Anton Perera

COMPUTATIONAL CHEMIST

Profile

- Skilled computational chemist with expertise in materials chemistry, computer-aided drug design, and a strong background in physical chemistry and chemical physics, contributing to multiple lead-author publications showcasing advanced computational techniques and understanding of experimental methodologies.
- Proficient in software and hardware integration, high-performance computing, and cutting-edge simulation tools, optimizing computational workflows and utilizing state-of-the-art technology to boost research efficiency and innovation.
- Adept at fostering interdisciplinary collaborations with experimentalists, using excellent communication and problem-solving skills to bridge the gap between theoretical predictions and experimental data, ensuring project success and promoting a collaborative research environment for scientific advancement.

Education

PhD in Chemistry, University of Kentucky, Lexington

AUGUST 2018 — SEPTEMBER 2023

Cumulative GPA: 3.84/4.00

PhD Advisors: Prof. Chad Risko, Prof. Susan Odom

Bachelor of Science in Chemistry, Institute of Chemistry Ceylon, Colombo

JANUARY 2012 — SEPTEMBER 2015

Graduated with honors (second class upper division)

Employment History

Graduate Research Assistant , University of Kentucky, Lexington

MAY 2019 — PRESENT

- Served as the lead computational chemist in the Odom lab producing three first-author and one lead computational author manuscripts (published and in-pipeline) and contributed to securing grant proposals performing computational simulations, theoretical calculations, and predictive modeling collaborating with experimental chemists from multiple universities and national labs across the USA, under the Joint Center for Energy Storage Research (JCESR), a Department of Energy (DOE) Energy Innovation Hub.
- Collaborated with computational chemists and experimentalists from Risko lab and other partnering institutions in understanding solvation, crystallization, and molecular packing of organic materials geared towards energy storage leading to two published and in-pipeline manuscripts as the lead computational author.
- Developed and validated computational workflows and tools for theoretical calculations and analysis of molecular dynamics simulations.

Graduate Teaching Assistant , University of Kentucky, Lexington

AUGUST 2018 — MAY 2019

- Conducted undergraduate general chemistry laboratory courses at the University of Kentucky.

Assistant Research Technologist , Industrial Technology Institute, Colombo

AUGUST 2017 — JUNE 2018

Details

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Links

LinkedIn | @AntonSPerera

Twitter | @AntonSPerera

Skills

Computational Chemistry

Molecular Dynamics (MD)

Ab-initio and DFT quantum calculations

Computational Materials Chemistry

Computer-aided Drug Design (CADD)

Cheminformatics

Python

Machine Learning

Schrodinger software

Quantitative Structure-Property/Activity Relationship (QSAR/QSPR)

High Performance Computing

- Served as the computational lead in the project, *in-silico* and *in-vitro* screening of natural products against enzymes responsible for common diseases leading to three technical abstracts in international conferences and multiple grant reports.
- Implemented a computational workflow with GPU acceleration for mining and *in-silico* screening of a natural product database and trained chemists to continue similar projects.
- Collaborated with multiple scientists within the institute in developing cosmeceuticals from natural product extracts leading to two peer-reviewed manuscripts (published and in review).

Graduate Teaching Assistant, Institute of Chemistry Ceylon, Colombo

JULY 2016 — JULY 2017

- Pioneered the establishment of the Computational Research and Learning Center (CRLC) at the Institute of Chemistry and conducted and mentored multiple research projects leading to presentations in three research symposia in Sri Lanka and overseas.
- Served as the Assistant Secretary of Educational Affairs at the Institute of Chemistry Ceylon from 2016 to 2017.
- Served as the teaching assistant in charge of the Computational Research and Learning Center (CRLC) at the Institute of Chemistry.

Selected Publications

Perera, A. S., Suduwella, T. M., Attanayake, N. H., Jha, R. K., Eubanks, W. L., Shkrob, I. A., Risko, C., Kaur, A. P., & Odom, S. A. (2022). Large variability and complexity of isothermal solubility for a series of redox-active phenothiazines. *Materials Advances*, *3*(23), 8705–8715.

Stumme, N., **Perera, A. S.**, Horvath, A., Ruhunage, S., Duffy, D. H., Koltonowski, E. M., Tupper, J., Dzierba, C., McEndaffer, A. D., Teague, C. M., Risko, C., & Shaw, S. K. (2023). Probing Redox Properties of Extreme Concentrations Relevant for Nonaqueous Redox-Flow Batteries. *ACS Applied Energy Materials*, *6*(5), 2819–2831.

Liyanaararchchi, G. D., **Perera, A. S.**, Samarasekera, J. K. R. R., Mahanama, K. R. R., Hemalal, K. D. P., Dlamini, S., Perera, H. D. S. M., Alhadidi, Q., Shah, Z. A., & Tillekeratne, L. M. V. (2022). Bioactive constituents isolated from the Sri Lankan endemic plant Artocarpus nobilis and their potential to use in novel cosmeceuticals. *Industrial Crops and Products*, *184*(May), 115076.

Affiliations

American Chemical Society (ACS)

MARCH 2021 — PRESENT

Associate Member

Institute of Chemistry Ceylon (IChemC)

MARCH 2016 — PRESENT

Associate Member

Electrochemical Society (ECS)

MARCH 2020 — PRESENT

University of Kentucky Student Chapter | President-2021, Vice president-2020

Royal Society of Chemistry (RSC)

2014 — 2016

Affiliate undergraduate member

University of Kentucky Chemistry Graduate Students' Association

AUGUST 2018 — PRESENT

Treasurer | 2021-2022