Geemi P. Wellawatte

Email: **gwellawatte@gmail.com** ***Website: https://geemi725.github.io/***
Phone: **+41 76 786 4993** ***LinkedIn: https://www.linkedin.com/in/geemiw***

Education

University of Rochester — *Rochester, NY*
Ph.D,in 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

Post-Doctoral Researcher — *July, 2023 - Current*
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

Extracting human interpretable structure-property relationships in chemistry using XAI and large language models **G. P. Wellawatte**, P. Schwaller *Submitted (2023)*

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. *Submitted 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, 13, 3697-3705*

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, 11, 9524-9531*
[*]*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, 5(51): 2367*

Oral Presentations

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

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

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 andrew.white@rochester.edu
University of Rochester, Rochester, NY.

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