

Duwage Charitha Perera

website

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WORK EXPERIENCE

Postdoctoral Fellow

Indiana University
(Advisor: Philip Shushkov)

Bloomington, IN

February 2023

EDUCATION

University of Maine

Ph.D. in Chemistry, GPA 3.9/4.0
(Advisor: Jayendran C. Rasaiah)

Orono, ME

December 2022

University of Ruhuna

B Sc. (Special) – Specialized Chemistry and Mathematics

Matara, Sri Lanka

August 2014

RESEARCH INTEREST

DFT studies of small cluster systems

H₂ production from water splitting on ZnO and ZnO-Graphene Oxide nanoclusters.

Dynamics of water splitting reaction on ZnO nanocluster.

Acetic acid decarboxylation reaction on Mg(OH)₂ and MgO nanoclusters.

Computational studies on Molecular Qubits into quantum computing

Calculating spin relaxation time for molecular qubits using DFT

AIMD studies of metal cation interactions with glyphosate

Metal cation/cationic mixtures interactions with glyphosate molecule using ab initio molecular dynamic

PUBLICATIONS

Published

Duwage C. Perera and Jayendran C. Rasaiah, "Computational Study of H₂O Adsorption, Hydrolysis, and Water Splitting on (ZnO)₃ Nanoclusters Deposited on Graphene and Graphene Oxides", ACS Omega, 2023
<https://pubs.acs.org/doi/full/10.1021/acsomega.3c04882>

Duwage C. Perera and Jayendran C. Rasaiah, "Exchange Functionals and Basis Sets for Density Functional Theory Studies of Water Splitting on selected ZnO nanocluster catalysts", ACS Omega, 2022
<https://doi.org/10.1021/acsomega.1c05666>

Perera, D.C., Hewage, J.W. Rasaiah, J.C. Acetic acid and propionic acid decarboxylation on Mg(OH)₂ nanoclusters: a density functional theory study. J Mater Sci 2020, 55, 16914–16927
<https://doi.org/10.1007/s10853-020-05196-z>

Duwage C. Perera, Jinasena W. Hewage, Nalin de Silva, Theoretical study of catalytic decomposition of acetic acid on MgO nanosurface, Comput. Theor. Chem 2015, 1064, 1-6
<http://www.sciencedirect.com/science/article/pii/S2210271X15001619>

Farshad, Mohsen, **Duwege C. Perera**, and Jayendran C. Rasaiah. "Theoretical Study of the Stability, Structure, and Optical Spectra of Small Silver Clusters and Their Formation Using Density Functional Theory." *Phys. Chem. Chem. Phys.*, 2021 , <https://doi.org/10.1039/D1CP04070G>

Mitchell R. M. Bruce, Alice E. Bruce, Sarah E. Bernard, Andrew N. Bergeron, Ahmad A. L. Ahmad, Timothy A. Bruce, **Duwege C. Perera**, Shyam Pokhrel, Sfoog Saleh, Anna Tyrina, and Sudheera Yaparathne; Designing a Remote, Synchronous, Hands-On General Chemistry Lab Course, *Journal of Chemical Education*, 2021 <https://doi.org/10.1021/acs.jchemed.1c00559>

Manuscripts in preparation

Duwege C. Perera, Review article on Photocatalytic water splitting reaction: Impact on graphene-based materials, 2023 (Manuscript in preparation)

Duwege C. Perera, Review article on Overview of the Theoretical Studies on atmospheric CO₂ capturing methods, 2023 (Manuscript in preparation)

Duwege C. Perera, Applications and Recent studies on molecular Qubits: A Review Article , 2023 (Manuscript in preparation)

CONFERENCE PRESENTATIONS

ACS - NERM October 02-05, 2022
American Chemical Society North Eastern Regional Meeting Rochester, NY
Duwege C. Perera and Jayendran C. Rasaiah, Effect of Graphene Oxide on the photocatalytic properties of ZnO nanoclusters: A Theoretical Study(**Oral**)

