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

- Ph.D. candidate in computational materials science research with a demonstrated history in employing High-Performance Computing (HPC) and High-Throughput Computing (HTC) to perform first principles *ab-initio* electronic structure calculations for bulk material and heterostructures, primarily focusing on strongly correlated materials (SCMs) using beyond-DFT quantum many body Green's functions methods and Dynamical Mean Field Theory (DMFT).

- Expertise in electronic structure methods includes :
  - Calculating electronic, magnetic, optical, elastic, mechanical, thermal and vibrational properties of strongly/weakly correlated material.
  - Performing molecular dynamics simulations of strongly/weakly correlated material.
  - Design and characterization of state-of-the-art novel material with remarkable emergent properties.
  - Study of defects, vacancies and alloying in SCMs.

- Interested in materials useful for high-temperature superconductivity, magnetism, colossal magnetoresistance, metal to insulator transitions, ferromagnetism, thermomagnetic, spintronics, neuromorphic computing and energy applications.

- Skilled in the collaborative development of frameworks to facilitate electronic structure calculations along with their pre and post-processing (E.g.- PyProcar, DMFTwDFT).

- Experienced with multi-disciplinary research in fields including Materials Science, Space Physics, Photometry and Agriculture; a portrayal of versatility and multifacetedness.

- Fluent in C, C++, Fortran, Python, Bash, Matlab, Java, SQL

Education

Doctor of Philosophy (Physics) 2017–2021 (Exp.)
Department of Physics and Astronomy, West Virginia University, Morgantown, WV 26508, USA
GPA: 3.68/4.00
Thesis: *"Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives."*
Advisor: Aldo H. Romero

Master of Science (Physics) 2015–2017
Department of Physics and Astronomy, West Virginia University, Morgantown, WV 26508, USA

Bachelor of Science (Physics major and Mathematics minor)
Second Class Honors (Upper Division) - GPA: 3.40/4.00 2010–2014
Department of Physics, Faculty of Science, University of Peradeniya, Peradeniya, Sri Lanka

Research Experience

West Virginia University 2017 –current
Graduate Research Assistant (Computational Materials Science) Romero Group

Strongly Correlated Materials Research

- Developed the DMFTwDFT framework; an open-source, user-friendly framework to calculate electronic, vibrational and elastic properties in strongly correlated materials (SCMs) using DMFT (Dynamical Mean Field Theory) in combination with a variety of DFT codes including VASP, Siesta and Quantum Espresso interfaced through Maximally Localized Wannier Functions (MLWF) and a Continuous Time Quantum Monte Carlo (CTQMC) impurity solver. Based on the original implementation by Dr. Hyowon Park at the University of Illinois at Chicago. Additionally, maintained the code repository (collectively 35+ stars, 10+ forks) and community forum (10+ users).
- Implemented full charge self-consistent DFT+DMFT calculations within the DMFTwDFT framework for the DFT code Siesta in collaboration with Dr. Javier Junquera, a lead developer for 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.
- Carried out molecular dynamics simulations on SCMs using our in-house MDWC code.
- Studied the effect of symmetrically induced oxygen vacancies based on site occupation disorder in strongly correlated rare earth nickelate perovskites using a combination of DFT and DMFT and identified potential metal-to-insulator transitions. Further studied the minimum energy pathways for oxygen vacancy diffusion using Nudged Elastic Band theory (NEB) within DMFT for these vacancies.
- Investigated the electronic properties of strongly correlated oxynitrides perovskites and Heusler alloys.
- Applied virtual crystal approximation (VCA) within DMFT to study alloying/ defects in SCMs.

