Nikita Fedik

computational chemist

Birth date: 09/11/1994
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Google Scholar
ResearchGate
Github
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EDUCATION

PhD — Utah State University, US
2018 > present

Professor: Alexander I. Boldyrev.
Major: Physical/Computational Chemistry.
GPA: 4.0

Specialist — Southern Federal University, Russia
2012 > 2017

5-year course in Fundamental and Applied Chemistry graduated with honors.
GPA=4.0

SCHOLARSHIPS

Summer Internship
2020, Los Alamos National Laboratory

Cargill Global Scholars
2014-2017, USA-Russia

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

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

President's Scholarship
2016, Russia

WORK EXPERIENCE

Graduate Research Assistant — 2021 > present
Los Alamos National Laboratory/Utah State University, US

Generation of quantum chemical big data and training supervised machine learning models.
Projects: ML-parametrized semiempirical methods for transition metals
Inclusion of long-range effects into ML-potentials
Interfacing quantum-chemistry codes with active learning framework

Graduate Research Assistant — 2018 > present
Utah State University, US

Chemical bonding of novel materials and clusters. Among other systems, we designed:
- mechanically trapped polycatenanes built of new carbon allotrope C_{18}
- $Na^- \rightarrow BH_3$ dative bond, a first synthesized example of Lewis adduct with electron-donating alkalide
- B≡B triple bond in synthesized $B_2Al_3^-$, isoelectronic analogue of N_2 molecule

I am also responsible for advancement of computing infrastructure and built from scratch a small supercomputer PRAGUE (Ubuntu, Slurm, 15 computing nodes). Both my proposals for computational time at CHPC (University of Utah) won 200k of CPU time:
- Capturing Relevant Properties of Clusters and Materials with Machine Learning
- Application of Artificial Intelligence in Clusters and 2D- and 3D-Materials

Graduate Research Assistant — summer 2020
Los Alamos National Laboratory, US

Summer Internship supported by Center for Non-linear Studies. I was responsible for generating dataset of transition metal organometallics. Furtherly, it was used for ML-parametrization of existing semi-empirical methods.

Graduate Research Assistant — summer 2018
Institute of Physical Organic Chemistry (IPOC), Russia — 2019

Design of new polyfunctional 2D materials and new boron architectures. We predicted:
- B supertetrahedral cages, stabilized by spherical aromaticity
- magnetic 2-D monolayer built of tetrahedral units

Undergraduate Research Assistant — 2012 > 2017
Southern Federal University, Russia

Computational study of NO-donating mechanism in furoxans. We proved that it goes through radical mechanism, in contrast to common believe of anionic pathway. I was also involved in study of pericyclic reactions mechanisms.

AWARDS

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

SKILLS

MACHINE LEARNING	QUATUM CHEMISTRY	PYTHON	ARTICLE WRITING
DATA SCIENCE	MOLECULAR DESIGN	BASH	HPC COMPUTING

CLASSES AND WORKSHOPS

· CHEM5100 Computational Chemistry	Prof. Steve Scheiner	A	Fall 2018
· CHEM6010 Quantum Chemistry	Prof. Alexander Boldyrev	A	Fall 2018
· CHEM6020 Molecular Spectroscopy	Prof. Alexander Boldyrev	A	Soring 2019
· CHEM7020 Statistical Mechanics	Prof. Alexander Boldyrev	A	Fall 2020
· STAT6685 Deep Learning Theory and Applications	Prof. Kevin Moon	in progress	Fall 2021
· Tutorial Workshop: Machine Learning in Materials	Data Science Institute, Columbia University		Dec 2020
· UNIX Tools: Data, Software and Production Engineering	edX		May 2021
· IBM Artificial Intelligence Engineering, Specialization	Coursera		in progress
· Data Analysis with Python, Certificate	Coursera		in progress

TEACHING EXPERIENCE

- CHEM 1225 Chemical Principles in Lab II under Dr. Douglas Harris supervision — Fall 2018
- CHEM 1225 Chemical Principles in Lab II under Dr. Robert Alumbaugh supervision — Fall 2019
- CHEM 1225 Chemical Principles in Lab II under Dr. Robert Alumbaugh supervision — Fall 2020

- 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

PUBLICATIONS

2021

1. The Rise of Neural Networks for Materials and Chemical Dynamics
   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**).

2. Band Gap Engineering and 14 Electron Superatoms in 2D Superoctahedral Boranes B_4X_2 (B, N, P, As, Sb)
   N. Fedik, D. Steglenko, A. Muñoz-Castro, R. M. Minyaev, V. I. Minkin
   The Journal of Physical Chemistry C, **2021**, *125(31)*, 17280-17290.

3. Spherical aromaticity in inorganic chemistry
   M. Kulichenko, **N. Fedik**, N. V. Tkachenko, A. Muñoz-Castro, Z-M. Sun, A. I. Boldyrev
   Aromaticity, edited by Israel Fernandez, Elsevier, **2021**, 447-489.

4. Bridging Aromatic/Antiaromatic Units: Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-Metal Clusters from Bonding and Magnetic Analyses
   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**

2020

5. "Bottled" spiro-doubly aromatic trinuclear $[Pd_2Ru]^+$ complexes
   M. Kulichenko, **N. Fedik**, A. Monfredini, A. Muñoz-Castro, D. Balestri, A. I. Boldyrev, G. Maestri
   Chemical Science, **2020**, *12(1)*, 477-486.

6. Boron-made N_2: Realization of a B≡B Triple Bond in the $B_2Al_3^-$ Cluster
   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.

7. Reply to the Comment on "Realization of Lewis Basic Sodium Anion in the $NaBH_3^-$ Cluster"
   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.

