Uthpala Herath

Department of Physics and Astronomy
West Virginia University
135 Willey St, Morgantown
Morgantown, WV 26506
+1 (304)-216-2535

ukh0001@mix.wvu.edu
uthpalaherath.github.io
github.com/uthpalaherath
linkedin.com/in/uthpalaherath
orcid.org/0000-0002-4585-3002

Summary

- Computational materials scientist with a demonstrated history in employing High-Performance Computing (HPC) and High-Throughput Computing (HTC) to perform first principles *ab-initio* 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).
- Interests lie in strongly correlated materials (SCMs) useful for semiconductors, Mott transitions, high-T_c superconductivity, magnetism, quantum and neuromorphic computing, electro-chemical devices and energy applications.
- Skilled in the design and characterization of novel materials together with collaborative code development.

Education

Doctor of Philosophy (Physics) 2015–2022 (expected)
Department of Physics and Astronomy, West Virginia University, USA
Thesis Topic: *"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

Research Experience

West Virginia University 2015–present
Graduate Research Assistant (Computational Materials Science) Romero Group

- Developed and maintain 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).
- 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).
- Applied Virtual Crystal Approximation within DMFT to study strongly correlated alloys/defects.
- Co-developed the popular electronic structure pre/post-processing code `PyProcar`.
- Implemented the Equation of State analysis and Abinit interface along with pressure corrections in VASP for the mechanical property analysis code `MechElastic`. Extended the original code as a Python library.
- Co-developed the constrained molecular dynamics simulations code `MDWC`. Implemented post-processing tools.
- Contributed to PyChemia; our in-house open-source Python library for materials structural search.
- Successfully secured allocation of computing resources in Stampede2 and Bridges super-computing clusters by coordinating the research group efforts in preparing the XSEDE grant proposal for three consecutive years (2018, 2019, 2020). Assisted PI in securing grant for DOE-EPSCOR Project :*"Searching optimal strongly correlated materials for neuromorphic computing."* by preparing the grant proposal.
- Mentored a post-doc in the group on the usage of the DMFTwDFT framework to treat strongly correlated materials.

Skills

- **First principles *ab-initio* calculations** :
  Hands on experience with Density Functional Theory (DFT) codes - *VASP, Siesta, Abinit, Elk, Quantum Espresso for DFT, DFT+U, Hybrid functionals, GW calculations. Investigating intriguing novel properties of bulk/2D material and heterostructures.*
- **Code development and application to research** :
  ◦ Treating SCMs with DMFT using `DMFTwDFT`, Quantum Monte Carlo methods (CTQMC), Hubbard model, Anderson Impurity model, Maximally Localized Wannier Functions (MLWF's) with `wannier90` and tight-binding Hamiltonians.
  ◦ Electronic structure calculation pre-processing and analysis with `PyProcar` and `PyChemia`.
  ◦ Investigating mechanical properties of materials with `MechElastic`.
  ◦ Constrained Molecular Dynamics Simulations with `MDWC`.
- **Materials research methods and tools** :
  Hands-on experience with VTST tools, DiSPy, SOD, Pymatgen, phonopy, VESTA, gnuplot, Xmgrace, xcrysden, VCA, CPA, SPRKKR, Tightbinding Hamiltonians.
- **Computational methods** :
  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.
- **Programming languages** : Python, Fortran, C, C++, Bash, Matlab.
- **Libraries** : BLAS, LAPACK, FFTW, GSL.
- **Graphics and Publishing** : Latex, Markdown, Photoshop, Premiere, After Effects, Illustrator.
- **Languages** : English (Bilingual proficiency), Sinhala (Native proficiency), Tamil (Elementary proficiency).
- **Soft skills** : Creative problem solving, Leadership, Organization, Communication, Teamwork, Networking, Flexibility.

Selected Publications

1. 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,* 107778 (Dec. 2020).
2. **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).
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).

Please visit my Google Scholar profile for an updated list of publications.
`https://scholar.google.com/citations?user=m6VPFYoAAAAJ&hl=en&authuser=1`

Selected Awards and Honors

• Ovshinsky Travel Award for the APS March Meeting **(2021)**
• Robert T. Bruhn Physics Research Award at West Virginia University **(2020)**

Selected Presentations

- **Uthpala Herath**, Pedram Tavadze, He Xu, Eric Bousquet, Sobhit Singh, Reese Boucher, Logan Lang, Freddy Farah, Francisco Muñoz and Aldo H Romero
  "A tutorial on PyProcar: A Python library for electronic structure pre/post-processing"
  Rutgers University, June 25th, 2021 (INVITED VIRTUAL TALK)
- **Uthpala Herath**, Vijay Singh, Benny Wah, Xingyu Liao, Hyowon Park and Aldo H. Romero
  "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 (VIRTUAL TALK)