

Duwage Charitha Perera

website

Email: charitha.perera@maine.edu

EDUCATION

University of Maine

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

Orono, ME

December 2022 Expected

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.

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, "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>

Farshad, Mohsen, **Duwage 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, **Duwage 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>

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>

Manuscripts on preparation

Duwage C. Perera and Jayendran C. Rasaiah, A theoretical study on the nanoclustered graphene oxide and ZnO as photocatalysts for water splitting reaction, 2022 (Manuscript on preparation)

Duwage C. Perera and Jayendran C. Rasaiah, Reaction pathways for water splitting on (ZnO)₃ nanoclusters: A theoretical study, 2022 (Manuscript on preparation)

Duwage C. Perera and Jayendran C. Rasaiah, Effect of graphene oxide towards the H₂ production from the hydrolyzed (ZnO)₃ nanocluster at the ground and first excited triplet state: A DFT Study, 2022 (Manuscript on preparation)

CONFERENCE PRESENTATIONS

ACS National Meeting

August 22-26, 2021

American Chemical Society

Atlanta, GA

Duwage 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

Duwage 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

Duwage 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

Duwage 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

Duwage 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

Duwage 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

APS March meeting March 06, 2019
American Physical Society Boston, MA
Duwage C. Perera (**Oral**) and Jayendran C. Rasaiah, Density Functional Theory Study of Water Splitting on ZnO Catalyst Adsorbed on Graphene Oxide

256th ACS National Meeting August 19-23, 2018
American Chemical Society Boston, MA
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**)

GRS & GRC Meeting July 21-27, 2018
Gordon Research Seminar and Conference Holderness, NH
Duwage C. Perera and Jayendran C. Rasaiah, Ab initio calculations of catalytic water splitting with ZnO catalyst(**Poster**)

ACTC July, 2017
American Conference on Theoretical Chemistry Boston, MA
Duwage C. Perera and Jayendran C. Rasaiah, Quantum Mechanical Studies of Catalytic effects on water splitting on ZnO clusters(**Poster**)

CRYSTAL Workshop July, 2017
Minnesota workshop on ab initio modelling in solid state chemistry with CRYSTAL Minneapolis, MN
Duwage C. Perera and Jayendran C. Rasaiah, Quantum Mechanical Studies of Catalytic effects on water splitting on ZnO clusters(**Poster**)

ACS - NERM October 06, 2016
American Chemical Society North Eastern Regional Meeting Binghamton, NY
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**)

WORKSHOPS & SUMMER SCHOOLS

Telluride School of Theoretical Chemistry July 29 – August 03, 2019
Telluride, CO

GERA Energy workshop, March meeting APS March 03, 2019
Boston, MA

CITL teaching pilot 5 months program January - May, 2019
University of Maine, Orono, ME

MolSSI software Summer School, Virginia Tech July-August 2017
Blacksburg, VA

The Minnesota Workshop on ab initio modeling in Solid State Chemistry July 2017
Minnesota, MN

ES-2017, Electronic Structure Workshop June 2017
Princeton, NJ

EXPERIENCE

Teaching Assistant

University of Maine

January 2016 – Present

Orono, ME

* General Chemistry undergraduate courses (CHY 123 & CHY 124)

Teaching Assistant

University of Ruhuna

2014 – 2015

Matara, Sri Lanka

* Physical Chemistry, Inorganic Chemistry Organic Chemistry undergraduate courses

AWARDS

The Outstanding Teaching Assistant in General Chemistry Award

University of Maine

2018-2019 Academic year

Orono, ME

Won the third place in 3MT (3 Minute Thesis) competition

University of Maine

March 25, 2018

Orono, ME

Wiley Outstanding Poster Award

Minnesota Workshop on ab initio modeling in Solid State Chemistry with CRYSTAL

July 2017

Minnesota, MN

National Research Council (NRC) merit award

For scientific publication for Computational and theoretical chemistry 2015, Vol 1064, pp 1-6

December 2017

Sri Lanka

GRANTS

GERA workshop travel grant

March meeting APS

2019

Boston, MA

Graduate Student Government (GSG) travel grant in spring cycle

University of Maine

2019

Orono, ME

TECHNICAL SKILLS

Languages: Python, C/C++, FORTRAN

Packages: Gaussian 09/16, Gauss view 05/06, NAMD, VMD, Mathematica, Gromacs, GaussSum, Matlab, CP2K

Platform: Unix/Linux, Microsoft Windows, LibreOffice

Graphics: Gnuplot

Instruments: Bomb calorimeter, UV-Vis spectrometer, Flame photometer

Libraries: Pandas, NumPy, Matplotlib

OUTREACH

Certified Publons Academy Peer Reviewer

Completed the Peer Reviewed Course on 01 June 2021

2021

Executive Committee Member in Forum on Outreach and Engage in Public (FOEP) 2020 – 2021

American Physical Society (APS)

Executive Committee Member in Forum on Graduate Student Affairs (FGSA)

American Physical Society (APS)

2019 – 2021

Member of Covid Research and Resources Group (CRRG) <i>American Physical Society (APS)</i>	2019 – 2021
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

American Chemical Society (ACS)	2016 – Present
American Physics Society (APS)	2018 - Present
Forum on Graduate Student Affairs (FGSA APS)	2018 - Present
University of Maine Graduate Student Government (GSG)	2016 - Present
University of Maine Women in Academia	2017 - Present
University of Maine Association for Computing Machinery-Women <i>(ACM-W) student chapter</i>	2017 - Present
Golden Key honor society member	2019 - Present