistry and Materials, Telluride Science Research Center, USA
17. From Organics to Organometallics: Transfer Learning Interatomic Potentials
2022, invited talk, International Conference on Chemical Bonding (ICCB-22), USA

16. Understanding and Designing Chemical Bonding: Synergy of Experiment and Computations
2022, invited 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