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
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) and High-Throughput Computing (HTC) for electronic structure calculations and molecular dynamics simulations. Specialized in developing advanced beyond-DFT quantum many-body Green's functions methods, including Dynamical Mean Field Theory (DMFT) and the GW Approximation (GWA), to explore materials critical to semiconductors, spintronics, neuromorphic computing, optics, photovoltaics, and energy applications. Proficient in the design, characterization, and collaborative development of novel material solutions, aiming to drive innovation and sustainability in technology.

Education

Doctor of Philosophy (Physics) 2015–2022
Department of Physics and Astronomy, West Virginia University, USA
Dissertation: *"Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives."*

Master of Science (Physics) 2015–2017
Department of Physics and Astronomy, West Virginia University, USA

Bachelor of Science (Physics major and Mathematics minor) 2010–2014
Department of Physics, Faculty of Science, University of Peradeniya, Sri Lanka

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.
- **Development and application of materials research methods and tools** :
  ◦ DMFTwDFT, ELSI (ELectronic Structure Infrastructure), Wannier90, Impurity Solvers and QMC methods, Tightbinding Hamiltonians, Phonopy
  ◦ Materials 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** : Python, Matlab, Fortran, C/C++, Bash
- **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
- **Grant Writing** : Successful in securing research grants spanning 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 management, and Mentorship.
- **Languages** : English (Full professional proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)

Research Experience

Duke University 2022 –present
Postdoctoral Associate (Computational Materials Science) 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 Continuous Integration (CI) 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. 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 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"*.

West Virginia University 2017 –2022
Graduate Research Assistant (Computational Condensed Matter Physics) Romero Group

Strongly Correlated Materials Research

- Developed the `DMFTwDFT` framework, significantly lowering the barrier to entry for researchers studying strongly correlated materials by enabling user-friendly integration of DFT and DMFT. This framework has interfaces for 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.
- Conducted electronic structure calculations to unveil the electronic properties of transition and rare-earth correlated nickelate perovskites, leveraging `DMFTwDFT`.
- 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 a method for studying alloying/defects in strongly correlated materials using a novel interface between the virtual crystal approximation (VCA) and DMFT.
- Carried out molecular dynamics simulations of strongly correlated nickelate perovskites utilizing the open-source code `MDWC` to investigate their behavior on longer time scales.

Contribution to materials research frameworks

- 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 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 through debugging and post-processing tool development.
- Contributed to `PyChemia`; an open-source Python library for materials structural search through debugging and developing interfaces to DFT codes.

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 :*"Searching optimal strongly correlated materials for neuromorphic computing"* (2019) and grants for allocations on NSF XSEDE supercomputing resources (2018-2020), showcasing grant writing expertise and the ability to secure funding for cutting-edge research projects.