

Maksim Kulichenko, Ph.D.

Santa Fe, NM | kulichenko.mb@gmail.com | (435) 512-1450 | [Personal website](#) | [Google Scholar](#)

SUMMARY

- Computational chemistry expert specializing in machine learning potentials and atomistic data acquisition
- Interdisciplinary collaborator with experience working with experimental data
- Author of 23 publications in peer-reviewed journals including 13 first-author papers

SKILLS

Technical Skills:

- Programming: Python (proficient) | C++ (basics)
- Shell Scripting: Bash
- Operating Systems: Linux | Windows
- Machine Learning Tools: PyTorch | Scikit-Learn
- Data Analysis Tools: Pandas | NumPy | MySQL
- Computational Chemistry Packages: GAUSSIAN | ASE | VASP | ORCA | MOPAC | RDKit | MAESTRO
- High Performance Computing: SLURM

Machine Learning Expertise:

- Machine learning in the context of interatomic potentials and molecular dynamics
- Physics-based ML models
- Uncertainty quantification for atomistic data acquisition

Computational Chemistry Expertise: Molecular dynamics | Structural minima search | Photoelectron spectroscopy | Multireference quantum chemistry | Non-linear optical properties | Chemical bonding

Chemical Systems Expertise: Gas phase molecules | Bulk materials | Amino acids | Peptides | Metalorganic complexes | Transition metal compounds | Charged ions | Hydrated particles | Ionic crystals | 2D sheets

Communication: Technical writing | Public speaking | Teaching & Mentorship | International collaborations

EDUCATION

PhD | Chemistry (Computational Chemistry) | Utah State University, Logan, UT 2022

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

BSc (with Honors) | Applied Mathematics and Physics | Moscow State University, Russia 2018

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

OPEN-SOURCE PROJECTS

PYSEQM

2023

A PyTorch-based package for semi-empirical quantum chemical simulations

Repository: <https://github.com/lanl/PYSEQM/tree/develop>

Contributions:

- Implemented Extended Lagrangian Born-Oppenheimer Molecular Dynamics engine (method for accelerated density matrix propagation)
- Implemented the support of open-shell calculations
- Generated reactive atomistic dataset for training the ML-interfaced semiempirical Hamiltonian
- Code refactoring

Active Learning Framework

2020 – 2023

A framework for atomistic data sampling via ensemble-based active learning

Repository: <https://github.com/lanl/ALF/tree/main>

Contributions:

- Implemented an uncertainty-driven sampler for a diverse chemical data acquisition

EXPERIENCE

Los Alamos National Laboratory, Physics and Chemistry of Materials (T-1) Division 2022 – present

Director's Postdoc Fellow

- Developed physics-based ML models
- Developed molecular dynamics methods
- Performed ML-assisted molecular dynamics
- Performed chemical data sampling
- Conducted statistical analysis of data sets

Los Alamos National Laboratory, Physics and Chemistry of Materials (T-1) Division 2020 – 2022

Graduate Research Assistant position at USU funded by LANL.

- Performed atomistic simulations via ML potentials
- Performed atomistic data generation
- Applied uncertainty quantification for atomistic data sampling

Utah State University, Department of Chemistry & Biochemistry 2018 – 2022

Graduate Research/Teaching Assistant

- Conducted structural minima search of atomic clusters
- Collaborated with experimentalists (photoelectron spectroscopy)
- Conducted analysis of non-linear optical properties of materials
- Performed electronic structure analysis in molecules and solids

Los Alamos National Laboratory, Physics and Chemistry of Materials (T-1) Division Summer 2020

Intern

- Developed advanced data sampling techniques for machine learning potentials

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

Intern

- Conducted quantum chemical study of efficient reaction pathways involving carbene-like molecules

