Joseph A. Makowski

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Summary

- Computational scientist with expertise in physical modeling, machine learning, statistical analysis, and high-performance computing.

- Author of seven peer-reviewed publications and co-writer of a funded NIH R15 grant ($507k), demonstrating independent execution, technical leadership, and project delivery

- Background spans computational chemistry, applied mathematics, statistical modeling, and scientific software development, with a strong record of interdisciplinary collaboration and communication.

- Skilled in designing automated, reproducible analytical workflows; integrating simulations with experimental data; and building tools that accelerate scientific insight.

Education

Duquesne University *Aug. 2021 – Dec. 2025*

Ph.D., Computational Chemistry and Biophysics Pittsburgh, Pennsylvania

Bethany College *Sep. 2017 – May 2021*

B.S., Chemistry; Minors in Mathematics and Theoretical Physics Bethany, West Virginia

Coursework Highlights

- Machine Learning
- Statistical Computing
- Numerical Analysis
- Nonlinear Dynamics and Chaos
- Simulation Methods
- Algebra/Analysis/Topology
- Protein–Nucleic Acid Interactions
- Graph Theory and Algorithms
- Cheminformatics

Technical Skills

Computational Methods: Molecular dynamics simulations; enhanced sampling and free-energy methods; quantum chemistry (HF, MP2/MPn, DFT, CC); multivariate statistics; machine learning (supervised/unsupervised); Markov state models; Bayesian parameter estimation and uncertainty quantification; likelihood-free inference and Approximate Bayesian Computation (ABC); Markov chain Monte Carlo (MH, Gibbs, HMC/NUTS); chain-of-states methods (NEB, GSM); topological data analysis (persistent homology); foundational bioinformatics; high-performance computing.

Libraries: `numpy`, `scipy`, `scikit-learn`, `pandas`, `matplotlib`, `mdtraj`, `ripser`, `persim`, `networkx`, `deeptime`, `Biostrings`, `DECIPHER`, `BiocManager`, `adegenet`, `stringr`, `ape`, `BLAS`, `LAPACK`.

Technologies & Software: GNU/Linux (HPC environments), SLURM, Gaussian 16, GaussView, NAMD, AmberTools, CHARMM, VMD (Tcl/Tk scripting), bash, make, Jupyter, conda/venv, basic familiarity with OpenMP and CUDA.

Programming Languages: Python, Fortran, R, Tcl/Tk, Mathematica, MATLAB/Octave, LaTeX.

Experience

Math and Science Tutoring *2021 – Present*

Founder and Head Tutor Remote

– Provided sustained one-on-one instruction across mathematics, chemistry, physics, and quantitative subjects to students from middle school through university level, maintaining multiple long-term clients for years.

– Developed customized explanations and step-by-step walkthroughs of complex mathematical, chemical, and computational topics, strengthening students' analytical thinking and problem-solving independence.

– Achieved measurable long-term outcomes including substantial grade improvements, top-tier exam performance, accelerated mastery of quantitative problem-solving, and successful completion of independent technical or project-based work.

Rebel Labs, Inc. *Nov. 2025 – Jan. 2026*

Computational Chemistry Consultant Remote

– Designed early-stage technical architecture, ML workflows, and data-processing pipelines for an AI/ML platform aimed at accelerating computational chemistry.

– Led prototype development cycles; advised on algorithm design, model development, and data infrastructure across pre-seed R&D efforts.
– Provided strategic technical guidance that supported pre-seed fundraising and shaped long-term feasibility assessments.

Duquesne University, Evanseck Research Group *2021 – 2025*

Ph.D. Researcher, Computational Chemistry and Biophysics Pittsburgh, PA

– Built and deployed modeling pipelines used by multiple collaborators to generate publishable mechanistic predictions and validated computational results against NMR measurements.
– Built reproducible analysis pipelines for trajectory processing, feature engineering, dimensionality reduction, unsupervised clustering, and automated visualization.
– Implemented data-cleaning and analysis workflows used by multiple researchers, supporting several peer-reviewed publications.
– Collaborated with experimental scientists to design computational studies, validate predictions, and interpret results, enabling joint manuscripts and coordinated research milestones.

Duquesne University, Dept. Chemistry and Biochemistry *2021 – 2025*

Instructor and Research Mentor Pittsburgh, PA

– Taught multiple laboratory, recitation, and lecture courses, developing clear instructional materials and supporting student problem-solving across a wide range of backgrounds.
– Recognized by students and faculty for clarity in explaining complex chemical, computational, and mathematical concepts, and for strong technical communication when coordinating and training instructional staff.
– Delivered technical workshops on Python for research workflows, machine learning fundamentals, molecular data visualization, and chain-of-states modeling to undergraduate and graduate researchers.
– Mentored more than ten students (undergraduate and graduate) in computational modeling, quantum chemistry, molecular dynamics, and data analysis, guiding project design, execution, and interpretation.
– Provided individualized technical coaching enabling students to perform independent HPC jobs, molecular simulations, transition-state searches, and RNA structural analyses.

Selected Publications

‡Shared first authorship

- Matzel, T.‡, **Makowski, J.**‡, et al. *RNA* (2025). DOI: 10.1261/rna.080576.125
- Wirtz Martin, M.‡, **Makowski, J.**‡, et al. *Nucleic Acids Research* (2025). DOI: 10.1093/nar/gkaf552
- Kensinger, A., **Makowski, J.**, et al. *ACS Phys. Chem. Au* (2025). DOI: 10.1021/acsphyschemau.5c00031
- **Makowski, J.**‡, Kensinger, A.‡, et al. *ACS Phys. Chem. Au* (2023). DOI: 10.1021/acsphyschemau.3c00008
- Frye, C., Shine, M., **Makowski, J.**, et al. *Journal of Medical Virology* (2022). DOI: 10.1002/jmv.28141

Honors & Awards

Bayer Fellowship (2025); Highest Impact Factor Publication Awards (2024, 2025); "Above and Beyond" Teaching Assistant Award (2024); NSF REU (2019, 2020); J.S.V. Allen Memorial Prize in Physics (2021); WV NASA Space Grant Fellowship (2018–2019).