

# 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

**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

Morgantown, WV

Aug, 2015 - May, 2022

### BSc in Physics

Department of Physics, University of Peradeniya

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

Peradeniya, Sri Lanka

Jul, 2010 - Dec, 2014

## Work Experience

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

Postdoctoral Associate (Computational Materials Science)

Durham, NC

May, 2022 - Present

- Contributed to the advancement of materials science databases and frameworks, including HybriD<sup>3</sup>, MatD<sup>3</sup>, and Springer Materials.
- 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 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

Graduate Research Assistant (Computational Condensed Matter Physics)

Morgantown, WV

Aug, 2017 - May, 2022

- Developed the DMFTwDFT framework, significantly advancing the study of strongly correlated materials. Maintained a code repository and a user forum with 35+ global users, with a publication cited 25+ times.
- Led research on oxygen vacancies in rare-earth nickelate perovskites, with implications for neuromorphic computing and micro-electronics.
- Pioneered techniques to investigate alloying/defects in strongly correlated materials, significantly improving computational resource efficiency.
- Mentored a postdoc and 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 and a global user forum of 290+ users, with a publication cited 270+ times.
- Developed MechElastic, an open-source Python library for calculating elastic properties of materials, maintaining a repository and a user forum of 45+ global users, with a publication cited 85+ 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

Aug, 2015 - May, 2017

- Taught 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

**Method development**  
**Version control/build systems**  
**Programming environments**  
**Grant writing**  
**Languages**  
**Interests**

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