Uthpala Herath, Ph.D.

Computational Physicist · Postdoctoral Associate

Department of Mechanical Engineering and Materials Science, Duke University

(304) 216-2535 | uthpala.herath@duke.edu | www.uthpalaherath.com | uthpalaherath | Google Scholar

Summary

Innovative computational physicist with **10 years** of experience leveraging high-performance computing for advanced materials research. Specializes in the development and application of frameworks utilizing beyond-DFT methods to design, characterize, and advance novel materials critical to semiconductors, spintronics, neuromorphic computing, electronics, optics, photovoltaics, and energy applications. Proven leader and mentor in pioneering collaborative projects, securing over **$1.1 million** in grants, publishing research recognized with **450+ citations**, and developing open-source tools adopted by **380+ 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 — *Morgantown, WV*

Department of Physics and Astronomy, West Virginia University — *Aug, 2015 - May, 2022*

Advisor: Dr. Aldo H. Romero

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 — *Morgantown, WV*

Department of Physics and Astronomy, West Virginia University — *Aug, 2015 - Aug, 2017*

B.Sc. in Physics — *Peradeniya, Sri Lanka*

Department of Physics, University of Peradeniya — *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*

- Enhanced materials science databases (`HybriD`^{3}, `MatD`^{3}, and Springer Materials) by refining critical features for improved functionality.
- Led the integration of relativistic spin-orbit coupling into periodic GWA within the DFT code, `FHI-aims` and conducted comprehensive GWA benchmarks exploring compound semiconductors and heavy-element materials for electronics and energy applications.
- Developed a novel Δ-SCF method in `FHI-aims` and `ELSI` to study high-temperature superfluorescence in collaboration with experimentalists, facilitating advanced research in quantum computing and optics.
- Coordinated a global initiative to enhance `FHI-aims` and `ELSI` usability through code development efforts, 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 open-source `DMFTwDFT` framework, significantly advancing the study of strongly correlated materials through the many-body Green's functions method, DMFT. Maintained a code repository and a user forum with 40+ global users, with a publication cited 30+ times.
- Led research on the effects of oxygen vacancies and hydrogen doping on metal-insulator transitions and diffusion in rare-earth nickelate perovskites, with implications for neuromorphic computing and microelectronics.
- Developed neural network-based interatomic potentials capturing DMFT-level accuracy for strongly correlated materials, enabling large-scale MD simulations across diverse time and length scales through the interface of `DMFTwDFT` and BLAST frameworks.
- Implemented a symmetry based method to investigate alloying/defects in strongly correlated materials with higher computational efficiency.
- Developed the open-source electronic structure pre/post-processing tool `PyProcar`, maintaining a code repository and a global user forum of 290+ users, with a publication cited 300+ times.
- Developed `MechElastic`, an open-source Python library for calculating elastic properties of materials, maintaining a repository and a user forum of 50+ global users, with a publication cited 100+ times.
- Developed `MDWC`; an 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*

- Developed and applied a C/C++ particle tracer code to perform 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.

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*

- Utilized telescopic data to construct a novel Color-Magnitude Diagram (CMD) of the globular cluster M53, mapping Blue Straggler stars using CCD Aperture Photometry and PSF (Point Spread Function) Fitting Photometry methods with the IRAF (Image Reduction and Analysis Facility) system.

Department of Physics, University of Peradeniya — *Peradeniya, Sri Lanka*

Undergraduate Research Student | Advisor: Dr. P. Samarasekara — *Jan, 2013 - Dec, 2013*

- Investigated the traits, synthesis methods, functionalization, and applications of nano-magnets.

Skills

First principles (*ab-initio*) electronic structure calculations

- Expertise in developing and applying electronic structure codes ***FHI-aims***, *VASP, Siesta, Abinit, Elk, and Quantum Espresso* for DFT, DFT+U, molecular dynamics, and many-body Green's functions methods (GWA, DMFT) for materials research
- Skilled in the analysis of electronic, structural, vibrational, magnetic, mechanical, thermal, and optical properties of multi-dimensional materials
- Proficient in studying properties of 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, workflows and analysis (**PyProcar**, **PyChemia**, **MechElastic**, Materials Project, Pymatgen, AFLOW, AiiDA, 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, matplotlib)
- Vacancy, defect and alloying methods (Virtual Crystal Approximation (VCA), Coherent Potential Approximation (CPA), Site Occupation Disorder (SOD))

Programming environments

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

Data science

- FAIR data management, data mining, regression analysis, data analysis
- Database management systems (SQL, MongoDB)
- Python libraries for data science (Numpy, SciPy, Pandas, NetworkX, regex)

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), 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

Languages

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

Teaching & mentorship

Postdoctoral Associate (Duke University) *May, 2022 - Present*

- Guided students in using HPC clusters for electronic structure calculations with the **FHI-aims** code while providing hands-on training with Python, Fortran, and Bash for advanced materials research.
- Led students in the design and implementation of the **HybriD**^{3} materials database and **MatD**^{3} framework.
- **ME511: Computational Materials Science** - Developed computational modules and assisted students with technical and physics-based questions.

