Geemi P. Wellawatte

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Education

University of Rochester — *Rochester, NY*
Ph.D, Chemistry — *2020-2023*

University of Rochester — *Rochester, NY*
M.S, Chemistry — *2018-2020*

University of Colombo — *Colombo, Sri Lanka*
B.S, Special Degree in Computational Chemistry (First Class Honors) — *2013-2017*

Experience

AI Technical Lead; Fellowship Program — *September, 2025 - Current*
FutureHouse — *San Francisco, CA*

Member of Technical Staff — *September, 2024 - September, 2025*
FutureHouse — *San Francisco, CA*

Post-Doctoral Researcher — *July, 2023 - August, 2024*
Advisor: Prof. Philippe Schwaller
The Laboratory of Artificial Intelligence (LIAC) — *EPFL, Switzerland*

- Research Focus: Large language models to accelerate scientific research in Chemistry, Explainable AI for chemistry

Graduate Research Assistant — *Jan, 2019 - May, 2023*
Advisor: Prof. Andrew White
Department of Chemistry, University of Rochester — *Rochester, NY*

- Research Focus: Explainable AI for molecular models, deep-learning for coarse-grained molecular dynamics

Graduate Teaching Assistant — *Aug, 2018 - Aug, 2019*
Department of Chemistry, University of Rochester — *Rochester, NY*

Teaching Assistant — *Feb, 2017 - Feb, 2018*
Department of Chemistry, University of Colombo — *Colombo, Sri Lanka*

Selected Honors & Awards

D. E. Shaw Research Graduate and Postdoc Women's Fellowship
May 26, 2022 - May 27, 2022

Esther M. Conwell Graduate Fellowship, Department of Chemistry, University of Rochester
August 2021-August 2022

MolSSI Covid-19 Seed Fellowship, Molecular Sciences Software Institute, VA
July 2020-December 2020

Sherman-Clarke Fellowship, Department of Chemistry, University of Rochester
August 2018-August 2019

Journal Publications

Training a Scientific Reasoning Model for Chemistry S. Narayanan, J. D. Braza, R. Griffiths, A. Bou, **G. P. Wellawatte**, M. C Ramos, L. Mitchener, M. M. Pieler, S. G. Rodriques,

A. D. White *NeurIPS maintrack Accepted (2025)*

Human interpretable structure-property relationships in chemistry using explainable machine learning and large language models **G. P. Wellawatte**, P. Schwaller. *Communications Chemistry (2025)*

BixBench: a Comprehensive Benchmark for LLM-based Agents in Computational Biology L. Mitchener, J. M. Laurent, B. Tenmann, S. Narayanan, **G. P. Wellawatte**, A. D. White, L. Sani, S. G. Rodriques, *arXiv preprint (2025)*

Aviary: training language agents on challenging scientific tasks S. Narayanan, J. D. Braza, R. Griffiths, ... **G. P. Wellawatte**, ... S. G. Rodriques, A. D. White. *arXiv preprint (2025)*

ChemLit-QA: a human evaluated dataset for chemistry RAG tasks **G. P. Wellawatte**[*], H. Guo[*], M. Lederbauer, A. Borisova, M. Hart, M. Brucka,, P. Schwaller. *Machine Learning Science & Technology (2025)*
[*]*Equal contribution*

Neural Potentials of Proteins Extrapolate Beyond Training Data **G. P. Wellawatte**, G. M. Hocky, A. D. White. *The Journal of Chemical Physics (2023)*

A Perspective on Explanations of Molecular Prediction Models **G. P. Wellawatte**, H. A. Gandhi, A. Sheshadri, A. D. White. *Journal of Chemical Theory and Computation (2023).*

Why does that molecule smell? A. Sheshadri, H. A. Gandhi, **G. P. Wellawatte**, A. D. White. *arXiv preprint (2022)*

Assessment of chemistry knowledge in large language models that generate code A. D. White, G. M. Hocky, H. A. Gandhi, M. Ansari, S. Cox, **G. P. Wellawatte**, S. Sasmal, Z. Yang, K. Liu, Y. Singh, W. J. P. Ccoa *Digital Discovery (2023)*

