Hashan C. Peiris

Ph.D. Candidate - Materials Science and Computational Modeling
Binghamton, NY 13902 | 607 - 297 - 8459 | mpeiris1@binghamton.edu
LinkedIn | GitHub | Google Scholar | ORCiD

ACCOMPLISHMENTS

- **Advanced Computational Research**: Led and collaborated on projects employing DFT, AIMD, and ML to model cathode interfaces, PFAS degradation reaction pathways, solvation dynamics, and thermal-mechanical stability, resulting in 6 publications in high-impact journals (more pending), and 10+ conference presentations.
- **Real world work experience at manufacturing plants:**
  - Certified inspector of pressure valves at Chevron plant
  - Quality control and failure analysis at Michelin wheel manufacturing facility
  - Industrial internship for production and bottling of gases N_2, O_2, and C_2H_2
- **Interdisciplinary Collaborations**: Successfully partnered on projects merging experimental and computational methods—addressing topics from PFAS degradation to Au–S bond energetics—to support breakthrough research initiatives.
- **High-Performance Computing**: Provisioned, installed, and optimized compute nodes while managing key software tools (VASP, Quantum Espresso, DeePMD, USPEX) to enhance research capabilities and drive simulations.
- **Funding & Grant Success**: Authored and contributed to grant proposals securing support from agencies such as NSF, IEEC, SRC, and XSEDE/ACCESS, significantly boosting resources for research.
- **Academic Excellence & Recognition**: Achieved first-class honors in BSc Eng. in MSE, earned a fully funded Ph.D. scholarship, and received multiple awards for excellence in MSE.
- **Mentoring & Teaching**: Guided undergraduate and graduate students through research projects and served as a Graduate Teaching Assistant, fostering technical growth and scientific communication skills.

SKILLS

Programming & Tools	**Python, Visual Basic, Git, Bash, LaTeX, MATLAB** **HPC hardware setup and utilities**
Software	**VASP, DeePMD, USPEX, Quantum Espresso, LAMMPS, Orca** **VSCode, Linux, SolidWorks, Abaqus, AutoCAD, MS Office**
Certifications	**ASNT SNT-TC-1A** (Non-Destructive Testing: PT, UT, RT, MT) – *exp. 2022* **API 510** (Pressure Vessel Inspection) – *exp. 2023* **CIMA (UK):** Passed Finalist; Awaiting PER Qualification (*ACMA*) **Machine Learning:** Predictive Analysis for Business Decisions (*IEEE*)
Soft skills	• **Proposal writing and funding/resource acquisition, project management** • **Applying software and hardware toolkits to real world problems in novel materials** • **Experimental design and performance for root cause analysis and identifying mechanisms** • **Effective scientific communication with talks and presentations** • **Effective collaborations with local and remote teams** • **Managing multiple projects and working independently.** • **Skilled in FEA, DFT and AIMD/ML analysis applied to real world chemistry problems** • **ML interatomic potential development; Data processing and analysis**

EDUCATION

Binghamton University, State University of New York — **New York**
Ph.D. Candidate in Materials Science & Engineering — *Expected Summer/Fall 2025*
Advisor: Dr. Manuel Smeu | Cumulative GPA: 3.8

University of West London — **London, UK**
Master of Business Administration — *Oct 2019*

University of Moratuwa — **Moratuwa, SL**
Bachelor of Science in Materials Science & Engineering — *Dec 2018*
First Class Honors, Summa Cum Laude
Advisor: Dr. Indika De Silva | Cumulative GPA: 3.71 | Dean's List Semesters 2, 5, 7, and 8

Chartered Management Accountants (UK) — **UK**
Chartered Management Accountant (Awaiting PER) — *Oct 2016*

PROFESSIONAL & RESEARCH EXPERIENCE

Binghamton University **Binghamton, NY**

Graduate Research Assistant – Projects *Dec 2022 - Present*

- Modeling of the chemical activity on Ni/Co-rich interfaces of NMC-811 cathodes using DFT, and large scale AIMD simulations. Findings published in a *Cell Reports Physical Science* journal article and an additional manuscript in prep.
- Study of the dynamics of solvation shells of Li/Ca based salts in the electrolyte and at the cathode interface using DFT/AIMD models. Findings were published in a journal article in *Colloids and Surfaces: Physicochemical and Engineering Aspects*. An ML accelerated Ca-based solvation dynamics study is ongoing.
- Investigation of thermo-mechanical stability of Sn-based soldering alloys using DFT/ML-based approaches. Findings published in multiple conferences and submitted IEEC and SRC proposals for funding based on outcomes from the study. Ongoing work.
- *Collaboration* - Investigating the unexpected degradation mechanisms of PFAS chemicals (PVDF) in TMA used in ALD-based coatings. Our findings were published in ACS *Applied Interfaces & Materials.*
- *Collaboration* - Simulating break junction simulations of Au probes in single-molecule junctions using AIMD/DFT and ML to elucidate the number of anchor groups vs. electronic transport in the junction. Manuscript in prep.
- *Collaboration* – Studied the energetics of Au-S bond breaking in Au surfaces via experimental and DFT based approaches. Manuscript in prep.
- *Collaboration* – Provided computational backing to experimentally confirmed high-pressure nitrous oxide reduction by a Cu(II) carbon nitride electrocatalyst framework. Manuscript submitted to *JACS* and under review.
- Provisioning, installation and optimization of high-performance compute nodes and integration into Spiedie compute cluster at Binghamton University
- Compilation and optimization of compute code (VASP, Linux, QE, DeePMD, USPEX etc.) as required for personal and group research needs.
- Authored and contributed to successful annual grant proposals to secure funding and computational resources, obtaining support from funding agencies (NSF, IEEC, SRC) and XSEDE/ACCESS for compute.