AWARDS

1. Journal of Materials Chemistry C Poster Prize Conference on Excited State Processes, Santa Fe, NM	2023
2. Director's Postdoctoral Fellowship , Los Alamos National Lab Selections are made based on academic and research accomplishments, the strength of the proposed research, as well as their potential impact at the Laboratory.	2022
3. Teng Scholarship , Utah State University This one-year award is given to an exemplary graduate student in the Department of Chemistry and Biochemistry.	2022
4. Outstanding Graduate Student in Chemistry , Utah State University The award is given to a student within their last year of graduate study in chemistry, who has demonstrated outstanding research and academic achievement.	2022
5. Winner of Universiade "Lomonosov" in fundamental physical and chemical engineering , Moscow, Russia	2018
6. Recipient of Increased State Academic Scholarship , Moscow State University <i>Selection criteria:</i> Scholarship is awarded for noteworthy academic, research, social, cultural, creative, and/or athletic achievements.	2017

OUTREACH ACTIVITY

1. Co-organized an annual workshop "Machine Learning and Informatics for Chemistry and Materials" Event webpage	2022, 2023
2. <i>Mentored a Summer Student</i> , Los Alamos National Laboratory, NM	2023
3. <i>Recruited graduate students</i> Utah State University, UT	2020-2021
4. <i>Build a departmental computer cluster which is used by graduate students for research and by undergrads for Physical Chemistry labs</i> Utah State University, Chemistry & Biochemistry department, UT	2019
5. <i>Was a member of a student council</i> Moscow State University	2014-2018
6. <i>Participated in the organization of All-Russian Science Festival NAUKA 0+</i> Moscow, Russia	2014, 2015

PUBLICATIONS

The full publication list can be found on my [Google Scholar page](#):

23 published articles

Citations –306 (Google Scholar)

h-index – 12

1. "NEXMD v2.0 Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations"
J. Chem. Theory Comput. (2023) Accepted, DOI: 10.1021/acs.jctc.3c00583
 (IF=6.6)
2. "Semi-Empirical Shadow Molecular Dynamics: A PyTorch implementation"
M. Kulichenko, K. Barros, N. Lubbers, N. Fedik, G. Zhou, S. Tretiak, B. Nebgen, A.M.N. Niklasson 1 citation
J. Chem. Theory Comput. (2023) 19, 3209, DOI: 10.1021/acs.jctc.3c00234
 (IF=6.6)
3. "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)
4. "Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials"
M. Kulichenko, N. Lubbers, J. S. Smith, Y. W. Li, R. Messerly, S. Tretiak, K. Barros, B. Nebgen 4 citations
Nat. Comput. Sci. (2023) 3, 230, DOI: 10.1038/s43588-023-00406-5
5. "Extending machine learning beyond interatomic potentials for predicting molecular properties" 21 citations
 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) *Invited review*
6. "Photoelectron Spectroscopy and Theoretical Study of Di-Copper-Boron Clusters: Cu_2B_3^- and Cu_2B_4^- " 3 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)
7. "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)
8. "Probing Copper-Boron Interactions in the Cu_2B_8^- Borozene Complex" 4 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)
9. "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 <i>J. Phys. Chem. A</i> (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 Chemistry"
10. "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 <i>Eur. J. Inorg. Chem.</i> (2021) 41, 4239, DOI: 10.1002/ejic.202100519 (IF=2.5)	6 citation Invited review
11. "The Rise of Neural Networks for Materials and Chemical Dynamics" M. Kulichenko , J. S. Smith, B. Nebgen, Y. W. Li, N. Fedik, A. I. Boldyrev, N. Lubbers, K. Barros, S. Tretiak <i>J. Phys. Chem. Lett.</i> (2021) 12, 6227, DOI: 10.1021/acs.jpcllett.1c01357 (IF=6.5)	33 citations Invited perspective Featured on the issue cover
12. Chapter: "Spherical aromaticity in inorganic chemistry" M. Kulichenko , N. Fedik, N. 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	1 citation Invited chapter
13. "Designing Molecular Electrides from Defective Unit Cells of Cubic Alkaline Earth Oxides" M. Kulichenko , A. N. Utenyshev, K. V. Bozhenko <i>J. Phys. Chem. C</i> (2021) 125, 17, 9564, DOI: 10.1021/acs.jpcc.1c02710 (IF=4.1)	3 citations
14. "Double σ -Aromaticity in a Planar Zinc-Doped Gold Cluster: Au_9Zn^- " M. Kulichenko , W.-J. Chen, Y.-Y. Zhang, C.-Q. Xu, J. Li, L.-S. Wang <i>J. Phys. Chem. A</i> (2021) 125, 21, 4606, DOI: 10.1021/acs.jpca.1c02954 (IF=2.9)	12 citations
15. "Bottled spiro-doubly aromatic trinuclear $[\text{Pd}_2\text{Ru}]^+$ complexes" M. Kulichenko , N. Fedik, A. Monfredini, A. Muñoz-Castro, D. Balestri, A. I. Boldyrev, G. Maestri <i>Chem. Sci.</i> (2021) 12, 477-486, DOI: 10.1039/D0SC04469E (IF=9.8)	14 citations
16. " σ -aromaticity in MoS_2 monolayer" M. Kulichenko , A. I. Boldyrev <i>J. Phys. Chem. C</i> (2020) 124, 11, 6267, DOI: 10.1021/acs.jpcc.0c00533 (IF=4.1)	22 citations
17. "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)

