Maksim Kulichenko

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- Director's Postdoc Fellow
- Physics and Chemistry of Materials (T-1) Group, Los Alamos National Laboratory
- Personal website: https://m-kulichenko.github.io/
- Google Scholar profile: https://scholar.google.com/citations?user=5QlRU5wAAAAJ&hl

Research Interests

Applications of Machine Learning in chemistry, chemical bonding, spectroscopy

Education

PhD — Utah State University, Logan, Utah 2018 — 2022

Department of Chemistry and Biochemistry

Major: Chemistry

Advisor: Alexander I. Boldyrev

Thesis: *Stability, Electronic Structure, and Nonlinear Optical Properties in Clusters and Materials: A Synergistic Experimental-Computational Analysis*

BSc (with Honors) — Lomonosov Moscow State University, Moscow, Russia 2014 — 2018

Department of Fundamental Physical and Chemical Engineering

Major: Applied Mathematics and Physics

Thesis: *Reactions of insertion in bond $MY_n+H_2=MY_nH_2$ (M=C, Si, Al, B and Y=H, F, Cl), $MY^+ + H_2 = MYH_2^+$ (M=C, Si and Y=H, F, Cl): quantum chemical study.*

Skills & Abilities

Programming:

Python (proficient), C++ (basics)

Machine Learning:

Toolkits: PyTorch, Scikit-Learn, NumPy, SciPy, Pandas

Machine learning in the context of interatomic potentials

Uncertainty quantification for atomistic data acquisition

Computational Chemistry:

Proficient in the following computational chemistry packages: ASE, GAUSSIAN, VASP, ORCA, ADF, ABINIT, MAESTRO, HIPNN

Molecular dynamics (*ab initio*/DFT and ML-based)

Structural global minima search

Computational spectroscopy

Multireference quantum-chemical calculations

Computational analysis of non-linear optical properties

Bonding analysis in molecules and solids

Other:

Experience with High Performance Computing (via SLURM)

SQL (MySQL basics)

Experience in SSH servers building and remote-control software configuration (WinSCP, OpenSSH)

Open-Source Projects

PYSEQM 2023

Description: A PyTorch-based package for semi-empirical quantum chemical simulations
Repository: https://github.com/lanl/PYSEQM/tree/develop
Contributions:

- Implementation of Extended Lagrangian Born-Oppenheimer Molecular Dynamics engine
- Implementation of the support of open-shell calculations
- Generation of reactive dataset for training ML model interfaced with semiempirical Hamiltonian
- Code refactoring

Active Learning Framework 2020 – 2023

Description: A framework for atomistic data sampling via ensemble-based active learning
Repository: https://github.com/lanl/ALF/tree/main
Contributions:

- Implementation of an uncertainty-driven sampler for a diverse chemical data acquisition

Experience

Director's Postdoc Fellow, Los Alamos National Lab 2022 – present

Research topic: applications of machine learning in atomistic simulations

Graduate Contractor, Los Alamos National Lab 2020 – 2022

Graduate Research Assistant position at USU funded by Los Alamos National Lab.
Topic: applications of machine learning in atomistic simulations

Graduate Research/Teaching Assistant — Utah State University 2018 – 2022

Research topic: computational chemistry

Summer Internship — Los Alamos National Lab, NM Summer 2020

Internship topic: Development of sampling techniques for machine learning potentials

Internship — Institute of Problems of Chemical Physics of Russian Academy of Sciences 2017 - 2018

Internship topic: quantum chemical investigation of efficient reaction pathways

Publications

The full publication list can be found on my Google Scholar page:
22 published articles
Citations –301 (Google Scholar)
h-index – 12

1. Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation — 1 citation

   M. Kulichenko, K. Barros, N. Lubbers, N. Fedik, G. Zhou, S. Tretiak, B. Nebgen, A.M.N. Niklasson
   J. Chem. Theory Comput. (2023) 19, 3209, DOI:10.1021/acs.jctc.3c00234 (IF=6.6)

2. 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
   Accepted in the Journal of Chemical Physics (2023) (IF=4.3)

3. Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials — 4 citations

   M. Kulichenko, N. Lubbers, J. S. Smith, Y. W. Li, R. Messerly, S. Tretiak, K. Barros, B. Nebgen
   Nat. Comput. Sci. (2023) 3, 230, DOI: 10.1038/s43588-023-00406-5

4. Extending machine learning beyond interatomic potentials for predicting molecular properties — 20 citations *Invited review*

   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
   Nat. Rev. Chem. (2022) DOI: 10.1038/s41570-022-00416-3 (IF=34.0)

5. Photoelectron Spectroscopy and Theoretical Study of Di-Copper–Boron Clusters: $Cu_2B_3^-$ and $Cu_2B_4^-$ — 1 citation