8. Can aromaticity be a kinetic trap? Example of mechanically interlocked aromatic polycatenanes built of cyclo[18]carbon
   N. Fedik, M. Kulichenko, D. Steglenko, A. I. Boldyrev
   Chemical Communications, **2020**, *56(18)*, 2711-2714.

9. Periodic F-defects on the MgO Surface as Potential Single-Defect Catalysts with Non-Linear Optical properties
   M. Kulichenko, **N. Fedik**, D. Steglenko, R. M. Minyaev, V. I. Minkin, A. I. Boldyrev
   Chemical Physics, **2020**, *532*, 110680.

2019

10. Expansion of aromaticity magnetic criteria on multi-layer structures. Magnetic response and spherical aromaticity of Matryoshka-like $[Sn@Cu_{12}@Sn_{20}]^{12-}$ cluster
    M. Kulichenko, **N. Fedik**, A. Muñoz-Castro, A. I. Boldyrev
    Chemistry – A European Journal, **2019**, *26(10)*, 2263-2268.

11. Realization of Lewis Basic Sodium Anion in the $NaBH_3^-$ Cluster
    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**)

12. Structure and Bonding in $[Sb@In_8Sb_{12}]^{3-}$
    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**)

13. Hydrated Sulfate Clusters $SO_4^{2-}(H_2O)_n$ (n=1-40): Charge Distribution through Solvation Shells and Stabilization
    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 $[Pd_3Sn_8Bi_6]^{4-}$
    N. Fedik, M. Kulichenko, A. I. Boldyrev
    Chemical Physics, **2019**, *522*, 134-137 (**Front cover**).

15. New Inorganic Molecular Electride Mg_4O_3: Structure, Bonding and Nonlinear Optical Properties
    M. Kulichenko, **N. Fedik**, K. V. Bozhenko, A. I. Boldyrev
    Chemistry – A European Journal, **2019**, *25(20)*, 5311-5315.

16. 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
    N. Fedik, A. I. Boldyrev, A. Muñoz-Castro
    Physical Chemistry Chemical Physics, **2019**, *21(45)*, 25215-25219.

17. Superoctahedral two-dimensional metallic boron with peculiar magnetic properties
    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.

18. Comprehensive study of nitrofuroxanoquinolines. New perspective donors of NO molecules
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.

19. Structure and bonding of new boron and carbon superpolyhedra
O. A. Gapurenko, R. M. Minyaev, **N. Fedik**, V. V. Koval, A. I. Boldyrev, V. I. Minkin
Structural Chemistry, **2019**, *30(3)*, 805-814.

2018

20. Insight into The Nature of Rim Bonds in Coronene
N. Fedik, A. I. Boldyrev
The Journal of Physical Chemistry A, **2018**, *122(43)*, 8585-8590.

2017

21. Thiol-induced nitric oxide donation mechanisms in substituted nitrobenzofuroxans
M. E. Kletskii, O. N. Burov, **N. Fedik**, S. V. Kurbatov
Nitric Oxide, **2017**, *62*, 44-51.

2016

22. 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
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.

23. 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 Hetererocylic Compounds, **2016**, *52(09)* «Perycylic reactions in organic chemistry», 700-710.

24. Synthesis and Study of Conformation of 8-Hydroxy-2-(2-(Pyridin-4-Yl)Vinyl)Quinoline By NMR Spectroscopy Correlation
D. A. Svetlichnyy, **N. Fedik**
St. Petersburg State University, **2016**, *3(61)*, 171-179 (DOI: 10.21638/11701/spbu04.2016.205).

2015

25. 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.

26. 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 Hetererocylic Compounds, **2015**, *51(11/12)*, 997-1007.

27. 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 *Heterocylic Compounds*, **2015**, *51(11/12)*, 951-960.

28. 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 Heterocylic Compounds; **2015**, *51(10)*, 903-912.

PRESENTATIONS

2021

1. Size does not matter: Machine learning potentials trained on X_n stoichiometries are applicable for X_{n+m} systems
   oral presentation, ACS Spring 2021 National Meeting, USA

2020

2. From data to machine learning models: design of interatomic potentials
   oral presentation, Utah State University, USA

2019

3. Machine learning parametrization of empirical and semiempirical methods for improving transition metal chemistry
   oral presentation, Los Alamos National Laboratory, USA
4. Artificial intelligence driven exploration of potential energy surfaces
   oral presentation, Utah State University, USA
5. Dualism of electronically enriched boron clusters: From transmutation to nitrogen to formation of inverse Lewis pair
   poster presentation, ACS Fall 2019 National Meeting, USA, San Diego

2018

6. Coronene's conundrum in organic chemistry. Is it finally solved?
   oral presentation, Utah State University, USA
7. About educational system in the USA and graduate study experience at Utah State University
   oral presentation, Institute of Physical and Organic Chemistry (IPOC), Russia

2017

8. Search for new NO-donors by methods of quantum chemistry
   oral presentation, Institute of Physical and Organic Chemistry (IPOC), Russia
9. Quantum chemical study of NO donation mechanisms
   oral presentation, Institute of Physical and Organic Chemistry (IPOC), Russia

2016

10. Furoxans as NO donating drugs: theoretical study
    oral presentation, Southern Federal University, Russia

11. Study of reactivity of alkaloid berberine derivatives
    oral presentation, Institute of Physical and Organic Chemistry (IPOC), Russia

2015

12. Mechanisms of nucleophilic substitution in alkaloid berberine as potential drug
    oral presentation, Southern Federal University, Russia

2014

13. Structure of 8-hydrxoquinoline derivatives as ligands for OLEDs
    oral presentation, Institute of Physical and Organic Chemistry (IPOC), Russia