Geemi P. Wellawatte

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Phone: **(585) 732 5438**

Website: https://geemi725.github.io/
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

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

Overview: Structural Explanations for Molecular Prediction Models **G. P. Wellawatte**, H. A. Gandhi, A. Sheshadri, A. D. White. *Submitted 2022*

Why the Smell? Exploring Structure-Odor Relationships Using Explainable AI A. Sheshadri, H. A. Gandhi, **G. P. Wellawatte**, A. D. White. *Submitted 2022*

Do Language Models Know Chemistry? 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 *ChemRxiv. 2022*

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

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: 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 &   *Graduate Student Advisory Committee, University of Rochester*   *November, 2021 -*
AFFILIATIONS   *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   *Prof. Andrew White*
CONTACT   Associate Professor of Chemical Engineering   andrew.white@rochester.edu
University of Rochester, Rochester, NY.   *Phone:* 585 276 7395

Prof. Ignacio Franco
Associate Professor of Chemistry,   ignacio.franco@rochester.edu
University of Rochester, Rochester, NY.   *Phone:* 585 275 8209

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