Model Agnostic Generation of Counterfactual Explanations for Molecules **G. P. Wellawatte**, A. Sheshadri, A. D. White. *Chemical Science (2022)*

Graph neural network based coarse-grained mapping prediction **G. P. Wellawatte**[*], Z. Li[*] ,M. Chakraborty, H. A. Gandhi, C. Xu, A. D. White. *Chemical Science (2020)*
[*]*Equal contribution*

HOOMD-TF: GPU-Accelerated, Online Machine Learning in the HOOMD-blue Molecular Dynamics Engine
R. Barrett, M. Chakraborty, D. Amirkulova, H. Gandhi, **G. P. Wellawatte**, A. D. White. *The Journal of Open Source Software (2020)*

Oral Presentations

December 14, 2024: AI4Mat Workshop, Neurips
Accepted Talk: **ChemLit-QA: A human evaluated dataset for chemistry RAG tasks**

May 16, 2024: SIMPLAIX Workshop
Invited Talk: **Explainable AI in Chemistry**

February 29, 2024: AGI-Leap Summit
Invited Talk: **Extracting human interpretable structure-property relationships in chemistry using XAI and large language models**

May 18, 2023: Summer of Chemical Theory @WashU 2023
Invited Talk: **Extrapolating with CG neural potentials**

March 28, 2023: ACS Spring Conference
Invited Talk: (On behalf of Andrew White); **Can CG neural potentials extrapolate beyond training data?**

November 22, 2022: EPFL ISIC ML Seminar
Invited Talk: **Model Agnostic Counterfactual Explanations for Molecular Property Predictions**

October 04, 2022: ACS NERM 2022
Computational Tools for Materials Science: **Molecular model agnostic counterfactual explanations (MMACE) in explainable AI**

April 29, 2022: ICLR 2022
Invited Talk: Deep Generative Models for Highly Structured Data Workshop; **Model Agnostic Counterfactual Explanations for Molecules**

February 01, 2022: M_2D_2 2022
Invited Talk: Molecular Modeling And Drug Discovery M_2D_2 Seminar Series; **Model Agnostic Counterfactual Explanations for Molecules**

August 22, 2021: ACS 2021
Division of Computers in Chemistry; **Predicting coarse-grained (CG) mappings using graph neural networks: Applications in CG molecular dynamics**

June 16, 2021: MTSM 2021
Session: Applications of Machine Learning, Contributed Speech; **Applications of Machine Learning in Coarse-Grained (CG) Molecular Dynamics (MD)**

April 26, 2021: Virtual Talk, Univeristy of Rochester,
Third year talk, Chemistry Department; **Developing Coarse-Grained Models Using Machine Learning**

November 16-20, 2020: Virtual AIChE Annual Meeting
Forum Plenary: Computational Molecular Science and Engineering Forum; **Theory and application of graph neural networks for molecular modeling**

Internships

May 31, 2022 - August 26, 2022
Molecular Modeling and Cheminformatics Intern;
Merck, Rahway, NJ, USA

Summer 2022(Declined Offer)
DAAD-RISE Professional Intern;
ABB Corporate Research, Germany

Leadership & Affiliations

AI4Mat Workshop, Neurips, Organizing Committee *July, 2024 - December 2024*

AI4Mat Workshop - Vienna, Organizing Committee *May, 2024 - July 2024*

ML4Molecules-ELLIS Workshop, Organizing Committee *October, 2023 - December 2023*

ACS Fall Graduate Student Symposium, Planning Committee *May, 2021 - August 2022*
Treasurer

Graduate Student Advisory Committee, University of Rochester *November, 2021 - May,2022*
Graduate Student Representative

Title IX Education Assessment Committee, University of Rochester *July, 2020 - May,2021*
Graduate Student Representative

Graduate Student Association, University of Rochester *June, 2019 - May,2021*
Treasurer

References for Contact

Prof. Andrew White
Associate Professor
FutureHouse, San Francisco, CA.
andrew@futurehouse.org

Prof. Philippe Schwaller
Assistant Professor
EPFL, Switzerland
philippe.schwaller@epfl.ch