Contribution to materials research frameworks

- Development of PyProcar; a robust, open-source Python library used for pre- and post-processing of the electronic structure data coming from DFT calculations. Based on the original implementation by Dr. Aldo Romero and Dr. Francisco Muñoz. Additionally, maintained the code repository (75+ stars, 40+ forks) and community forum (130+ users).
- Contributed to MechElastic; An open-source Python library to calculate elastic properties of materials. Implemented the Equation of State analysis and Abinit interface along with pressure corrections in VASP. Maintained the code repository (15+ stars, 10+ forks) and the community forum (15+ users). Original implementation by Dr. Sobhit Singh.
- Contributed to MDWC; our in-house command line open-source Python program for constrained molecular dynamics simulations. Involved in debugging and post-processing tool development. Based on the implementation by Dr. Arturo Hernandez.
- Contributed to PyChemia; our in-house open-source Python library for materials structural search. Based on the implementation by Dr. Guillermo Avendano-Franco.

Assist in grant proposal writing

- XSEDE proposal for allocation of computing resources in Stampede2 and Bridges super-computing clusters. (2018, 2019, 2020) - ACCEPTED
- DOE-EPSCOR Project :*"Searching optimal strongly correlated materials for neuromorphic computing."* (2019) - ACCEPTED

West Virginia University 2016 –2017
Graduate Research Assistant (Computational Space Physics)) Tu Group

The effect of magnetic field line curvature scattering on the rapid loss of ring current ions

- Performed test particle simulations to quantify cumulative FLC scattering of ring current ions. Based on these simulation results, a physical parameterization for the FLC scattering was attempted to be incorporated into the RAM-SCB model.
- Received hands-on experience with a C, C++ based in-house particle tracer code.
- Presented preliminary results at the 2017 GEM conference in Portsmouth, VA.

Arthur C. Clarke Institute for Modern Technologies, Sri Lanka 2014
Intern - Space Applications Division

Identification of Blue Stragglers in the globular cluster M53 using CCD photometry
Advisors : Mr. S. Gunasekara, Dr. T. Ranawake

- Worked in conjunction with an expert team of scientists at the Space Applications division of ACCIMT to perform an extensive study of globular cluster characteristics using Aperture Photometry and PSF (Point Spread Function) Fitting Photometry methods with the IRAF (Image Reduction and Analysis Facility) system.
- Telescopic data of the globular cluster M53 was used to construct a novel Color-Magnitude Diagram (CMD) of the cluster, which was in turn utilized to study its stellar population, mainly focusing on the Blue Straggler Star population.

University of Peradeniya, Sri Lanka 2012–2013
Undergraduate Research Student - Department of Physics, Faculty of Science

Nano Magnets and their Applications
Advisor : Prof. P. Samarasekara

- Investigated the traits, synthesis methods, functionalization and applications of Nano Magnets.

Teaching Experience

- **Volunteer Instructor**, Department of Physics and Astronomy at West Virginia University 2017-present
  Occasionally covered for Dr. Aldo Romero's (thesis advisor) graduate level Quantum Mechanics class.
- **Graduate Teaching Assistant**, Department of Physics and Astronomy at West Virginia University 2015-2017
  Conducted lab and office hours on electrostatics, electromagnetism and optics for STEM undergraduate students in Physics 112. Graded exams and homework.
- **Graduate Teaching Assistant**, Department of Physics at University of Peradeniya, Sri Lanka 2014-2015
  Conducted lab and tutorial sessions for STEM undergraduate students. Graded exams and homework.

Skills

- **First principles *ab-initio* calculations** :
  ◦ Density Functional Theory (DFT) codes - *VASP, Siesta, Abinit, Elk, Quantum Espresso for DFT, DFT+U, Hybrid functionals, GW calculations*
  ◦ Electronic, vibrational, magnetic, mechanical, elastic, thermal and optical properties of bulk material and heterostructures.

