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

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| **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 MYn+H2=MYnH2 (M=C, Si, Al, B and Y=H, F, Cl), MY++H2=MYH2+ (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

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| **PYSEQM** 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 | ****2023**** |
| **Active Learning Framework** 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 | ****2020 – 2023**** |

# Experience

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| **Director’s Postdoc Fellow, Los Alamos National Lab** Research topic: applications of machine learning in atomistic simulations | ****2022 – present**** |
| **Graduate Contractor, Los Alamos National Lab** Graduate Research Assistant position at USU funded by Los Alamos National Lab. Topic: applications of machine learning in atomistic simulations | ****2020 – 2022**** |
| **Graduate Research/Teaching Assistant** — Utah State University Research topic: computational chemistry | ****2018 – 2022**** |
| **Summer Internship** — Los Alamos National Lab, NM Internship topic: Development of sampling techniques for machine learning potentials | ****Summer 2020**** |
| **Internship** — Institute of Problems of Chemical Physics of Russian Academy of Sciences Internship topic: quantum chemical investigation of efficient reaction pathways | ****2017 - 2018**** |

# Publications

The full publication list can be found on my [**Google Scholar page**](https://scholar.google.com/citations?hl=en&user=5QlRU5wAAAAJ&view_op=list_works):

22 published articles

Citations –301 (Google Scholar)

h-index – 12

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| 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) |
| 1. 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) |
| 1. 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 |
| 1. 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) |
| 1. Photoelectron Spectroscopy and Theoretical Study of Di-Copper–Boron Clusters: Cu2B3– and Cu2B4– | 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) |
| 1. On the Structures and Bonding of Copper Boride Nanoclusters, Cu2Bx– (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) |
| 1. Probing Copper-Boron Interactions in the Cu2B8– 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) |

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| 1. Photoelectron Spectroscopy of Size-Selected Bismuth-Boron Clusters: BiBn- (n = 6-8) | 13 citations  *Published as part of the special issue “125 Years of The Journal of Physical Chemistry”* |
| 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) |
| 1. 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  *Eur. J. Inorg. Chem.* (2021) 41, 4239, DOI: 10.1002/ejic.202100519 (IF=2.5) | 14 citations |
| 1. The Rise of Neural Networks for Materials and Chemical Dynamics | 32 citations  *Invited perspective Featured on the issue cover* |
| **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) |
| 1. 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 |
| 1. Designing Molecular Electrides from Defective Unit Cells of Cubic Alkaline Earth Oxides | 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) |
| 1. Double σ-Aromaticity in a Planar Zinc-Doped Gold Cluster: Au9Zn- | 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) |
| 1. Bottled spiro-doubly aromatic trinuclear [Pd2Ru]+ complexes | 14 citations |
| **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) |
| 1. σ-aromaticity in MoS2 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) |
| 1. 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) |
| 1. 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) |
| 1. 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) |
| 1. 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.jpcb.9b01744 (IF=3.0) |
| 1. 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) |
| 1. 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) |
| 1. 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

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| **21 reviews**  **Journal list can be found on my** [**Web of Science page**](https://www.webofscience.com/wos/author/record/AAA-3477-2022)**.** |

# Outreach Activity

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| **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

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| **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 MYn + H2 = MYnH2 (M = C, Si, Al, B and Y = H, F, Cl), MY+ + H2 = MYH2+ (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

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| **Director’s Postdoc 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** |
| **Teng Scholarship**, Utah State University  This one-year award is given to an exemplary graduate student in the Department of Chemistry and Biochemistry. | **2022** |
| **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** |
| **Winner of Universiade “Lomonosov” in fundamental physical and chemical engineering**, Moscow, MSU. | **2018** |
| **Recipient of Increased State Academic Scholarship**, Moscow State University  *Selection criteria*: Scholarship is awarded for noteworthy academic, research, social, cultural, creative, and/or athletic achievements. | **2017** |