

Uthpala Herath, Ph.D.

POSTDOCTORAL ASSOCIATE · COMPUTATIONAL PHYSICIST

Department of Mechanical Engineering and Materials Science, Duke University

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Summary

Innovative computational physicist with **9 years** of experience leveraging high-performance computing for advanced materials research. Specializes in the development and application of frameworks utilizing beyond-DFT Green's Functions methods to design, characterize, and advance novel materials critical to semiconductors, spintronics, neuromorphic computing, optics, photovoltaics, and energy applications. Proven leader and mentor in pioneering collaborative projects, securing over **\$1.1 million** in grants and developing open-source tools with **430+ citations** and **350+ global users**. Dedicated to applying advanced computational, problem-solving, and leadership skills to spearhead transformative projects in materials research and beyond.

Education

Ph.D. in Computational Condensed Matter Physics

Department of Physics and Astronomy, West Virginia University

Morgantown, WV

Aug, 2017 - May, 2022

Dissertation: "Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives"

M.Sc. in Computational Condensed Matter Physics

Department of Physics and Astronomy, West Virginia University

Morgantown, WV

Aug, 2015 - Aug, 2017

B.Sc. in Physics

Department of Physics, University of Peradeniya

Peradeniya, Sri Lanka

Jul, 2010 - Dec, 2014

Research experience

Department of Mechanical Engineering and Materials Science, Duke University

Durham, NC

Postdoctoral Associate - Blum Group (Computational Materials Science)

May, 2022 - Present

- Improved the functionality and features of materials science databases and frameworks; HybriD³, MatD³, and Springer Materials.
- Led the integration of relativistic spin-orbit coupling to periodic GWA in the DFT code, FHI-aims, enhancing the exploration of semiconductor and renewable energy materials with heavy elements.
- Developed a novel Δ -SCF method, in collaboration with experimentalists to detect superfluorescence, facilitating advanced studies in quantum optics and nano-medicine.
- Spearheaded a global effort to enhance FHI-aims and ELSI usability, including the implementation of a CI pipeline utilizing Docker and integrating cutting-edge eigen solvers and density matrix solvers.

Department of Physics and Astronomy, West Virginia University

Morgantown, WV

Graduate Research Assistant - Romero Group (Computational Condensed Matter Physics)

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 30+ 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.
- 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 100+ times.
- Developed MDWC; a command line open-source Python program for constrained molecular dynamics simulations and PyChemia; an open-source Python library for materials structural search through debugging, simulation, and testing.

Department of Physics and Astronomy, West Virginia University

Morgantown, WV

Graduate Research Assistant - Tu Group (Computational Space Physics)

Jan, 2016 - May, 2017

- Performed test particle simulations to quantify the effect of magnetic field line curvature scattering on the rapid loss of ring current ions in Earth's magnetosphere.
- Received hands-on development experience with a C, C++ based in-house particle tracer code.

Arthur C. Clarke Institute for Modern Technologies

Moratuwa, Sri Lanka

Intern (Space Applications Division) | Advisors: Mr. S. Gunasekara, Dr. T. Ranawake

Jan, 2014 - Dec, 2014

- Worked in conjunction with an expert team of scientists at the Space Applications division of ACCIMT to perform an extensive study of globular cluster characteristics using CCD Aperture Photometry and PSF (Point Spread Function) Fitting Photometry methods with the IRAF (Image Reduction and Analysis Facility) system to map Blue Stragglers stars in the globular cluster M53.
- Utilized telescopic data of the globular cluster M53 to construct a novel Color-Magnitude Diagram (CMD) of the cluster.

Department of Physics, University of Peradeniya

Peradeniya, Sri Lanka

Undergraduate Research Student | Advisor: Prof. P. Samarasekara

Jan, 2013 - Dec, 2013

- Investigated the traits, synthesis methods, functionalization and applications of Nano Magnets.

Leadership & outreach

Council Member - Duke University Postdoc Association (DUPA)

Jul, 2022 - Present

- Organized and led events bringing postdocs from different backgrounds together fostering interdisciplinary research collaborations.