Graduate Teaching Assistant/ Research Assistant (West Virginia University) *Aug, 2015 - May, 2022*

- Mentored a postdoc and graduate students in performing electronic structure calculations using the **DMFTwDFT**, **PyProcar**, **MechElastic** frameworks and DFT codes (VASP, Abinit, Siesta, Elk, and Quantum Espresso) on HPC clusters.
- **PHYS651, PHYS652: Quantum Mechanics I & II** - Served as the substitute lecturer to cover core topics in quantum mechanics through delivering lectures and leading class discussions.
- **PHYS112: General Physics 2** - Conducted lab sessions and office hours for this calculus-based physics course covering topics in electrostatics, magnetism, and optics receiving recognition as a highly effective TA.
- **ASTR106: Descriptive Astronomy** - Graded homework and exams for this introductory astronomy course.

Instructor (University of Peradeniya) *Dec, 2014 - May, 2015*

- **PH211: Vibrations and AC Theory** - Conducted office hours to assist enrolled students. Graded homework and exams.
- **PH230: Quantum Mechanics and Atomic Physics** - Delivered lectures and led class discussions.
- **PH280: General Physics Laboratory I** - Conducted physics lab and tutorial sessions. Graded homework and exams.

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 $SmNiO_3$. *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. Biliroglu, 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* (2024).

In preparation

1. Chakraborty, R., Herath, U., & Blum, V. HybriD^3: A Curated Materials Database for Hybrid Organic-Inorganic Semiconductors.
2. Zhang, M.-Y., Herath, U., Merz, F., Yao, Y., Rampp, M., Ren, X., Blum, V., & Scheffler, M. All-electron periodic GW method in numeric atom-centered basis framework: a thorough benchmark.
3. Herath, U., Singh, V., Bhat, S. S., Park, H., & Romero, A. H. Stability and diffusion of oxygen vacancies in $LaNiO_3$: a DMFT study. *arXiv*.
4. Herath, U., Bhat, S., Singh, V., Park, H., & Romero, A. H. Investigating strongly correlated alloys via Dynamical Mean Field Theory.

Selected presentations

1. HybriD^3: A Collaborative Platform for Curating Hybrid Perovskite Data. *Duke, NCSU, UNC DMREF Collaboration Meeting, Raleigh, NC. November 6, 2024 (ORAL-INVITED)*
2. Database for Hybrid Perovskites: HybriD^3. *NREL CHOICE Meeting, Golden, CO. November 1, 2024 (ORAL-INVITED)*
3. A tutorial on PyProcar: A Python library for electronic structure pre/post-processing. *Rutgers University, Piscataway, NJ. June 25, 2021 (ORAL-INVITED)*
4. Recent Developments in PyProcar: A Python library for electronic structure pre/post-processing. *APS March Meeting. March 15-19, 2021 (ORAL)*
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 (ORAL)*
6. PyProcar: A Python library for electronic structure pre/post-processing. *Carolina Science Symposium, University of California, Merced. November 12-13, 2020 (ORAL)*
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 (ORAL)*
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*

- 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 TACC 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* *Oct, 2018 - Mar, 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 PSC Bridges, Bridges2 and 374,942 node-hours on TACC 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

Sigma Xi Scientific Research Honor Society Associate Membership *Feb, 2025*

- Inducted in recognition of scholarly achievements and contributions to the advancement of materials research.

Ovshinsky Travel Award *Feb, 2021*

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

Robert T. Bruhn Physics Research Award *May, 2019*
- 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

Applied Data Science with Python (University of Michigan)* *Jan, 2025 - Apr, 2025*
- In-depth training in applying statistical, machine learning, information visualization, text analysis, and social network analysis techniques for data science, employing Python libraries including scikit-learn, nltk, and networkx.

Emerging Leaders Institute (Duke University) *Jan, 2025 - Mar, 2025*
- Developed communication, self-awareness, professional adaptability, project management, interdisciplinary teamwork, and leadership skills through an eight-week professional development program.

Introduction to Machine Learning (Duke University)* *Jan, 2025 - Feb, 2025*
- Gain a foundational understanding of machine learning models including logistic regression, convolutional neural networks, and natural language processing through hands-on experience implementing them with PyTorch to solve complex problems across various fields.

OITE Management Short Course (National Institute of Environmental Health Sciences (NIEHS)) *Jun, 2024*
- Received training on management principles through small group discussions and case studies.

Responsible Conduct of Research - Staff (CITI/ Duke University) *Jul, 2022*
- Received training on core norms, principles, regulations, and rules governing the practice of research including authorship, collaborative research, conflicts of interest, human subjects, and research misconduct.

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 while addressing their needs and celebrating their accomplishments.

Organizer - FHI-aims Developers' and Users' Meeting *Aug 2, 2023 - Aug 4, 2023*
- Organized the FHI-aims Developers' and Users' Meeting in Hamburg, Germany, cultivating a vibrant community and promoting 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 local community.
- 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 suggest treatments in collaboration with the Sri Lanka Department of Agriculture leading to improvements in crop production.

* In progress

References

Dr. Volker Blum
Department of Mechanical Engineering and Materials Science
Duke University
volker.blum@duke.edu
(919) 660 5279

Dr. Aldo H. Romero
Department of Physics and Astronomy
West Virginia University
aldo.romero@mail.wvu.edu
(304) 293-6317

Dr. Hyowon Park
Department of Physics
University of Illinois at Chicago
hyowon@uic.edu
(312) 996-8913

Dr. Sobhit Singh
Department of Mechanical Engineering
University of Rochester
s.singh@rochester.edu
(304) 282-6862