

# Uthpala Herath, Ph.D.

POSTDOCTORAL ASSOCIATE · COMPUTATIONAL MATERIALS SCIENTIST

Department of Mechanical Engineering and Materials Science, Duke University

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## Summary

Innovative and results-driven Computational Materials Scientist with a Ph.D. in Physics, specializing in high-performance computing applications for advanced materials research. Proven leadership in pioneering methodologies and collaborative endeavors aimed at driving technological advancements and sustainability. Eager to leverage extensive analytical, problem-solving, and leadership capabilities to foster transformative growth and sustainable practices within a forward-thinking environment.

## Education

### PhD in Physics

Department of Physics and Astronomy, West Virginia University

Morgantown, WV

2015 - 2022

**Awards:** APS Ovshinsky Award, Robert T. Bruhn Physics Research Award, Office of the Provost Graduate Student Award, Eberly College of Arts and Sciences Graduate Student Award

### BSc in Physics

Department of Physics, University of Peradeniya

Peradeniya, Sri Lanka

2010 - 2014

**Positions held:** President of the Astronomy Society, Editor of the Physics Society, Faculty Representative of the Ceylon Drama Society

## Work Experience

### Department of Mechanical Engineering and Materials Science, Duke University

Durham, NC

Postdoctoral Associate (Computational Materials Science)

May 2022 - Current

- Led integration of relativistic spin-orbit coupling in the DFT code, FHI-aims, enhancing semiconductor and renewable energy materials research.
- Developed a novel method, in collaboration with experimentalists to detect superfluorescence, facilitating advanced studies in quantum optics and nano-medicine, culminating in a high-impact submission to Nature Photonics.
- Spearheaded a global effort to enhance FHI-aims and ELSI (high-performance eigen-value solver library) usability, including the implementation of a CI pipeline utilizing Docker.
- Organized the FHI-aims Developers' and Users' Meeting in Hamburg, Germany, fostering collaboration and knowledge exchange.
- Secured a collaborative grant worth over \$125,000 on the NSF-funded TACC Frontera supercomputer, underlining grant writing and project management skills.

### Department of Physics and Astronomy, West Virginia University

Morgantown, WV

Graduate Research Assistant (Computational Condensed Matter Physics)

2017 - 2022

- Developed the DMFTwDFT framework, significantly advancing the study of strongly correlated materials. Maintained a code repository with 65+ stars and 15+ forks and a user forum with 35+ global users, with a publication cited 20+ times.
- Led research on oxygen vacancies in rare-earth nickelate perovskites, with implications for neuromorphic computing.
- Pioneered techniques to investigate alloying/defects in strongly correlated materials, significantly improving computational resource efficiency.
- Mentored a postdoc and multiple graduate students, demonstrating a commitment to developing the next generation of scientists.
- Developed the electronic structure pre/post-processing tool PyProcar, maintaining a code repository with 160+ stars, 70+ forks, and a global user forum of 260+ users, with a publication cited 230+ times.
- Developed MechElastic, an open-source Python library for calculating elastic properties of materials, maintaining a repository with 40+ stars, 20+ forks, and a user forum of 45+ global users, with a publication cited 60+ times.
- Secured interdisciplinary research grants from DOE-EPSCOR and NSF-funded XSEDE supercomputers amounting to over \$350,000, showcasing collaborative grant writing expertise and the ability to secure funding for cutting-edge research projects.

Graduate Teaching Assistant

2015 - 2017

- Led a graduate-level quantum mechanics course, showcasing the capability to make complex subjects accessible and comprehensible.
- Conducted lab sessions and office hours on electrostatics, electromagnetism and optics for STEM students receiving recognition as a highly effective TA.

## Leadership and Volunteering Experience

- Organized and led events bringing postdocs from different backgrounds together fostering interdisciplinary research collaborations as a council member of the Duke University Postdoctoral Association (DUPA).
- Volunteered with the Physics and Astronomy Graduate Students' Organization (PAGSO) at WVU in outreach programs enhancing public literacy in science across the state, demonstrating skills in public communication, educational outreach, and community service.
- Organized a vigil at WVU in memory of the Easter Sunday attack victims in Sri Lanka building inter-faith cohesion.
- Led the charity program, *Let Them Smile*, improving the education of under-privileged students in rural schools across Sri Lanka.
- Conducted lectures, planetary observation sessions and workshops to promote science and astronomy in Sri Lanka.
- Developed a computational framework to diagnose plant disease and treatment in collaboration with the Sri Lanka Department of Agriculture improving crop production.

## Skills and Interests

<b>Method development</b>	Development and application of MD, DFT, GWA and DMFT frameworks for advanced materials research
<b>Version control/build systems</b>	Git, Gitlab CI, Travis CI, Docker, Apptainer, CMake, CTest and Unit testing
<b>Programming environments</b>	Python, Matlab, Fortran, C/C++, Bash, Java, SQL, MongoDB, GPU programming (CUDA), HPC, MPI and Linux
<b>Grant writing</b>	Secured grants exceeding \$475,000 across multiple funding agencies including NSF and DOE
<b>Languages</b>	English (native or bilingual proficiency), Sinhala (native or bilingual proficiency), Tamil (elementary proficiency)
<b>Interests</b>	Camping, backpacking, reading, exploring new cities and joining various Meetup groups to expand networks