Organizer - FHI-aims Developers' and Users' Meeting

Aug 2, 2023 - Aug 4, 2023

- Served in the organizing committee of the FHI-aims Developers' and Users' Meeting in Hamburg, Germany.
- This leadership position underscored the commitment to fostering a vibrant community of developers and users, enhancing collaboration and knowledge exchange.

Outreach Volunteer - Physics and Astronomy Graduate Student Organization (PAGSO), WVU

Aug, 2015 - May, 2022

- Volunteered in physics outreach programs enhancing public literacy in science across West Virginia, demonstrating skills in public communication, educational outreach, and community service.

Coordinator - Condensed Matter Seminar, Department of Physics and Astronomy, WVU

May, 2018 - May, 2022

- Coordinated weekly seminar sessions bridging sub-disciplines within the condensed matter research community.

Member - Sri Lankan Student's Organization (SLSA), WVU

Jan, 2018 - May, 2022

- Planned events to share Sri Lankan cultural and heritage experience with the rest of the university.
- Organized a vigil in memory of the Easter Sunday terrorist attack victims in Sri Lanka building inter-faith cohesion.

President - Astronomy Society of University of Peradeniya

Jan, 2014 - Dec, 2014

- Organized "Water Rocket Challenge 2014"; the first-ever water rocket competition held at University of Peradeniya.
- Conducted lectures, planetary observation sessions and workshops to promote science and astronomy in Sri Lanka.
- Volunteered for United Nations World Space Week through public outreach programs.

Junior Editor - Physical Society of University of Peradeniya

Jan, 2013 - Dec, 2013

- Compiled academic articles for the scientific journal "Echo" issued by the society.

Faculty Representative - The Ceylon Drama Society of University of Peradeniya

Jan, 2012 - Dec, 2012

- Organized drama competitions engaging students from various backgrounds.

Volunteer - Let Them Smile

Aug, 2010 - Dec, 2014

- Led charity programs focused on improving the education of under-privileged students in rural schools across Sri Lanka.

Volunteer Software Developer - Department of Agriculture, Sri Lanka

Jan, 2010 - Dec, 2010

- Developed a computational framework to diagnose plant disease and treatment in collaboration with the Sri Lanka Department of Agriculture improving crop production.

Teaching & mentorship

Postdoctoral Associate (Duke University)

May, 2022 - Present

- Mentored graduate and undergraduate students on the usage of electronic structure calculations and computational tools for advanced materials research.
- ME 511** - Developed computational modules and provided assistance to students for the graduate level *Computational Materials Science* course.

Graduate Teaching Assistant/ Research Assistant (West Virginia University)

Aug, 2015 - May, 2022

- Mentored a postdoc and multiple graduate students in condensed matter physics research, demonstrating a commitment to developing the next generation of scientists.
- PHYS 651, PHYS 652** - Substitute lecturer for graduate-level quantum mechanics courses.
- PHYS 112** - Conducted lab sessions and office hours for electrostatics, electromagnetism, and optics for STEM students receiving recognition as a highly effective TA.
- ASTR 106** - Graded homework and exams for an undergraduate introductory astronomy course.

Graduate Teaching Assistant (University of Peradeniya)

Dec, 2014 - May, 2015

- Conducted physics lab and tutorial sessions for STEM undergraduate students. Graded exams and homework.

Skills

First principles (ab-initio) electronic structure calculations

- Expertise in developing and applying electronic structure codes including *FHI-aims*, *VASP*, *Siesta*, *Abinit*, *Elk*, *Quantum Espresso* for Density Functional Theory (DFT), DFT+U, Hybrid functionals, GWA, and DMFT calculations
- Skilled in the analysis of electronic, vibrational, magnetic, mechanical, elastic, thermal and optical properties of bulk/2D material and heterostructures
- Advanced proficiency in studying strongly correlated materials using DMFT