18. "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)

19. "Expansion of aromaticity magnetic criteria on multi-layer structures. Magnetic response and spherical aromaticity of Matryoshka-like [Sn@Cu₁₂@Sn₂₀]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)

20. "Hydrated Sulfate Clusters SO₄²⁻(H₂O)_n (n = 1–40): Charge Distribution Through Solvation Shells and Stabilization" 29 citations

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

21. "High-Resolution Photoelectron Imaging of IrB₃⁺: Observation of a p-Aromatic B₃⁺ Ring Coordinated to a Transition Metal" 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)

22. "Two Names of Stability: Spherical Aromatic or Superatomic Intermetalloid Cluster [Pd₃Sn₈Bi₆]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)

23. "Inorganic Molecular Electride Mg₄O₃: 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](#).

CONFERENCES AND TALKS

1. Invited Talk: "Improving Atomistic Simulations with Semi-Empirical Quantum Mechanics and Machine Learning" 2023
 International Conference on Chemical Bonding, Kauai, HI

2. Talk: "Improving Atomistic Simulations with Semi-Empirical Quantum Mechanics and Machine Learning" 2023
Workshop "Machine Learning and Informatics for Chemistry and Materials", Telluride, CO
3. Poster: "Semi-Empirical Molecular Dynamics with Extended Lagrangian" 2023
Conference on Excited State Processes, Santa Fe, NM
4. Talk: "Uncertainty Driven Dynamics for Active Learning of Interatomic Potentials" 2022
Workshop "Machine Learning and Informatics for Chemistry and Materials", Telluride, CO
5. Invited Talk: "Accelerating Data Generation for Machine Learning Potentials by Biasing Towards Regions of Uncertainty" 2022
International Conference on Chemical Bonding, Kauai, HI
6. Talk: "Diversification of ML Datasets via Bias Potentials as Functions of Uncertainty" 2021
Lightning Talks at Los Alamos National Lab
7. Talk: "Diversification of ML Datasets via "Uncertainty" as a Bias Potential" 2021
ACS Conference
8. Poster: "Elusive Electrides. From Solids to Molecules" 2019
ACS National Meeting, San Diego, CA
9. Poster: "Quantum chemical study of reactions of insertion in bond $MY_n + H_2 = MY_nH_2$ ($M = C, Si, Al, B$ and $Y = H, F, Cl$), $MY^+ + H_2 = MYH_2^+$ ($M = C, Si$ and $Y = H, F, Cl$)" 2017
XXIV International Conference of Students and Young Scientists "Lomonosov", Moscow, Russia

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