Geemi P. Wellawatte

Email: **gwellawa@ur.rochester.com** ***Website: https://geemi725.github.io/***
Phone: **(585) 732 5438** ***Twitter: https://twitter.com/GWellawatte***

Education

University of Rochester — *Rochester, NY*
Ph.D, Candidate in Chemistry — *2020-Present*

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

Graduate Research Assistant (Year IV) — *January, 2019 - present*
Advisor: Prof. Andrew White
Department of Chemistry, University of Rochester — *Rochester, NY*

- **Research Focus**: Using all-atom and coarse-grained molecular dynamics with machine learning to understand chemistry and design materials

Graduate Teaching Assistant
Department of Chemistry, University of Rochester — *Rochester, NY*

- *Physical Chemistry-I (CHM 251)* — *Fall 2019*
- *Quantum Chemistry-I (CHM 451)* — *Fall 2019*
- *Energy, Science, Tech & SO (CHM 286)* — *Spring 2019*
- *Chemistry Concepts, Systems & Practicals I (CHM 131)* — *Fall 2018*

Demonstrator
Department of Chemistry, University of Colombo — *Colombo, Sri Lanka*

- *Physical Chemistry Laboratory-I* — *Semester-I, 2017*
- *Computational Chemistry Laboratory-I* — *Semester-I, 2017*
- *Physical Chemistry Laboratory-I* — *Semester-II, 2017*
- *Computational Chemistry Laboratory-I* — *Semester-II, 2017*
- *Computational Chemistry Laboratory, Msc.* — *Semester-I, 2017*
- *Computational Chemistry Laboratory, Msc.* — *Semester-II, 2017*

Professional Qualifications

Charted Institute of Marketing (CIM),UK-Professional Postgraduate Diploma in Marketing(Level 7) — *2015*

Charted Institute of Marketing (CIM), UK-Professional Diploma in Marketing (Level 6) 2014

Charted Institute of Marketing (CIM), UK-Professional Certificate in Marketing (Level 4) 2012

Geemi P. Wellawatte ***Email:*** **gwellawa@ur.rochester.edu**

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

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, 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

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: 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

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

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

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

Transportation Advisory Committee, University of Rochester *May, 2020 - May,2021*
Graduate Student Representative

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

Chemical Society, University of Colombo, Sri Lanka *April, 2016- April, 2017*
Vice President

Varsity Rowing Crew, University of Colombo, Sri Lanka *March, 2012- March, 2015*
Oarswoman/Cox

References for Contact

Prof. Andrew White
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University of Rochester, Rochester, NY.
andrew.white@rochester.edu
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Prof. Ignacio Franco
Associate Professor of Chemistry,
Associate Professor of Physics,
Leonard Mandel Faculty Fellow
University of Rochester, Rochester, NY.
ignacio.franco@rochester.edu
Phone: 585 275 8209

Prof. Alan M. Grossfield
Associate Professor of Department of Biochemistry and Biophysics
University of Rochester, Rochester, NY.
alan_grossfield@urmc.rochester.edu
Phone: 585 276 4193

Prof. Wolf-Udo Schröder
Professor of Chemistry, Professor of Physics
University of Rochester, Rochester, NY.
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