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, 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* calculations** :
  ◦ Proficient in the development and application of Density Functional Theory (DFT) codes - *FHI-aims* ***(in-house code)****, VASP, Siesta, Abinit, Elk, Quantum Espresso for DFT, DFT+U, Hybrid functionals, GW calculations*
  ◦ Experienced in investigating intriguing novel electronic, vibrational, magnetic, mechanical, elastic, thermal and optical properties of bulk/2D material and heterostructures.
- **Experienced in the development and application of materials research methods and tools** :
  ELSI Interface, DMFTwDFT, Wannier90, Impurity Solvers and Quantum Monte Carlo Methods, Tightbinding Hamiltonians, PyProcar, PyChemia, MechElastic, AFLOW, VTST Tools, DiSPy, Nudged Elastic Band (NEB) method, Site Occupation Disorder (SOD) method, Molecular Dynamics Simulations, Pymatgen (Python Materials Genomics), phonopy, Graphical tools (VESTA, gnuplot, Xmgrace, xcrysden), Vacancy, defect and alloying methods - *Virtual Crystal Approximation (VCA), Coherent Potential Approximation (CPA), SPRKKR*.
- **Programming languages** : Python, Matlab, Fortran, C, C++, Bash
- **Computational methods and libraries** : Linux/Unix systems, High-performance computing (HPC), High-throughput computing (HTC), Parallel computing with OpenMP and MPI, Regression analysis, Differential solvers and Integrators, Numerical analysis algorithms, Object-oriented and Procedural programming paradigms, BLAS, LAPACK, SCALAPACK, FFTW, GSL
- **Supercomputing clusters experience**: TACC Frontera, NERSC Perlmutter and Cori, WVU Thorny Flat and Spruce Knob, XSEDE Bridges2 and Stampede2, LANL HPC
- **Version Control and CI** : Git, Docker, Apptainer, CMake
- **Languages** : English (Full professional proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)
- **Soft skills** : Creative problem solving, Leadership, Organization, Communication, Teamwork, Flexibility, Networking, Time management, Mentorship Scientific grant writing (NSF and DOE)

Research Experience

Duke University 2022 –present
Postdoctoral Associate (Computational Materials Science) 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.
- Implementation of a method to study static particle excitations through the delta-SCF method in FHI-aims and ELSI Interface.
- 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 2017 –2022
Graduate Research Assistant (Computational Condensed Matter Physics) 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+ 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 `Aiida`) 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+ 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`; a open-source Python library for materials structural search through debugging and developing interfaces to DFT codes.