Development and application of materials research methods and tools

- DMFTwDFT, ELSI, Wannier90, Impurity Solvers and QMC methods, Tightbinding Hamiltonians, Phonopy
- Materials discovery and analysis (PyProcar, PyChemia, MechElastic, Pymatgen, AFLOW, Atomate2)
- Transition state and diffusion analysis (VTST Tools, DiSPy, Nudged Elastic Band (NEB) method)
- Molecular dynamics simulations (MDWC, VMD, Jmol, qAgate)
- Graphical visualization (VESTA, gnuplot, Xmgrace, xcrysden)
- Vacancy, defect and alloying methods (Virtual Crystal Approximation (VCA), Coherent Potential Approximation (CPA), Site Occupation Disorder (SOD), SPRKKR)

Programming environments

- Python, Matlab, Fortran, C/C++, Bash, Java, SQL, MongoDB, Django, GPU programming (CUDA)

Computational methodologies

- Linux/Unix systems, High-Performance Computing (HPC) experience with major supercomputing clusters (TACC, PSC, NERSC), High-Throughput Computing (HTC), Parallel computing (OpenMP and MPI), Regression analysis, Differential solvers and integrators, Numerical analysis algorithms, Object-oriented and procedural programming paradigms, Scientific libraries (LAPACK, BLAS, SCALAPACK, FFTW, GSL)

Version control, CI and build systems

- Git, Gitlab CI, Travis CI, Docker, Apptainer, CMake, CTest and Unit testing

Graphics and Publishing

- Latex, Markdown, Zotero, Adobe Creative Suite (Photoshop, Premiere, After Effects, Illustrator), Microsoft Office

Soft skills

- Demonstrated abilities in creative problem solving, leadership, organization, communication, teamwork, flexibility, networking, time and resource management, and mentorship

Languages

- English (Native or bilingual proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)

Publications

1. Bhat, S. S., Singh, V., Herath, U., Varughese, B., Sankaranarayanan, S. K. R. S., Park, H., & Romero, A. H. Dynamical correlations leading to site and orbital selective Mott insulator transition in hydrogen doped **SmNiO₃**. *Phys. Rev. B* **109**.20, 205124 (May 2024).
2. Lang, L., Tavadze, P., Tellez, A., Bousquet, E., Xu, H., Muñoz, F., Vasquez, N., Herath, U., & Romero, A. H. Expanding PyProcar for new features, maintainability, and reliability. *Computer Physics Communications* **297**, 109063 (2024).
3. Singh, S., Lang, L., Dovale-Farelo, V., Herath, U., Tavadze, P., Coudert, F.-X., & Romero, A. H. MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. *Computer Physics Communications* **267**, 108068 (2021).
4. Singh, V., Herath, U., Wah, B., Liao, X., Romero, A. H., & Park, H. DMFTwDFT: An open-source code combining Dynamical Mean Field Theory with various density functional theory packages. *Computer Physics Communications* **261**, 107778 (2021).
5. Herath, U., Tavadze, P., He, X., Bousquet, E., Singh, S., Muñoz, F., & Romero, A. H. PyProcar: A Python library for electronic structure pre/post-processing. *Computer Physics Communications* **251**, 107080 (2020).

SUBMITTED

1. Biliriglu, M., Seyitliyev, D., Kotyrov, M., Abdelsamei, M., Qin, X., Findik, G., Alma, G. A., Herath, U., Lei, L., Chai, J., Mehta, Y., Swan, A., Temnov, V., Blum, V., So, F., & Gundogdu, K. Two-Step Phase Transition in Superfluorescence of Lead-Halide Perovskites. *Submitted to Nature* (2023).

IN PREPARATION

1. Herath, U., Singh, V., Bhat, S. S., Park, H., & Romero, A. H. Stability and diffusion of oxygen vacancies in LaNiO₃: a DMFT study. *arXiv* (2022).
2. Herath, U., Bhat, S., Singh, V., Park, H., & Romero, A. H. Investigating strongly correlated alloys via Dynamical Mean Field Theory.