ACS National Meeting August 22-26, 2021
American Chemical Society Atlanta, GA
Duwege C. Perera and Jayendran C. Rasaiah, Reaction pathways for the hydrolysis of (ZnO)₃ nanoclusters on graphene oxide as a key step for water splitting reaction– A DFT study (**Oral**)
<https://doi.org/10.1021/scimeetings.1c00964>

University of Maine Student Symposium April 16, 2021
University of Maine Orono, ME
Duwege C. Perera (**Oral**), and Jayendran C. Rasaiah, Exchange Functionals and Basis Sets for Density Functional Theory Study of ZnO Nano clusters in Photocatalytic Reactions
<https://video.maine.edu/media/Kaltura+Capture+recording+-+March+25th+2021>

Saint Anselm College April 09, 2021
Manchester, NH
Duwege C. Perera (**Oral, Invited**), and Jayendran C. Rasaiah, A Density Functional Study of Water Splitting Reaction Pathway on ZnO Nanoclusters

Webinar on nanotechnology, iNano 2020 October 19-20, 2020
Phronesis LLC Virtual
Duwege C. Perera and Jayendran C. Rasaiah, Density Functional Theory Study of the Effect of Graphene Oxide (GO) on the Hydrolysis Reaction of ZnO Nanoclusters with Water(**Poster**)

LatinXChem Twitter Conference September 7, 2020
LatinXChem Virtual
Duwege C. Perera and Jayendran C. Rasaiah, The Effect of Graphene Oxide in Adsorption of Water on ZnO Clusters: A DFT Study(**Poster**) <https://twitter.com/dcharitha/status/1302946538956763137>

University of Maine Student Symposium April 10, 2019
University of Maine Orono, ME
Duwege C. Perera (**Oral**), Jinasena W. Hewage and Jayendran C. Rasaiah, Theoretical study and design of a catalytic reaction using density functional theory: Acetic acid decarboxylation in the gas phase and on Mg(OH)₂ nanosurfaces

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| APS March meeting <i>American Physical Society</i> Duwage C. Perera (Oral) and Jayendran C. Rasaiah, Density Functional Theory Study of Water Splitting on ZnO Catalyst Adsorbed on Graphene Oxide | March 06, 2019 Boston, MA |
| 256th ACS National Meeting <i>American Chemical Society</i> Duwage C. Perera, Jinasena W. Hewage and Jayendran C. Rasaiah, Theoretical study of the thermal decomposition of acetic acid on Mg(OH) ₂ nano surface using DFT(Poster) | August 19-23, 2018 Boston, MA |
| GRS & GRC Meeting <i>Gordon Research Seminar and Conference</i> Duwage C. Perera and Jayendran C. Rasaiah, Ab initio calculations of catalytic water splitting with ZnO catalyst(Poster) | July 21-27, 2018 Holderness, NH |
| ACTC <i>American Conference on Theoretical Chemistry</i> Duwage C. Perera and Jayendran C. Rasaiah, Quantum Mechanical Studies of Catalytic effects on water splitting on ZnO clusters(Poster) | July, 2017 Boston, MA |
| CRYSTAL Workshop <i>Minnesota workshop on ab initio modeling in solid state chemistry with CRYSTAL</i> Duwage C. Perera and Jayendran C. Rasaiah, Quantum Mechanical Studies of Catalytic effects on water splitting on ZnO clusters(Poster) | July, 2017 Minneapolis, MN |
| ACS - NERM <i>American Chemical Society North Eastern Regional Meeting</i> Duwage C. Perera, Jinasena W. Hewage and Jayendran C. Rasaiah, Ab initio studies of Magnesium Hydroxide Nanoparticles as potential catalysts for thermal decomposition of Acetic Acid(Poster) | October 06, 2016 Binghamton, NY |