Graduate Teaching Assistant *January 2020 - Dec 2022; Intermittent*

- Deliver laboratory-based and discussion-based teaching sessions, managed experiments, and supported student learning in all assigned courses (PHYS 121/122/131/132).
- Served as a Computational TA providing technical support to graduate students (PHYS 568)

Chevron Lubricants Lanka PLC **Colombo, Sri Lanka**

API certified Inspector for Pressure Relieving Devices (consulting) *Mar 2019 - June 2019*

- Conducted certified inspections, testing, and certification of Pressure Safety Valves (PSVs) and Pressure Relief Valves (PRVs) at processing facilities.
- Advised on maintenance and testing protocols while overseeing the plant performance and safety.
- Supervision of establishing maintenance SOPs and regulatory testing to ensure compliance with API 510 standards.

University of Moratuwa **Colombo, Sri Lanka**

Graduate Research/Teaching Assistant *Jan 2019 – Dec 2019*

- Modeled the molecular behavior of glass-metal specimens using classical simulation tools (LAMMPS, VMD), contributing to deeper insights into metallic glass properties using hybrid forcefields.
- Performed AFM pico-indentation experiments on amorphous specimens in contact mode to evaluate force/displacement responses and assess mechanical characteristics and verify computational models.

Undergraduate Research *Jan 2018 – Dec 2018*

- Designed and implemented a custom stress applicator setup and corrosion chamber for highly corrosive environment simulations and conducted exposure tests on carbon steel in corrosive $H_2S_{(aq)}$ conditions.
- Analyzed the depletion of load-carrying capabilities in sheet metal by performing microstructural analysis of corrosion layer development using SEM/EDS.
- Developed a predictive model for the degradation of pipeline steel's load-bearing capacity in highly corrosive (wet sour) environments. Published research work in the journal Engineer (Sri Lanka).

Camso Loadstar (Pvt) Ltd. (Wheel Manufacturing Div.) - Michelin **Ja-Ela, Sri Lanka**

Trainee Engineer *June 2017 - Dec 2017*

- Inspected incoming raw materials including steel plates and welding materials, while monitoring warehousing procedures.
- Evaluated weldments for wheels and wheel components to ensure quality standards were met.
- Conducted secondary quality assurance using sample preparation, light microscopy (LM), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX)

- Performed nondestructive testing (NDT) techniques (PT, UT, RT) and documented reports on failed wheel components/assemblies pre- and post-production.
- Responsible for failure analysis on wheels and assemblies from customer returns, providing detailed reports to management and engineering divisions.

Industrial Gases (Pvt) Ltd. **Colombo, Sri Lanka**

Internship *July 2015 – Aug 2015*

- Worked in gas production and bottling for N_2, O_2, and C_2H_2, ensuring efficient processing and quality output.
- Processed orders, loaded shipments, and inspected returned gas cylinders while supporting maintenance tasks.
- Supported the installation of a new N_2 storage terminal at Ceylon Breweries, boosting operations and distribution.

PUBLICATIONS

Journal Articles (links)

