Nikita Fedik

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

	Sante Fe, NM			Google Scholar: Nikita Fedik
	435-512-6637			ResearchGate: Nikita-Fedik
	personal: nikitafedik@gmail.com work: nfedik@lanl.gov			Publons: nikita-fedik
	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	Gaussian, ORCA, PSI4, VASP
solid-state calculations, 2D/3D materials	AdNDP, AIMAll, MultiWFN
multireference calculations	ASE, phonopy, aenet, hippynn, cclib
molecular dynamics, large-scale simulations	
molecular design and chemical bonding	

MACHINE LEARNING

machine learning interatomic potentials	Python
data generation and visualization	numpy, sklearn, pytorch, skorch, matplotlib

SYSTEM ADMINISTRATION/POWER USER

deployment of small HPC clusters	Unix-shell, bash, ssh, Slurm
Windows and Linux machines	Adobe Photoshop, VSCode
networks, remote access, NFS storage	Jekyll, web/UI basics
schemes, illustrations, computer graphics	

WORK EXPERIENCE

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

T-1 /CNLS at Los Alamos National Laboratory, US

- Developer of PYSEQM, GPU-accelerated quantum mechanics code interfaced with ML for model tuning
- Implementing module for excited state simulations: GPU-enabled Davidson algorithm for efficient matrix diagonalization in Krylov subspace
- Designed ideas and data to challenge ML in transition path sampling
- First-authored review in *Nature Chemistry Review* to guide enthusiast on incorporating ML for molecular property prediction

- Conceptualized a Perspective connecting ML and old-fashioned parametric quantum-mechanics (*featured and selected as cover image of JCP issue*)

Graduate Research Assistant **2018 - 2022**

Utah State University, US

- Computationally designed first of a kind chemical bond in $NaBH_3^-$ (synthesized, 20+ follow-up studies)
- Suggested first of a kind design of mechanically interlocked carbon rings (50+ citations)

Graduate Research Assistant **summer 2020**

Los Alamos National Laboratory, CNLS, US

- Designed organometallic dataset for machine learning interatomic potentials

Graduate Research Assistant **summer 2019**

Institute of Physical Organic Chemistry, Russia **summer 2018**

- Contributed to computational discovery of magnetic flat boron material

Undergraduate Research Assistant **2012 - 2017**

Southern Federal University, Russia (Laboratory of Medicinal Chemistry)

- Discovered the mechanism of vasodilating NO-release in furoxans
- Contributed to the strategy of alkaloid berberine functionalization

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

MANAGEMENT EXPERIENCE

Organizer of International Workshop "*Machine Learning in Chemical and Materials Sciences 2024*" **planned in 2024**

Center for Nonlinear Studies, Los Alamos National Laboratory, USA

Mentorship of summer graduate intern **2023**

Los Alamos National laboratory, USA

- Vitor Grizzi, University of Illinois at Urbana-Champaign

Session Chair at *International Conference on Chemical Bonding 2023* **2023**

session: Clusters and Spectroscopy, Lihue, USA

Visit of Dr. James Stewart (Mr. Mopac) **2023**

host, Los Alamos National Laboratory

Session Chair at *Machine Learning and Informatics for Chemistry and Material*

hands-on-workshop, Telluride, USA

Session Chair at *International Conference on Chemical Bonding 2022* **2023**

session: Bonding for Quantum Technology, Lihue, USA

Assembly and administration of small computing cluster PRAGUE **2019-2022**
author of idea and administrator, Utah State University, USA
- 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**
Utah State University, US

- Maksim Kulichenko, now PhD
- Nikolay Tkachenko, now PhD

Mentorship of new undergraduate students **2015-2017**
Southern Federal University, Russia

- 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
demonstrator, Sothern Federal University, Russia

V Southern Festival of Science **2014**
presenter, Southern Federal University, Russia

EXTRA TRAINING

CS50: Intro to Computer Science, *Harward University, online* **in progress**

Introduction to Molecular Modeling in Drug Discovery, *Schrödinger* **2022**

Machine Learning and Informatics for Chemistry and Materials, *Telluride Science Research Center* **2021**

UNIX Tools: Data, Software and Production Engineering, *edX* **2021**

Python for Scientists and Engineers, *Enthought (live session)* **2021**

Machine Learning Mastery Workshop, *Enthought (live session)* **2021**

Tutorial Workshop: Machine Learning in Materials, *Data Science Institute, Columbia University* **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 **2016**
Southern Federal University, Russia

Commemorative medal for merits in science **2016**
Rostov Area Government, Russia

Superior Academic Achievement and Leadership **2015**
Cargill, Inc., USA-Netherlands

SCHOLARSHIPS

Teng Endowed Fellowship **2021**
Utah State University, USA

Summer Internship at Center for Nonlinear Studies (CNLS) **2020**
Los Alamos National Laboratory, USA

Cargill Global Scholars Program **2014-2016**
Cargill, Inc., USA-Russia

Science Merit Scholarship **2015-2017**
Southern Federal University, Russia)

Congress of Russian Americans Scholarship **2014-2016**
USA-Russia

Scholarship of private bank Center-Invest **2016, 2015, 2014**
Southern Russia

Scholarship of Rostov Area Governor **2016, 2015**
Russia

President's Scholarship **2016**
Southern Federal University, Russia

REVIEWING ACTIVITY

Reviewer for Journals: ChemPhysChem, Chemical Communications, Daltron 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 B_4X_2 (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 $[Pd_2Ru]^+$ 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 N_2: Realization of a B≡B Triple Bond in the $B_2Al_3^-$ 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 $NaBH_3^-$ 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 $[Sn@Cu_{12}@Sn_{20}]^{12-}$ 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 $[Sb@In_8Sb_{12}]^{3-}$ — 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 $SO_4^{2-}(H_2O)_n$ (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 $[Pd_3Sn_8Bi_6]^{4-}$ — 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 $[Au_{13}]^{5+}$ and $[MAu_{12}]^{4+/6+}$(M= Pd, 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 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.

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-NMe_2/-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.

5. Mechanisms For the Formation of Five-Membered Rings In Ethene Addition Reactions with Azomethine Ylide and Allyl Anion IF = 1.5
M. E. Kletskii, O. N. Burov, N. Fedik, S. V. Kurbatov
Chemistry of Hetererocylic Compounds, 2016, 52(09) «Perycylic reactions in organic chemistry», 700-710.

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. Kletskii, **N. Fedik**, A. N. Lisovin, S.V. Kurbatov
Chemistry of Hetererocylic 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. Kletskii, **N**. **Fedik**, A. N. Lisovin, S. V. Kurbatov
Chemistry of Heterocylic 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. Kletskii, **N. Fedik**, K. F. Suzdalev
*Chemistry of Heterocylic Compound*s, **2015**, 51(10), 903-912.

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-Hydrxoquinoline Derivatives as Ligands For Oleds
2014, *oral presentation*, Institute of Physical and Organic Chemistry (IPOC), Russia