

# Uthpala Herath, Ph.D.

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## Summary

- Computational materials scientist with a demonstrated history in employing High-Performance Computing (HPC) and High-Throughput Computing (HTC) to develop and perform electronic structure calculations and molecular dynamics simulations for bulk/2D materials and heterostructures using beyond-DFT quantum many-body Green's functions methods including Dynamical Mean Field Theory (DMFT) and the GW Approximation.
- Interests lie in materials useful for semiconductors, spintronics, neuromorphic computing, photovoltaics and energy applications.
- Skilled in the design and characterization of novel materials together with collaborative code development.

## 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 :**
  - Proficient in the development and application of Density Functional Theory (DFT) codes - *FHI-aims, VASP, Siesta, Abinit, Elk, Quantum Espresso for DFT, DFT+U, Hybrid functionals, GWA, and DMFT calculations.*
  - Experienced in investigating intriguing novel 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 Interface, 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
- **Languages :** English (Full professional proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)
- **Grant Writing :** Successfully secured research grants spanning multiple funding agencies including National Science Foundation (NSF) and Department of Energy (DoE)
- **Soft skills :** Creative problem solving, Leadership, Organization, Communication, Teamwork, Flexibility, Networking, Time management, Mentorship

### Duke University

Postdoctoral Associate (Computational Materials Science)

2022 –present

Blum Group

#### Electronic structure method development

- Development of electronic structure methods to study heavy elements with relativistic effects useful for novel semiconductor and renewable energy materials through the implementation of Periodic GW with relativistic spin-orbit coupling in the electronic structure code FHI-aims.
- Implemented a method to study static particle excitations through the  $\Delta$ -SCF method in FHI-aims and ELSI Interface leading to an article submission to Nature Photonics.
- Established code stability, usability, performance and implemented bug fixes in FHI-aims and ELSI Interface through collaboration with developers from around the globe.
- Enhancement of the ELSI Interface library including the implementation of the CI through Docker and the integration of updated eigen solvers and density matrix solvers.
- Served in the organizing committee for the FHI-aims Developers' and Users' Meeting held in Hamburg, Germany.
- Successfully secured a grant of 46,000 node-hours on the NSF funded TACC Frontera supercomputing cluster for the project, *"Research and development of methods for many-body electronic structure theory and applications in FHI-aims"*.

### West Virginia University

Graduate Research Assistant (Computational Condensed Matter Physics)

2017 –2022

Romero Group

#### Strongly Correlated Materials Research

- Developed the DMFTwDFT framework enabling users to study properties of strongly correlated materials using DFT and DMFT with minimal technical expertise. Created interfaces to popular DFT codes (VASP, Quantum Espresso, Siesta) through Maximally Localized Wannier Functions (MLWF's) and tight-binding Hamiltonians. Maintain a code repository of 65+ stars, 15+ forks and a community forum of 35+ global users. Published article cited 20+ times.
- Implemented full charge self-consistent DFT+DMFT calculations within the DMFTwDFT framework for the DFT code Siesta. Interfaced Quantum Espresso with DMFTwDFT (both natively and through Aiiida) to perform one-shot DMFT calculations.
- Performed electronic structure calculations to study the electronic properties of transition and rare-earth correlated nickelate perovskites using DMFTwDFT.
- Investigated the effect of symmetrically induced oxygen vacancies based on site occupation disorder in strongly correlated rare-earth nickelate perovskites and identified potential metal-to-insulator transitions. Further studied the minimum energy pathways for oxygen vacancy diffusion using Nudged Elastic Band algorithm (NEB) within DMFT for these vacancies. Identified potential applications in neuromorphic computing and micro-electronics. Calculated total energies with self-energy corrections to train an atomic interaction potential based on artificial neural networks (ANN).
- Implemented a method to study alloying/defects in SCMs through an interface between the virtual crystal approximation (VCA) and DMFT.
- Carried out molecular dynamics simulations of SCMs using the open source code MDWC.

#### Contribution to materials research frameworks

- Developed the electronic structure pre/post-processing code PyProcar. Maintain a code repository of 160+ stars, 70+ forks and a community forum of 260+ global users. Published article cited 225+ times.
- Developed MechElastic; an open-source Python library to calculate elastic properties of materials and made it available as a Python library on PyPI. Implemented the Equation of State (EOS) analysis and Abinit interface along with pressure corrections in VASP. Maintain a code repository of 40+ stars, 20+ forks and a community forum of 45+ global users. Published article 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.
- 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).