Małgorzata Zofia Makoś

Postdoctoral Research Associate
Physical Sciences Directorate
Oak Ridge National Laboratory

Education

Southern Methodist University — Dallas, TX
Ph.D. in Computational and Theoretical Chemistry — 2017–2021

Cracow University of Technology — Cracow, Poland
B.E. in Physics, Specialization: New Materials and Nanotechnology — 2010–2014

Research Experience

Postdoctoral Research Associate
Advisor: Dr. Vanda Glezakou, Oak Ridge National Laboratory — 2023-current

Implementation of machine learning and data science algorithms to analyze the reaction mechanisms using global optimizer.

Postdoctoral Research Associate
Advisors: Dr. Roger Rousseau, Dr. Vanda Glezakou, Pacific Northwest National Laboratory — 2021-2023

Major work on chemical separations and CO_2 capture using classical and ab-initio molecular dynamics. Designing machine learning algorithms to predict the solvation energies.

Graduate Research Assistant
Advisor: Prof. Dr. Elfi Kraka, Southern Methodist University — 2017- 2021

Dissertation: Mechanistic Studies of Catalysis Through Quantum Chemical and Machine Learning Approaches

Graduate Research Fellowship
Advisors: Dr. Nicholas Lubbers, Dr. Justin S. Smith Los Alamos National Laboratory — 2020-2021

Analyzing reactions on the fly for a machine learning nanoreactor.

Undergraduate Research
Advisor: Dr. Jerzy Sanetra, Cracow University of Technology — 2013–2014

Construction and characteristic of organic electroluminescent diodes.

Skills

- Physics, computational chemistry, machine learning.
- Programming in Python (proficient, primary programming language), Fortran, C++ (entry-level).
- Python libraries I am proficient with: PyTorch, Keras, Scikit-learn, Pandas, NumPy, and MatPlotLib, Atomic Simulation Environment.
- Machine learning algorithms I have experience with: Support-Vector Machine, Convolutional and Recurrent Neural Networks, Generative Adversarial Network, Reinforcement Learning.
- Computational chemistry modeling using Gaussian, ORCA, Q-Chem, NAMD, Gromacs, CP2K.
- Quantum mechanical calculation using DFT, MP2, CCSD(T), CASPT2.

- Calculation of geometry optimization, transition states, reaction paths, potential energy surfaces, vibrational spectroscopic information, binding free energies.
- Parallel computing using: UNIX (Linux, Mac OS X) on Intel computer clusters.
- Proficiency with: git, LaTeX, MS Office.
- Scientific writing and presentation.

Selected Publications

The complete list of publications can be found here.

1. M.Z. Makoś, M. Freindorf, D. Sethio and E. Kraka; New Insights into Fe−H_2 and Fe−H^- Bonding of a [NiFe] Hydrogenase Mimic: a Local Vibrational Mode Study; Theor. Chem. Acc., 138, 2019
2. M.Z. Makoś, W. Zou, M. Freindorf, and E. Kraka; Metal-Ring Interactions in Actinide Sandwich Compounds: Combined the Normalized Elimination of the Small Component and Vibrational Spectroscopy Study; Mol. Phys., e1768314, 2020
3. M.Z. Makoś, M. Freindorf, Y. Tao, and E. Kraka; New Insigth into Au(I) Catalyzed Hydroalkoxylation of Allenes: a Unified Reaction Valley Approach Study; J. Org. Chem. 2021, 86, 5714−5726
4. M.Z. Makoś, N. Verma, E. C. Larson, M. Friendorf, and E. Kraka; Generative Adversarial Networks for Transition State Geometry Prediction; J. Chem. Phys. 2021, 155, 024116
5. M.Z. Makoś, P.K. Gurunathan, V.-A. Glezakou, R. Rosseau, S. Raugei, K. Kowalski; Benchmark Compuational Modeling of Ionization Potentials of the Ferrocene in the Condensed Phase; J. Phys. Chem. Lett. 2022, 13, 42, 10005–10010
6. S. Zhang, M.Z. Makoś, R. Jadrich, E. Kraka, K. Barros, B. Nebgen, S. Tretiak, O. Isayev, N. Lubbers, R. Messerly, J. Smith, ChemRxiv. Cambridge: Cambridge Open Engage; 2022.

Conference Presentations

- The 28^{th} Austin Symposium on Molecular Structure and Dynamics at Dallas TX — Feb. 2023
  poster presentation
- Gordon Conference on Chemical Separation — Aug. 2022
  poster presentation
- 2021 Postgraduate Research Symposium, Pacific Northwest National Laboratory — Aug. 2021
  poster - Top Post Doctorate Poster Presentation Award
- The 52^{nd} Local Section of the American Chemistry Society, University of North Texas — Apr. 2019
  oral presentation
- The 51^{st} Local Section of the American Chemistry Society, Southern Methodist University — Apr. 2018
  oral presentation

Workshops and courses

- **Applied Data Science Program** — Jun-Aug 2022
  Massachusetts Institute of Technology, MIT Professional Education
- **Quantum Computing Boot Camp** — Jul-Aug 2021
  Pacific Northwest National Laboratory, Richland WA
- **Machine Learning and Chemistry: Progress so far and Challenges on the Way Forward** — Nov. 2019
  Molecular Software Science Institute and University of Maryland, College Park MD

- **High-Performance Scientific Computation Workshop** Aug. 2019
  High-Performance Computing Center at Southern Methodist University, Dallas TX
- **Software Summer School** Jul-Aug 2019
  Molecular Software Science Institute and Texas Advanced Computer Center, Austin TX

Teaching

- Advanced Computational Chemistry Laboratory Fall 2018
  graduate course, Southern Methodist University
- General Chemistry Laboratory Fall 2017 –Spring 2018
  undergraduate course, Southern Methodist University
- Basics of Physics Laboratory Spring 2014
  undergraduate course, Cracow University of Technology

Professional Service

- **Scientific Journal Reviewer**
  Energies, MDPI;
  Symmetry, MDPI;
  Journal of Inorganic Chemistry, ACS.
- **Math and Science Mentor** (2021/2022)
  elementary/middle/high school, Team Battelle Math Mentors/Coaches at PNNL

Languages

- Polish - mother tongue
- English - highly proficient
- Russian - entry level

Links

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- scholar.google.com/Makos
- github.com/MZ-Makos
- ORCID: 0000-0002-6015-5608
- linkedin.com/malgorzata-makos

References

- Dr. Roger Rousseau
- Dr. Vassiliki-Alexandra (Vanda) Glezakou
- Dr. Elfi Kraka