

Uthpala Herath, Ph.D.

Department of Mechanical Engineering & Materials Science
Duke University
Box 90300 Hudson Hall
Durham, NC USA 27708
☎ +1 (304)-216-2535

✉ uthpala.herath@duke.edu
🌐 uthpalaherath.github.io
in linkedin.com/in/uthpalaherath
🐙 github.com/uthpalaherath
🆔 orcid.org/0000-0002-4585-3002

Summary

Experienced Computational Materials Scientist with a strong foundation in leveraging High-Performance Computing (HPC) & High-Throughput Computing (HTC) for electronic structure calculations & molecular dynamics simulations. Specializes in strongly correlated materials research, developing advanced beyond-DFT quantum many-body Green's functions methods, including Dynamical Mean Field Theory (DMFT) & the GW Approximation (GWA), to explore materials critical to semiconductors, spintronics, neuromorphic computing, optics, photovoltaics, and energy applications. Proficient in leading the design, characterization, and collaborative advancement of novel material solutions, aiming to drive innovation and sustainability in technology.

Education

Doctor of Philosophy (Physics) Department of Physics and Astronomy, West Virginia University, USA Dissertation: <i>"Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives."</i>	2015–2022
Master of Science (Physics) Department of Physics and Astronomy, West Virginia University, USA	2015–2017
Bachelor of Science (Physics major and Mathematics minor) Department of Physics, Faculty of Science, University of Peradeniya, Sri Lanka	2010–2014

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 (ELectronic Structure Infrastructure), Wannier90, Impurity Solvers and QMC methods, Tightbinding Hamiltonians, Phonopy
 - Materials discovery & analysis (PyProcar, PyChemia, MechElastic, Pymatgen, AFLOW)
 - 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 languages and platforms :** Python, Matlab, Fortran, C/C++, Bash, Java, SQL, MongoDB, 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 & Unit testing
- **Grant Writing :** Experienced in composing compelling grant proposals, successfully securing funding for cutting-edge scientific research across multiple funding agencies including National Science Foundation (NSF) and Department of Energy (DOE).
- **Soft skills :** Demonstrated abilities in Creative problem solving, Leadership, Organization, Communication, Teamwork, Flexibility, Networking, Time & resource management, and Mentorship.
- **Languages :** English (Native or bilingual proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)

Duke University

Postdoctoral Associate (Computational Materials Science)

2022 –present

Blum Group

Electronic structure method development

- Pioneered the integration of relativistic spin-orbit coupling to Periodic GWA in FHI-aims revolutionizing the exploration of novel semiconductors and renewable energy materials with heavy elements.
- Developed a novel Δ -SCF method within FHI-aims and ELSI to study particle excitations, enabling the detection of superfluorescence phenomena. This method, developed in collaboration with experimental researchers, holds promising applications in quantum optics and nano-medicine, culminating in a high-impact submission to Nature Photonics.
- Led a global collaborative effort to establish stability, usability, and performance of FHI-aims and ELSI improving code reliability and efficiency. Orchestrated the comprehensive enhancement of ELSI by implementing a CI pipeline with Docker and integrating cutting-edge eigen solvers and density matrix solvers.
- Played a key role in the organizing committee of the FHI-aims Developers' and Users' Meeting in Hamburg, Germany (2023). This leadership position underscored the commitment to fostering a vibrant community of developers and users, enhancing collaboration and knowledge exchange.
- Successfully secured a grant of 46,000 node-hours (equivalent to over \$125,000) on the NSF-funded TACC Frontera supercomputing cluster supporting the project, "*Research and development of methods for many-body electronic structure theory and applications in FHI-aims*", demonstrating proficiency in grant writing, resource management, and project planning.

Other experience

- As a council member of the Duke University Postdoctoral Associate (DUPA), organized and led events bringing postdocs from different backgrounds together fostering interdisciplinary research collaborations.

West Virginia University

Graduate Research Assistant (Computational Condensed Matter Physics)

2017 –2022

Romero Group

Strongly Correlated Materials Research

- Developed the DMFT \leftrightarrow DFT framework, significantly lowering the barrier to entry for researchers studying strongly correlated materials. Interfaced popular DFT codes (VASP, Quantum Espresso, Siesta), fostering a global community of users. Maintain a code repository with 65+ stars and 15+ forks and a user forum with 35+ global users, with a publication cited 20+ times.
- Investigated symmetrically induced oxygen vacancies based on site occupation disorder in strongly correlated rare-earth nickelate perovskites, identifying potential for neuromorphic computing and micro-electronics applications. This included studying minimum energy pathways for oxygen vacancy diffusion using the Nudged Elastic Band (NEB) algorithm within DMFT and developing an Artificial Neural Network (ANN) based atomic interaction potential.
- Implemented an innovative approach for analyzing alloying and defects in strongly correlated materials, utilizing a novel interface between the Virtual Crystal Approximation (VCA) and Dynamical Mean Field Theory (DMFT), substantially reducing the computational resources needed to investigate these complex systems.

Contribution to materials research frameworks

- Developed the electronic structure pre/post-processing tool PyProcarr, maintaining a code repository with 160+ stars, 70+ forks, and a global user forum of 260+ users, with a publication cited 225+ times.
- Developed MechElastic, an open-source Python library for calculating elastic properties of materials. The tool, available on PyPI, includes EOS analysis and an Abinit interface with pressure corrections for VASP, maintaining a repository with 40+ stars, 20+ forks, and a user forum of 45+ global users, with a publication cited 55+ times.
- Contributed to 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.

Other experience

- Mentored a postdoc and graduate students on electronic structure calculations and computational tools, demonstrating a commitment to developing the next generation of scientists.
- Successfully secured grant for DOE-EPSCOR Project : "*Applications of Nickelate perovskites for neuromorphic computing from electronic structure and Machine Learning*" (2019) as well as allocations on NSF-funded XSEDE supercomputing resources (2018-2021) amounting to over 30 million core-hours (equivalent to over \$350,000), showcasing grant writing expertise and the ability to secure funding for cutting-edge research projects.
- Volunteered in physics outreach programs enhancing public literacy in science across West Virginia, demonstrating skills in public communication, educational outreach, and community service.