   A. S. Pozdeev, W.-J. Chen, H. W. Choi, **M. Kulichenko**, D.-F. Yuan, A. I. Boldyrev, L.-S. Wang
   J. Phys. Chem. A, (2023), 127, 4888, DOI: 10.1021/acs.jpca.3c02417 (IF=2.9)

6. On the Structures and Bonding of Copper Boride Nanoclusters, $Cu_2B_x^-$ (x = 5–7)

   A. S. Pozdeev, W.-J. Chen, **M. Kulichenko**, H. W. Choi, A. I. Boldyrev, L.-S. Wang
   Solid State Sci.(2023) 142 ,DOI:10.1016/j.solidstatesciences.2023.107248 (IF=3.7)

7. Probing Copper-Boron Interactions in the $Cu_2B_8^-$ Borozene Complex — 3 citations

   M. Kulichenko, W.-J. Chen, H. W. Choi, D.-F. Yuan, A. I. Boldyrev, L.-S. Wang
   J. Vac. Sci. & Technol A (2022) 40,042201, DOI:10.1021/acs.jpca.1c05846 (IF=2.4)

8. Photoelectron Spectroscopy of Size-Selected Bismuth-Boron Clusters: BiB_n^- (n = 6-8) — 13 citations

W.-J. Chen, **M. Kulichenko**, H. W. Choi, J. Cavanagh, D.-F. Yuan, A. I. Boldyrev, L.-S. Wang

J. Phys. Chem. A (2021) 125, 31, 6751, DOI: 10.1021/acs.jpca.1c05846 (IF=2.9)

Published as part of the special issue "125 Years of The Journal of Physical

9. Bridging Aromatic/Antiaromatic Units. Recent Advances in Aromaticity and Antiaromaticity in Main-group and Transition-metal Clusters from Bonding and Magnetic analyses — 6 citation

Invited review

N. V. Tkachenko, I. A. Popov, **M. Kulichenko**, N. Fedik, Z.-M. Sun, A. Muñoz-Castro, A. I. Boldyrev — 14 citations

Eur. J. Inorg. Chem. (2021) 41, 4239, DOI: 10.1002/ejic.202100519 (IF=2.5)

10. The Rise of Neural Networks for Materials and Chemical Dynamics — 32 citations

M. Kulichenko, J. S. Smith, B. Nebgen, Y. W. Li, N. Fedik, A. I. Boldyrev, N. Lubbers, K. Barros, S. Tretiak

J. Phys. Chem. Lett. (2021) 12, 6227, DOI: 10.1021/acs.jpclett.1c01357 (IF=6.5)

Invited perspective Featured on the issue cover

11. Chapter: Spherical aromaticity in inorganic chemistry — 1 citation

Invited chapter

M. Kulichenko, N. Fedik, N. V. Tkachenko, Á. Muñoz-Castro, Z.-M. Sun, A. I. Boldyrev

Aromaticity - Modern Computational Methods and Applications, Elsevier (2021) Pages 447-489, DOI: 10.1016/B978-0-12-822723-7.00014-5

12. Designing Molecular Electrides from Defective Unit Cells of Cubic Alkaline Earth — 3 citations

M. Kulichenko, A. N. Utenyshev, K. V. Bozhenko

J. Phys. Chem. C (2021) 125, 17, 9564, DOI: 10.1021/acs.jpcc.1c02710 (IF=4.1)

13. Double σ-Aromaticity in a Planar Zinc-Doped Gold Cluster: Au_9Zn^- — 12 citations

M. Kulichenko, W.-J. Chen, Y.-Y. Zhang, C.-Q. Xu, J. Li, L.-S. Wang

J. Phys. Chem. A (2021) 125, 21, 4606, DOI: 10.1021/acs.jpca.1c02954 (IF=2.9)

14. Bottled spiro-doubly aromatic trinuclear $[Pd_2Ru]^+$ complexes

M. Kulichenko, N. Fedik, A. Monfredini, A. Muñoz-Castro, D. Balestri, A. I. Boldyrev, G. Maestri — 14 citations

Chem. Sci. (2021) 12, 477-486, DOI: 10.1039/D0SC04469E (IF=9.8)

15. σ-aromaticity in MoS_2 monolayer — 22 citations

M. Kulichenko, A. I. Boldyrev

J. Phys. Chem. C (2020) 124, 11, 6267, DOI: 10.1021/acs.jpcc.0c00533 (IF=4.1)

16. Can aromaticity be a kinetic trap? Example of mechanically interlocked aromatic polycatenanes built of cyclo[18]carbon — 49 citations

N. Fedik, **M. Kulichenko**, D. Steglenko, A. I. Boldyrev
Chem. Commun. (2020) 56, 2711-2714, DOI: 10.1039/C9CC09483K (IF=6.2)

17. Periodic F-defects on the MgO Surface as Potential Single-Defect Catalysts with Non-Linear Optical Properties — 15 citations