Selected presentations

1. HybriD³: A Collaborative Platform for Curating Hybrid Perovskite Data. *Duke, NCSU, UNC DMREF Collaboration Meeting, Raleigh, NC. November 6, 2024 (INVITED VIRTUAL TALK)*
2. Database for Hybrid Perovskites: HybriD³. *NREL CHOICE Meeting, Golden, CO. November 1, 2024 (INVITED VIRTUAL TALK)*
3. A tutorial on PyProcar: A Python library for electronic structure pre/post-processing. *Rutgers University, Piscataway, NJ. June 25, 2021 (INVITED VIRTUAL TALK)*
4. Recent Developments in PyProcar: A Python library for electronic structure pre/post-processing. *APS March Meeting. March 15-19, 2021 (VIRTUAL TALK)*
5. DMFTwDFT: An open-source code combining Dynamical Mean Field Theory with various Density Functional Theory packages. *APS Mid Atlantic Section Meeting. December 4-6, 2020 (VIRTUAL TALK)*
6. PyProcar: A Python library for electronic structure pre/post-processing. *Carolina Science Symposium, University of California, Merced. November 12-13, 2020 (VIRTUAL TALK)*
7. An ab-initio DFT+DMFT study of the effect of oxygen vacancies on structural, electronic and magnetic properties of rare-earth nickelate perovskites (RNiO₃). *APS March Meeting, Boston, MA. March 4-8, 2019 (TALK)*
8. Development of computational methods for the characterization of novel strongly correlated materials. *International Summer School on Computational Quantum Materials, Sherbrooke, Québec, Canada. May 27-June 8, 2018 (POSTER)*
9. The Effect of Magnetic Field Line Curvature Scattering on the Rapid Loss of Ring Current Ions. *Geospace Environment Modeling (GEM) conference, Portsmouth, VA. July 2017 (POSTER)*

Fellowships, Grants & Awards

FELLOWSHIPS

ORISE Fellowship

May, 2024 - May, 2025

- STEM fellowship awarded by Oak Ridge National Lab (ORNL) and US Department of Energy (DOE) to conduct materials research in collaboration with the National Energy Technology Laboratory (NETL).

Award: \$3,451.50 per month

GRANTS

NSF TACC Frontera Pathways - *Research and development of methods for many-body electronic structure theory and applications in FHI-aims*

Dec, 2023 - Dec, 2025

Role: PI

Grant ID: DMR23007

Award: \$64,060.65 (140,557 node-hours on Frontera)

NSF ACCESS Explore - *Benchmarking for “Effect of Molecular Motions on Structural Asymmetry and Electron Spin in 2D Hybrid Halide Perovskites”*

Jan, 2024 - Jan, 2025

Role: Co-PI

Grant ID: CHE240003

Award: \$4456.43 (200,000 ACCESS credits)

NSF XSEDE - *Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives*

2018 - 2023

Role: Lead contributor (Coordinated a team of graduate students at WVU to secure annual allocations of grant)

Grant ID: DMR140031

Award: \$352,243 (21,636,694 core-hours on Bridges2 and 374,942 node-hours on Stampede2)

DOE EPSCOR - *Applications of Nickelate perovskites for neuromorphic computing from electronic structure and Machine Learning*

Sep, 2020 - Aug, 2024

Role: Lead contributor

Grant ID: DOE DE-SC0021375

Award: \$690,000

AWARDS

Ovshinsky Travel Award

2021

- Awarded by the American Physical Society to fund registration for the APS March Meeting.

Robert T. Bruhn Physics Research Award

2020

- Awarded by the Department of Physics and Astronomy, West Virginia University to extend support to the research effort of a graduate or undergraduate student in the department in nanotechnology and material science.

Office of the Provost Graduate Student Travel Award

2018, 2019

- Awarded by the Office of the Provost, West Virginia University to fund travel to research conferences.

Eberly College of Arts and Sciences Graduate Student Travel Award

2018, 2019

- Awarded by the Eberly College of Arts and Sciences, West Virginia University to fund travel to research conferences.

Referee contributions

- Served as a peer-reviewer for the *Computer Physics Communications* journal (2022).
- Volunteered as a judge at the Virtual Summer Undergraduate Research Symposium organized by the Office of Undergraduate Research in the Mathematics and Physics Category at WVU (July, 2020).

Training & certifications

OITE Management Short Course

Jun, 2024

- Conducted by the National Institute of Environmental Health Sciences (NIEHS)

Responsible Conduct of Research - Staff - BASIC

Jul, 2022 - Jul, 2025

- Issued by the CITI program and completed through Duke RCR