1. **Polyvinylidene Fluoride (PVDF)–Trimethylaluminum (TMA) Chemistry: First-Principles Investigation and Experimental Insights**
   M. D. Hashan C. Peiris, Heran Huang, Hao Liu, and Manuel Smeu. ACS *Applied Materials & Interfaces* **17.3** (2025), pp. 4744–4753
2. **More isn't Always Better: When the Number of Anchor Groups Does Not Improve Charge Transport**
   Dylan Dyer, Kevin Batzinger, **Peiris, M. D. Hashan C.**, Rashmi Yohani Amarakoon Arachchige, Tarek H. El-Assaad, Sam LaMotte, Dominic V. McGrath, Manuel Smeu, and Oliver L. A. Monti (2024). *Under Revision.*
3. **High-Pressure Nitrous Oxide Reduction by an Atomically Precise Cu(II) Carbon Nitride Electrocatalyst**
   Krista M. Kulesa, Eric S. Wiedner, **Peiris, M.D. Hashan C.**, Manuel Quiroz, Patrick Crossland, Yaroslav Losovyj, John Anderson, Manuel Smeu, Lane A. Baker, and Jeremy M. Smith (2024). *Submitted to JACS.*
4. **Interfacial Chemistry of Ni-rich Cathodes: Electrolyte Reactivity, Oxygen States, and Degradation Mechanisms**
   Peiris, M. D. Hashan C., D. Liepinya, Hao Liu, and Manuel Smeu. *Cell Reports Physical Science* **5** (2024), p. 13.
5. **Computational determination of the solvation structure of $LiBF_4$ and $LiPF_6$ salts in battery electrolytes**
   Peiris, M. D. Hashan C., Scott Brennan, Diana Liepinya, Hao Liu, and Manuel Smeu. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* (2023), p. 131831
6. **Study of the Effect of Sulphide Stress Corrosion on the Load Bearing Capability of API 5L Grade B Steel used in Petroleum Pipelines**
   Peiris, M. D. Hashan C., W. L. Perera, and G. I. P. De Silva. *Engineer: Journal of the Institution of Engineers*, Sri Lanka **53.2** (2020), p. 13

Conference proceedings (select)

1. **APS Global Physics Summit 2025, M.D. Hashan C. Peiris** and Manuel Smeu, Molecular dynamics insights into Ca-based salts in organic electrolyte, *Anaheim, CA*, 2025 [Link].
2. **APS Global Physics Summit 2025, M.D. Hashan C. Peiris** and Manuel Smeu, Application of machine learning to accelerate materials research and discovery, *Anaheim, CA*, 2025 [Link].
3. **MRS Symposium 2024, M.D. Hashan C. Peiris** and Manuel Smeu, Computational determination of the solvation structure of $LiBF_4$ and $LiPF_6$ salts in battery electrolytes, *Binghamton, NY*, 2024.
4. **MRS Spring Meeting 2024, M.D. Hashan C. Peiris** and Manuel Smeu, First Principles Investigation into The Dynamics at Ca Anodes and Electrolyte Interfaces (***Invited***), *Seattle, WA*, 2024 [Link].
5. **APS March Meeting 2024, M.D. Hashan C. Peiris** and Manuel Smeu, First Principles Investigation of Stability, Structure Properties of Sn-Bi Based Alloys, *Minneapolis, MN*, 2024 [Link].
6. **APS March Meeting 2024, M.D. Hashan C. Peiris** and Manuel Smeu, Polyvinylidene fluoride (PVDF)-Trimethyl Aluminum (TMA) Chemistry: First-principles Investigation and Experimental Insights, *Minneapolis, MN*, 2024 [Link].
7. **APS March Meeting 2023, M.D. Hashan C. Peiris** and Manuel Smeu, First-principles investigation of Al2O3 cathode coatings on Co and Ni-rich cathodes, *Las Vegas, NV*, 2023 [Link].
8. **ACS Northeast Regional Meeting, M.D. Hashan C. Peiris** and Manuel Smeu, First principles-based study of the interactions of cathode materials with organic electrolytes, *Rochester, NY*, 2022 [Link].

HONORS & AWARDS

2020	***Ph.D. Scholarship**, Awarded a fully funded scholarship for Ph.D. studies in MSE*	*BU, NY*
2018	***D. Samson Rajapaksa Memorial Award**, MSE graduate with the highest final GPA.*	*UoM, SL*
2016	***Lanka Ceramic Limited Award** , MSE Student with the highest GPA at Semester 5 - 4.05/4.2*	*UoM, SL*

WORKSHOPS

Mar 2024	***APS Data Science for Physicists** I-II, - Data science in research, data analysis/visualization, CNN*	*Minneapolis*
Mar 2024	***LOBSTER School**, Applying crystal orbital Hamilton population (COHP) analysis using LOBSTER.*	*Helsinki*
Nov 2023	***Moving ions with VASP**, AIMD, ML force fields, phonons, and HPC topics.*	*Online*
Aug 2020	***Atomistic Simulations for Industrial Needs**, Applying atomistic simulations for industrial R&D, interatomic potential development, ML/AI integration, model coupling, and resource accessibility.*	*Online*

MENTORING & LEADERSHIP

Mentored undergrad/grad students

- Mentored an undergraduate student in conducting computational research during their summer research internship.
- Guidance to a graduate student on aligning their experimental research with computational work.

- Mentoring undergraduate and graduate students at the University of Moratuwa, inspiring junior researchers to pursue advanced research in materials science.

Society of Materials Engineering Students (SOMES - UoM) *Volunteer*

- Mentored high school students at a remote and disadvantaged public school in SL by providing academic support.

ADDITIONAL INFORMATION

Languages: Full proficiency in English and Sinhala, basic proficiency in Spanish

Three-year permit to work in the USA under STEM-OPT work authorization; eligible to self-petition for National Interest Waiver (NIW) application to obtain permanent residency beyond that timeframe.