M. Kulichenko, N. Fedik, D. Steglenko, R. M. Minyaev, V. I. Minkin, A. I. Boldyrev
Chem. Phys. (2020) 532, 110680, DOI: 10.1016/j.chemphys.2020.110680 (IF=2.3)

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 — 21 citations

M. Kulichenko, N. Fedik, A. I. Boldyrev, A. Muñoz-Castro
Chem. Eur. J. (2020) 26, 2263-2268, DOI: 10.1002/chem.201905088 (IF=5.2)

19. Hydrated Sulfate Clusters $SO_4^{2-}(H_2O)_n$ (n = 1–40): Charge Distribution Through — 29 citations

M. Kulichenko, N. Fedik, K. V. Bozhenko, A. I. Boldyrev
J. Phys. Chem. B (2019) 123, 18, 4065, DOI: 10.1021/acs.jpcb.9b01744 (IF=3.0)

20. High-Resolution Photoelectron Imaging of IrB_3^-: Observation of a p-Aromatic B_3^+ Ring — 21 citations

J. Czekner, L. F. Cheung, S. Kocheril, **M. Kulichenko**, A. I. Boldyrev, L.-S. Wang
Angew. Chem. *Int. Ed.* (2019) 58, 8877, DOI: 10.1002/anie.201902406 (IF=15.3)

21. Two Names of Stability: Spherical Aromatic or Superatomic Intermetalloid Cluster $[Pd_3Sn_8Bi_6]^{4-}$ — 16 citations *featured on the issue cover*

N. Fedik, **M. Kulichenko**, A. I. Boldyrev
Chem. Phys. (2019) 522, 134, DOI: 10.1016/j.chemphys.2019.02.015 (IF=2.3)

22. Inorganic Molecular Electride Mg_4O_3: Structure, Bonding and Nonlinear Optical Properties — 18 citations

M. Kulichenko, N. Fedik, K. V. Bozhenko, A. I. Boldyrev
Chem. Eur. J. (2019) 25, 5311-5315, DOI:10.1002/chem.201806372 (IF=5.2)

Peer Review Activity

21 reviews

Journal list can be found on my Web of Science page.

Outreach Activity

Co-organizer of an annual workshop "*Machine Learning and Informatics for Chemistry and Materials*" Event webpage: https://meetings.telluridescience.org/meetings/workshop-details?wid=1128	2022, 2023
Graduate students recruiting (USU)	2020-2021
Building a departmental computer cluster which is used by graduate students for research and by undergrads for Physical Chemistry labs (USU, Chemistry & Biochemistry department)	2019
Member of a student council (Moscow State University)	2014-2018
Participation in the organization of All-Russian Science Festival NAUKA 0+ (Moscow, Russia)	2014, 2015

Conferences and Talks

Workshop "Machine Learning and Informatics for Chemistry and Materials", Telluride, CO Talk Topic: Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials	2022
International Conference on Chemical Bonding, Hawaii Invited Talk Topic: Accelerating Data Generation for Machine Learning Potentials by Biasing Towards Regions of Uncertainty	2022
Los Alamos National Lab, Lightning Talks, Talk Topic: Diversification of ML Datasets via Bias Potentials as Functions of Uncertainty	2021
ACS Conference Live Speaker Presentation Topic: Diversification of ML datasets via "uncertainty" as a bias potential	2021
Los Alamos National Lab, Lightning Talks Talk Topic: Diversification of ML Datasets via Bias Potentials as Functions of Uncertainty	2020
ACS National Meeting at San Diego, CA Poster session Topic: Elusive Electrides. From Solids to Molecules	2019
XXIV International Conference of Students and Young Scientists "Lomonosov", Moscow, MSU Poster session Topic: Quantum chemical study of reactions of insertion in bond $MY_n + H_2 = MY_nH_2$ (M = C, Si, Al, B and Y = H, F, Cl), $MY^+ + H_2 = M_YH_2^+$ (M = C, Si and Y = H, F, Cl)	2017

Teaching Experience

CHEM 1225 Chemical Principles Lab II, Spring 2019

CHEM 1215 Chemical Principles Lab I, Spring 2020

CHEM 1215 Chemical Principles Lab I, Fall 2020

Evaluations in range 9-10

Awards

Director's Postdoc Fellowship, Los Alamos National Lab — 2022
Selections are made based on academic and research accomplishments, the strength of the proposed research, as well as their potential impact at the Laboratory.

Teng Scholarship, Utah State University — 2022
This one-year award is given to an exemplary graduate student in the Department of Chemistry and Biochemistry.

Outstanding Graduate Student in Chemistry, Utah State University — 2022
The award is given to a student within their last year of graduate study in chemistry, who has demonstrated outstanding research and academic achievement.

Winner of Universiade "Lomonosov" in fundamental physical and chemical engineering, Moscow, MSU. — 2018

Recipient of Increased State Academic Scholarship, Moscow State University — 2017
Selection criteria: Scholarship is awarded for noteworthy academic, research, social, cultural, creative, and/or athletic achievements.