

Geemi P. Wellawatte

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EDUCATION	<i>University of Rochester</i> Ph.D ,in Chemistry	<i>Rochester, NY</i> 2020-2023
	<i>University of Rochester</i> M.S , Chemistry	<i>Rochester, NY</i> 2018-2020
	<i>University of Colombo</i> B.S , Special Degree in Computational Chemistry (First Class Honors)	<i>Colombo, Sri Lanka</i> 2013-2017
EXPERIENCE	Graduate Research Assistant (Year IV) <i>Advisor: Prof. Andrew White</i> <i>Department of Chemistry, University of Rochester</i>	<i>January, 2019 - 2023</i> <i>Rochester, NY</i>
	<ul style="list-style-type: none">● Research Focus: Using all-atom and coarse-grained molecular dynamics with machine learning to understand chemistry and design materials	
	Graduate Teaching Assistant <i>Department of Chemistry, University of Rochester</i>	<i>Rochester, NY</i>
	<ul style="list-style-type: none">● <i>Physical Chemistry-I (CHM 251)</i>● <i>Quantum Chemistry-I (CHM 451)</i>● <i>Energy, Science, Tech & SO (CHM 286)</i>● <i>Chemistry Concepts, Systems & Practicals I (CHM 131)</i>	<i>Fall 2019</i> <i>Fall 2019</i> <i>Spring 2019</i> <i>Fall 2018</i>
	Demonstrator <i>Department of Chemistry, University of Colombo</i>	<i>Colombo, Sri Lanka</i>
	<ul style="list-style-type: none">● <i>Physical Chemistry Laboratory-I</i>● <i>Computational Chemistry Laboratory-I</i>● <i>Physical Chemistry Laboratory-I</i>● <i>Computational Chemistry Laboratory-I</i>● <i>Computational Chemistry Laboratory, Msc.</i>● <i>Computational Chemistry Laboratory, Msc.</i>	<i>Semester-I, 2017</i> <i>Semester-I, 2017</i> <i>Semester-II, 2017</i> <i>Semester-II, 2017</i> <i>Semester-I, 2017</i> <i>Semester-II, 2017</i>
PROFESSIONAL QUALIFICATIONS	<i>Chartered Institute of Marketing (CIM),UK-Professional Postgraduate Diploma in Marketing(Level 7)</i>	<i>2015</i>
	<i>Chartered Institute of Marketing (CIM), UK-Professional Diploma in Marketing (Level 6)</i>	<i>2014</i>
	<i>Chartered Institute of Marketing (CIM), UK-Professional Certificate in Marketing (Level 4)</i>	<i>2012</i>

SELECTED HONORS & AWARDS	<p><i>D. E. Shaw Research Graduate and Postdoc Women's Fellowship</i> May 26, 2022 - May 27, 2022</p> <p><i>Esther M. Conwell Graduate Fellowship, Department of Chemistry, University of Rochester</i> August 2021-August 2022</p> <p><i>MolSSI Covid-19 Seed Fellowship, Molecular Sciences Software Institute, VA</i> July 2020-December 2020</p> <p><i>Sherman-Clarke Fellowship, Department of Chemistry, University of Rochester</i> August 2018-August 2019</p>
JOURNAL PUBLICATIONS	<p><i>Neural Potentials of Proteins Extrapolate Beyond Training Data</i> G. P. Wellawatte, G. M. Hocky, A. D. White. <i>Submitted 2022</i></p> <p><i>A Perspective on Explanations of Molecular Prediction Models</i> G. P. Wellawatte, H. A. Gandhi, A. Sheshadri, A. D. White. <i>Journal of Chemical Theory and Computation</i> (2023).</p> <p><i>Why does that molecule smell?</i> A. Sheshadri, H. A. Gandhi, G. P. Wellawatte, A. D. White. <i>Submitted 2022</i></p> <p><i>Assessment of chemistry knowledge in large language models that generate code</i> 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 <i>Digital Discovery</i>. 2023</p> <p><i>Model Agnostic Generation of Counterfactual Explanations for Molecules</i> G. P. Wellawatte, A. Sheshadri, A. D. White. <i>Chemical Science</i>. 2022, 13, 3697-3705</p> <p><i>Graph neural network based coarse-grained mapping prediction</i> G. P. Wellawatte*, Z. Li*, M. Chakraborty, H. A. Gandhi, C. Xu, A. D. White. <i>Chemical Science</i>. 2020, 11, 9524-9531 *Equal contribution</p> <p><i>HOOMD-TF: GPU-Accelerated, Online Machine Learning in the HOOMD-blue Molecular Dynamics Engine</i> R. Barrett, M. Chakraborty, D. Amirkulova, H. Gandhi, G. P. Wellawatte, A. D. White. <i>The Journal of Open Source Software</i>. 2020, 5(51): 2367</p>
ORAL PRESENTATIONS	<p><i>March 28, 2023: ACS Spring Conference</i> Invited Talk (On behalf of Andrew White); Can CG neural potentials extrapolate beyond training data?</p> <p><i>November 22, 2022: EPFL ISIC ML Seminar</i> Invited Talk; Model Agnostic Counterfactual Explanations for Molecular Property Predictions</p> <p><i>October 04, 2022: ACS NERM 2022</i> Computational Tools for Materials Science: Molecular model agnostic counterfactual explanations (MMACE) in explainable AI</p> <p><i>April 29, 2022: ICLR 2022</i> Invited Talk: Deep Generative Models for Highly Structured Data Workshop; Model Agnostic Counterfactual Explanations for Molecules</p>

February 01, 2022: M₂D₂ 2022

Invited Talk: Molecular Modeling And Drug Discovery M₂D₂ 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

Graduate Student Advisory Committee, University of Rochester
May,2022

November, 2021 -

Graduate Student Representative

ACS Graduate Student Symposium Planning Committee for Fall 2022,
August 2022

May, 2021 -

Treasurer

Title IX Education Assessment Committee, University of Rochester
May,2021

July, 2020 -

Graduate Student Representative

Transportation Advisory Committee, University of Rochester
Graduate Student Representative

May, 2020 - May,2021

Graduate Student Association, University of Rochester
Treasurer

June, 2019 - May,2021

Chemical Society, University of Colombo, Sri Lanka
Vice President

April, 2016- April, 2017

Varsity Rowing Crew, University of Colombo, Sri Lanka
Oarswoman/Cox

March, 2012- March, 2015

REFERENCES FOR CONTACT

Prof. Andrew White

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University of Rochester, Rochester, NY.

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Prof. Ignacio Franco

Associate Professor of Chemistry,
University of Rochester, Rochester, NY.

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Prof. Alan M. Grossfield

Associate Professor of Department of Biochemistry
and Biophysics
University of Rochester, Rochester, NY.

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