Hashan Peiris

PhD Candidate, Materials Science | Researcher (Computational & Experimental) | MBA
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ACCOMPLISHMENTS

- **Research**: Led studies (DFT, AIMD, and ML with experimental backing) on electrode-electrolyte interfaces, chemical degradation, solvation, catalytic frameworks, and solder stability, leading to publications in high-impact journals.
- **Cross-Disciplinary Collaboration:** Bridged experimental and computational efforts to advance bulk and interface chemistry and degradation of materials studies.
- **High-Performance Computing:** Deployed and optimized compute nodes; managed VASP, Quantum Espresso, DeePMD, and USPEX to accelerate simulations.
- **Funding & Grants:** Secured 40M+ compute hours and funding via proposals to NSF, IEEC, SRC, and XSEDE/ACCESS
- **Academic Excellence & Recognition**: Received a First-class in BSc Eng., fully funded PhD, and multiple awards.
- **Mentoring & Teaching**: Guided undergraduate/graduate research and served as Graduate Teaching Assistant.

EDUCATION

Binghamton University, State University of New York — **New York**
Ph.D. Candidate in Materials Science & Engineering — *Spring 2026*
Advisor: Prof. 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: Prof. 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 — *Dec 2022 - Present*

- **Modeling of the chemical activity on Ni/Co-rich interfaces and oxide coatings of NMC-811 cathodes**
  - Initial findings published in *Cell Reports* and in *Colloids and Surfaces* on $LiNiO_2$ surface degradation.
  - Published research on chemo-mechanical properties of oxide coatings on Co-rich cathode surfaces.
  - Developed an ML accelerated interatomic potential to simulate Ca-based solvation dynamics in electrolytes.
- **Investigation of thermo-mechanical stability of Sn-based soldering alloys using DFT/ML-based approaches.**
  - Findings published in conferences (APS, EPS) and submitted IEEC and SRC proposals for funding. Ongoing work.
- **Collaborated** on multiple interdisciplinary computational research projects, including:
  - ***LabMonti*, Arizona State University** - Break junction simulations of Au electrodes in single-molecule junctions using AIMD/DFT and ML to elucidate the junction dynamics and electronic transport. Manuscript submitted to *Chem. Eur. J.*
  - **Liu Group, Binghamton University** - Degradation mechanisms of PFAS chemicals (PVDF) in TMA used in ALD-based coatings on NMC cathodes in Li-ion batteries. Findings published in ACS *Applied Interfaces & Materials.*
  - **Indiana University/PNNL** - 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 revision.
  - **Tohoku University, Japan** - Diffusion mechanism of Ca/Mg intercalant in MoO_3 cathodes for novel batteries.
- **Provisioning, installation of high-performance compute nodes and integration** into *Spiedie* compute cluster at BU.
- **Compilation and optimization of compute code** (VASP, Linux VM, QE, DeePMD, USPEX etc. on CPU/GPUs) as required.
- **Authored successful annual grant proposals to secure funding and computational resources**, obtaining support from funding agencies (NSF, IEEC, SRC) and XSEDE/ACCESS for compute (40M+ compute from 2020-2026).

Graduate Teaching Assistant — *January 2020 - Dec 2022*

- Deliver lab and discussion-based teaching, managed experiments, and supported student learning in Physics courses.
- 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*

- Responsible for the inspections, testing, and certification of Pressure Safety/Relief Valves (PSV/PRV).
- Supervision of the updated SOPs and regulatory testing to ensure compliance with the newer API-510 standard.

University of Moratuwa — **Colombo, Sri Lanka**

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

- Developed a model to corelate AFM pico-indentation on amorphous high entropy alloys (HEAs) specimens (contact) to evaluate F/d response, assess mechanical characteristics and verify using computational models (MD; LAMMPS).

Undergraduate Research — *Jan 2018 – Dec 2018*

- Design & fabricating a setup for accelerated wet-sour corrosion ($H_2S_{(aq)}$), exposure testing on carbon steel, FEA, and microstructural analysis using SEM/EDS/XRD to model time-corrosion based failure. Published research in the *Engineer*.

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

Trainee Engineer — *June 2017 - Dec 2017*

- Trained in QA/QC incoming raw materials including steel plates and welding materials, secondary inspections.
- Conducted secondary quality assurance on weldments using microscopy (LM/SEM), and X-ray spectroscopy (XRD/EDX)
- Performed nondestructive testing (NDT) evaluation (PT, UT, RT), FEA, and documentation on wheel failures pre/post-production.

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, trained in product processing and TQM.

PUBLICATIONS

Journal Articles

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. **When Dihedral Angles Mask Denticity in Molecular Conductance** Dylan D, Kevin B, **Peiris, M. D. Hashan C.**, Rashmi A.A, Tarek H. El-A, Sam L., Dominic V.M., Manuel S, and Oliver L. A. M (2025). *Accepted for publication in PCCP.*
3. **High-Pressure Nitrous Oxide Reduction by an Atomically Precise Cu(II) Carbon Nitride Electrocatalyst** Krista M. K, Eric S. W, **Peiris, M.D. Hashan C.**, Manuel Q, Patrick C, Yaroslav L, John A, Manuel S, Lane A. B, and Jeremy M. S (2025). *Submitted to JACS, being revised.*
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. **American Physicists Society (APS) - Global Physics Summit/March Meeting,**
   - **2025 – [Oral]** Molecular dynamics insights into Ca-based salts in organic electrolyte, *Anaheim, CA*, [Link].
   - **2025 – [Poster]** Application of machine learning to accelerate materials research and discovery, *Anaheim, CA*, [Link].
   - **2024 – [Oral]** PVDF-TMA Chemistry: First-principles investigation and experimental insights, *Minneapolis, MN*, **[Link].**
   - **2024 – [Poster]** Stability and structural properties of Sn-Bi based alloys, *Minneapolis, MN*, [Link].
   - **2023 – [Oral]** First-principles investigation of Al_2O_3 cathode coatings on Co and Ni-rich cathodes, *Las Vegas, NV*, 2023 [Link].
2. **Materials Research Society (MRS)**
   - **Spring 2024 [Oral]** First Principles investigation into dynamics at Ca Anodes and electrolyte interfaces (***Invited***), *Seattle, WA*, 2024 [Link].
   - **Fall 2024** Solvation structure of $LiBF_4$ and $LiPF_6$ salts in battery electrolytes, *Binghamton, NY*, 2024.
3. **ACS Northeast Regional Meeting (NERM) 2022** 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 (select)

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, IPs, ML/AI integration, model coupling, and resource accessibility.*	*Online*

MENTORING & LEADERSHIP

- Mentored undergraduates in conducting computational research during their summer research internship (REU-2022/2024/2025).
- **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.

SKILLS

Programming & Tools	**Python, PyTorch, TensorFlow, Visual Basic, Git, Bash, LaTeX, HPC hardware and utilities**
Software	**VASP, DeePMD, USPEX, Quantum Espresso, LAMMPS, Orca** **VSCode, Linux, SolidWorks, Abaqus, Ansys, 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** • **Effective scientific communication with talks and presentations** • **Effective collaborations with local and remote teams** • **Managing multiple projects and working independently.**

ADDITIONAL INFORMATION

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