

# Yatiwelle Koralalage Samuditha Sandaru Yatiwella

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## Academic Qualifications

- **University of South Carolina | Columbia, SC**  
Master of Science in Chemistry - Summer 2023 | 2019-Present  
**GPA 3.864/4.00**
- **University of Colombo | Sri Lanka** (<http://www.cmb.ac.lk>)  
Bachelor of Science (Honors) in Computational Chemistry | 2014-2017  
**GPA 3.04/4.00**  
Subjects
  - Chemistry
  - Applied Mathematics
  - Computer Science
  - Physics

## Research Experience

- **University of South Carolina - Research Project – 2019-2021**  
“Role of deformable mirror in multidimensional population-period transient spectroscopy”
  - Phase modulation using deformable mirror
  - Designing computer- based optical system using ray tracing program and budling up the optical setup**Supervisor:** Prof. Mark Berg, Professor,  
Department of Chemistry and Biochemistry, University of South Carolina
- **University of South Carolina - Research Project – 2021-2023**  
“Machine learning classification to predict the dimensionality of hybrid inorganic halide perovskites”-Thesis publication
  - Modeling different machine learning models to predict different properties on different organic chemical systems using smiles strings.
  - Data cleaning and processing
  - Small dataset handling.**Supervisor:** Prof. Christopher Sutton, Assistant Professor,  
Department of Chemistry and Biochemistry, University of South Carolina
- **University of Colombo - Research Project – 2017**  
“Theoretical investigation of Intercalation ability of small molecules with Graphene” - Thesis publication
  - Built optimized Graphene models and Intercalant compounds to use in intercalation process with different DFT method.
  - Intercalant were selected through there electron donor and acceptability.
  - Intercalated system was investigated for their structural and electronic property change.
  - Stabilization energy with interlayer distance were calculated alongside the stabilization energy and Density of States for each intercalated compound.**Supervisors:** Prof. Nalin de Silva, Senior Lecturer,  
Department of Chemistry, University of Colombo  
Prof. Rohini De Silva, Senior Lecturer,  
Department of Chemistry, University of Colombo

- **SLINTEC – Product Development for Ceylon Graphene Technologies – 2018/2019**
- The Product development process was based on Lab trials followed by Lab Analysis and different optimization methods which was supervised by SLINTEC ENGINEERING and SCIENCE teams
- Optimization of Graphene Oxide (GO) and reduced Graphene Oxide (rGO) as commercial product
- Analysis of vein Graphite, GO, rGO
- Mass scale production of GO and rGO
- Availability of rGO as a anti corrosive agent

#### Technical Skills

- **Computational Chemistry Related:**
- Monte Carlo Simulations
- Molecular dynamic Simulations
- Molecular Modeling
- Fortran, Java, Matlab, Python
- Software packages (Gaussian 98/03/09, HyperChem, RasMol, Hex, Winmopac, ChemDraw, Rdkit, Scikit learn, Mercury, Qchem, Psi4, Ray tracing, Overleaf)
- Working experience in Linux, Windows and Mac operating systems
- Mobile application development, Microsoft Office and general IT skills
- **Chemistry Related:**
- Chromatographic techniques  
Thin Layer Chromatography, Paper Chromatography, GC/MS, HPLC, Column Chromatography
- Spectroscopic techniques  
Atomic Absorption Spectroscopy, UV/Visible spectroscopy/Colorimetry, NMR, FT-IR, Raman Spectroscopy
- Other Instrumentation  
XPS, XRD, DTA, TGA, XRF, CHNS, SEM, IC-PMS, Particle size analyzer
- Qualitative & quantitative analysis of inorganic compounds (Cation/Anion Analysis)
- Qualitative & quantitative analysis of organic compounds (Functional Group Analysis)
- Complexometric titrations
- Potentiometric / Conductivity and PH Measurements
- Recrystallization / Distillation / Solvent Extraction Techniques

#### Presentations

- Conducted an oral presentation on “Photo Induced Charge Transfer” for the partial fulfillment of CH4002 – Seminars and Essay
- “Role of deformable mirror in multidimensional population-period transient spectroscopy”- Seminar 2020
- Poster presentation on the topic “Machine Learning assisted novel low dimensional perovskite material discovery” at SETCA 2023

#### Selected Extra-Curricular Activities

- Community Service Director Rotaract club Faculty of Science University of Colombo
- Member First XV Rugby Team University of Colombo
- Committee Member of Chemical Society University of Colombo, Sri Lanka in 2016/2017
- CO-Chief organizer of project SAHAS (Annual charity project organized by Chemical Society, University of Colombo, Sri Lanka in 2016)

	<ul style="list-style-type: none"> <li>University colors – 2016,2017</li> </ul>	
<b>Trainings attended</b>	<ul style="list-style-type: none"> <li>Leadership Training Conducted by University Grants Commission Sri Lanka</li> <li>XPS training Conducted by Product Specialist-XPS, Thermo Fisher Scientific India Pvt. Ltd</li> <li>ACS user awareness conducted by ACS representative</li> <li>Laser training conducted by University of South Carolina</li> <li>Chemical waste handling conducted by University of South Carolina</li> </ul>	
<b>Working Experience</b>	<ul style="list-style-type: none"> <li> <b>Teaching assistant   IChem   Sri Lanka</b>            Coordinating and document handling to acquire the accreditation for offering degree status         </li> <li> <b>Research Intern   SRI LANKA INSTITUTE OF NANOTECHNOLOGY (SLINTEC)</b>            Use chemistry knowledge to solve industrial problems (Material Analysis for Graphite, Charcoal, Activated Carbon)            Development and optimization of Graphene oxide and reduced Graphene oxide for Ceylon Graphene Technologies (CGTL)            Waste Management of Acids            Recovery of ethanol and Ether as low-grade solvents            Conducting research activities between SLINTEC and client sector (Lab analysis for different tea grades)         </li> <li> <b>Graduate Teaching Assistant   University of South Carolina   USA</b>            Conducted laboratory sessions for chemistry freshman students            Conducted laboratory sessions for chemistry honors students         </li> <li> <b>Temporary Instructor   University of South Carolina   USA</b>            Conducting laboratories for 200 non chemistry major students         </li> </ul>	
<b>Referees</b>	<ul style="list-style-type: none"> <li> <b>Prof. Mark A Berg,</b>            Professor Spectroscopy and Chemical Physics,            Department of Chemistry and Biochemistry,            University of South Carolina,            USA            Email: berg@sc.edu            Mobile: (803)777-1514         </li> </ul>	<ul style="list-style-type: none"> <li> <b>Prof. Tin Ge,</b>            Assistant Professor in Physical and Theoretical Chemistry,            Department of Chemistry and Biochemistry,            University of South Carolina,            USA            Email: tingg@mailbox.sc.edu            Mobile: (803)576-6508         </li> </ul>
	<ul style="list-style-type: none"> <li> <b>Prof. Dhammike Dissanayake,</b>            Professor in Chemistry,            Department of Chemistry,            Faculty of Science,            University of Colombo, Sri Lanka            Email: dpd@cmb.com            Mobile: +94712946635         </li> </ul>	