Maksim Kulichenko, Ph.D.

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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
- Version control: GitHub
- 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** 2023
   Conference on Excited State Processes, Santa Fe, NM
2. **Director's Postdoctoral 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.
3. **Teng Scholarship**, Utah State University 2022
   This one-year award is given to an exemplary graduate student in the Department of Chemistry and Biochemistry.
4. **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.
5. **Winner of Universiade "Lomonosov" in fundamental physical and chemical engineering**, Moscow, Russia 2018
6. **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.

OUTREACH ACTIVITY

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

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" — 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)

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" — 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

5. "Extending machine learning beyond interatomic potentials for predicting molecular properties" — 21 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)

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 *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 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 *Eur. J. Inorg. Chem.* (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 *J. Phys. Chem. Lett.* (2021) 12, 6227, DOI: 10.1021/acs.jpclett.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 *J. Phys. Chem. C* (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 *J. Phys. Chem. A* (2021) 125, 21, 4606, DOI: 10.1021/acs.jpca.1c02954 (IF=2.9)	12 citations
15. "Bottled spiro-doubly aromatic trinuclear $[Pd_2Ru]^+$ complexes" **M. Kulichenko**, N. Fedik, A. Monfredini, A. Muñoz-Castro, D. Balestri, A. I. Boldyrev, G. Maestri *Chem. Sci.* (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 *J. Phys. Chem. C* (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 $[Sn@Cu_{12}@Sn_{20}]^{12-}$ 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)

20. "Hydrated Sulfate Clusters $SO_4^{2-}(H_2O)_n$ (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.jpcb.9b01744
    (IF=3.0)

21. "High-Resolution Photoelectron Imaging of IrB_3^-: Observation of a p-Aromatic B_3^+ 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 $[Pd_3Sn_8Bi_6]^{4-}$ " — 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)

23. "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**.

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),* $MY^+ + H_2 = M_YH_2^+$ *(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