WORKSHOPS & SUMMER SCHOOLS

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| Telluride School of Theoretical Chemistry <i>Telluride, CO</i> | July 29 – August 03, 2019 |
| GERA Energy workshop, March meeting APS <i>Boston, MA</i> | March 03, 2019 |
| CITL teaching pilot 5 months program <i>University of Maine, Orono, ME</i> | January – May, 2019 |
| MolSSI Software Summer School, Virginia Tech <i>Blacksburg, VA</i> | July-August 2017 |
| The Minnesota Workshop on ab initio modeling in Solid State Chemistry <i>Minnesota, MN</i> | July 2017 |
| ES-2017, Electronic Structure Workshop <i>Princeton, NJ</i> | June 2017 |

EXPERIENCE

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| Teaching Assistant <i>University of Maine, Machias</i> • General Chemistry undergraduate courses (CHY 101) | August 2022 – December 2022 Machias, ME |
| Teaching Assistant <i>University of Maine</i> • General Chemistry undergraduate courses (CHY 123 & CHY 124) | January 2016 – May 2022 Orono, ME |
| Teaching Assistant <i>University of Ruhuna</i> • Physical Chemistry, Inorganic Chemistry Organic Chemistry undergraduate courses | 2014 – 2015 Matara, Sri Lanka |

AWARDS

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| The Outstanding Teaching Assistant in General Chemistry Award <i>University of Maine</i> | 2018-2019 Academic year <i>Orono, ME</i> |
| Won the third place in 3MT (3 Minute Thesis) competition <i>University of Maine</i> | March 25, 2018 <i>Orono, ME</i> |
| Wiley Outstanding Poster Award <i>Minnesota Workshop on ab initio modeling in Solid State Chemistry with CRYSTAL</i> | July 2017 <i>Minnesota, MN</i> |
| National Research Council (NRC) merit award <i>For scientific publication for Computational and theoretical chemistry 2015, Vol 1064, pp 1-6</i> | December 2017 <i>Sri Lanka</i> |

GRANTS

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| GERA workshop travel grant <i>March meeting APS</i> | 2019 <i>Boston, MA</i> |
| Graduate Student Government (GSG) travel grant in spring cycle <i>University of Maine</i> | 2019 <i>Orono, ME</i> |

TECHNICAL SKILLS

Languages: Python, C/C++, FORTRAN
Packages: Gaussian 09/16, Gauss view 05/06, NAMD, VMD, Mathematica, Gromacs, GaussSum, Matlab, CP2K, Orca, Quantum Espresso
Platform: Unix/Linux, Microsoft Windows, LibreOffice
Graphics: Gnuplot
Instruments: Bomb calorimeter, UV-Vis spectrometer, Flame photometer
Libraries: Pandas, NumPy, Matplotlib

OUTREACH

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| Elsevier Reviewer | 2023 |
| Leadership Team member in the Postdoctoral Association <i>Indiana University Bloomington, IN</i> | 2023 |
| Certified Publons Academy Peer Reviewer <i>Completed the Peer Reviewed Course on 01 June 2021</i> | 2021 |
| Executive Committee Member in Forum on Outreach and Engage in Public (FOEP) <i>American Physical Society (APS)</i> | 2020 – 2021 |
| Executive Committee Member in Forum on Graduate Student Affairs (FGSA) <i>American Physical Society (APS)</i> | 2019 – 2021 |
| Member of Covid Research and Resources Group (CRRG) <i>American Physical Society (APS)</i> | 2020 |
| Treasure of Graduate Student Government (GSG) <i>University of Maine</i> | 2019 – 2021 |
| Senator of Graduate Student Government (GSG) <i>University of Maine</i> | 2017 – 2019 |

MEMBERSHIPS

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| American Chemical Society (ACS) | 2016 – Present |
| American Physics Society (APS) | 2018 - Present |
| Forum on Graduate Student Affairs (FGSA APS) | 2018 - 2022 |

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| University of Maine Graduate Student Government (GSG) | 2016 - 2022 |
| University of Maine Women in Academia | 2017 - 2022 |
| University of Maine Association for Computing Machinery-Women <i>(ACM-W) student chapter</i> | 2017 - 2022 |
| Golden Key honor society member | 2019 - Present |