Duwage Charitha Perera

Email: charitha.perera@emaine.edu

Education

University of Maine — Orono, ME
Ph.D. in Chemistry, GPA 3.9/4.0 (Advisor:Jayendran C. Rasaiah) — *December 2021 Expected*

University of Ruhuna — Matara, Sri Lanka
B Sc. (Special) – Specialized Chemistry and Mathematics — *August 2014*

Research Interest

DFT studies of small cluster systems

Acetic acid decarboxylation reaction on $Mg(OH)_2$ and MgO nanoclusters and H_2 production from water on ZnO-Graphene Oxide nanoclusters

AIMD studies of metal cation interactions with glyphosate

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

Publications

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; Perera, Duwage; Rasaiah, Jayendran (2020): Theoretical Study of Stability, Structure, and Optical Spectra of Ultra-Small Silver Clusters Using Density Functional Theory, (Manuscript submitted to Journal of Physical Chemistry C) (ChemRxiv. Preprint: https://doi.org/10.26434/chemrxiv.13272443.v1)

Duwage C. Perera and Jayendran C. Rasaiah, Functional and Basis Set Comparison for Small ZnO Clsuters: A Theoretical Level Study, 2020 (Manuscript on preparation)

Conference Presentations

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/d_c*haritha*/*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 January 2016 – Present
University of Maine *Orono, ME*

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

Teaching Assistant 2014 – 2015
University of Ruhuna *Matara, Sri Lanka*

- Physical Chemistry, Inorganic Chemistry Organic Chemistry undergraduate courses

Awards

The Outstanding Teaching Assistant in General Chemistry Award 2018-2019 Academic year
University of Maine *Orono, ME*

Won the third place in 3MT (3 Minute Thesis) competition March 25, 2018
University of Maine *Orono, ME*

Wiley Outstanding Poster Award July 2017
Minnesota Workshop on ab initio modeling in Solid State Chemistry with CRYSTAL *Minnesota, MN*

National Research Council (NRC) merit award December 2017
For scientific publication for Computational and theoretical chemistry 2015, Vol 1064, pp 1-6 *Sri Lanka*

Grants

GERA workshop travel grant 2019
March meeting APS *Boston, MA*

Graduate Student Government (GSG) travel grant in spring cycle 2019
University of Maine *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

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) 2019 – 2021
American Physical Society (APS)

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

Treasure of Graduate Student Government (GSG) 2019 – 2021
University of Maine

Senator of Graduate Student Government (GSG) 2017 – 2019
University of Maine

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 2017 - Present
(ACM-W) student chapter

Golden Key honor society member 2019 - Present