- **Materials Research Methods and Tools** :
  ◦ DMFTwDFT - *An open-source framework to perform Dynamical Mean Field Theory (DMFT) calculations to study strongly correlated materials (SCMs), Mott transitions, mass renormalization effects, spectral functions.*
  ◦ Impurity Solvers and Quantum Monte Carlo Methods.
  ◦ PyProcar - *A robust, open-source Python library used for pre- and post-processing of the electronic structure data coming from DFT calculations.*
  ◦ PyChemia - *An open-source Python library for materials structural search.*
  ◦ MechElastic - *An open-source Python library to calculate elastic properties of materials.*
  ◦ VTST Tools - *Minimum Energy Pathways calculations.*
  ◦ Wannier90 - *Maximally Localized Wannier Functions.*
  ◦ Molecular Dynamics Simulations - *MDWC (A command line open-source Python program for constrained molecular dynamics simulations.), VMD, qAgate, Jmol.*
  ◦ Graphical tools - *VESTA (Visualization for Electronic Structure Analysis), gnuplot, Xmgrace, xcrysden.*
  ◦ Vacancy, defect and alloying methods - *sod (site occupation disorder), Virtual Crystal Approximation (VCA), Coherent Potential Approximation (CPA), SPRKKR.*
  ◦ Tightbinding Hamiltonians - *Employing Tightbinding Hamiltonians to study strongly correlated material.*
- **Programming languages** : C, C++, Fortran, Python, Bash, Matlab, Java, SQL
- **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
- **Libraries** : PyMatgen, phonopy, DiSPy, sod (site occupation disorder), numpy, scipy, pandas, matplotlib, BLAS, LAPACK, FFTW3, GSL
- **Operating systems** : Linux, MacOS, Windows
- **Graphics and Publishing** : Latex, Markdown, Adobe Photoshop, Adobe Premiere, Adobe After Effects, Adobe Illustrator
- **Version Control** : git, GitHub
- **Utilities** : vim, tmux, globus
- **Communications** : Slack, Zoom, Skype
- **Languages** : English (Full professional proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)
- **Soft skills** : Creative problem solving, Leadership, Organization, Communication, Teamwork, Empathy

Scholarships and Awards

- **Ovshinsky Travel Award for the APS March Meeting 2021** 2021
  Awarded by the American Physical Society to fund registration for the APS March Meeting in March, 2021.
- **Robert T. Bruhn Physics Research Award at West Virginia University** 2020
  Awarded by the Department of Physics and Astronomy to extend support to the research effort of a graduate or undergraduate student in the department in nanotechnology and material science.
- **Office of the Provost Graduate Student Travel Award** 2018, 2019
  Awarded by the Office of the Provost, West Virginia University to fund travel to research conferences.
- **Eberly College of Arts and Sciences Graduate Student Travel Award** 2018, 2019
  Awarded by the Eberly College of Arts and Sciences, West Virginia University to fund travel to research conferences.

Publications

1. **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. doi:https://doi.org/10.1016/j.cpc.2019.107080 (2020).

2. 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. doi:10.1016/j.cpc.2020.107778 (Dec. 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* 2020. arXiv: 2012.04758 `[cond-mat.mtrl-sci]`.
4. Herath, A. & **Herath, U.** Developing an Expert System for Plant Pest Diagnosis. *Annals of the Sri Lanka Department of Agriculture* **15,** 381 (2012).

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

Publications in progress

5. **Herath, U.,** Singh, V., Wah, B., Park, H. & Romero, A. H. A site occupation disorder study of oxygen vacancies in $LaNiO_3$.
6. **Herath, U.,** Singh, V., Wah, B., Park, H. & Romero, A. H. The effect of oxygen vacancies on strongly correlated nickelate perovskite oxides.
7. **Herath, U.,** Singh, V., Wah, B., Park, H. & Romero, A. H. A study of strongly correlated alloys through virtual crystal approximation within dynamical mean field theory.
8. Tavadze, P., Farah, F., Lang, L., Romestan, Z., Dovale-Farelo, V., **Herath, U.,** Singh, S. & Romero, A. H. Fermi3D: Expanding PyProcar's Fermi surface implementations.

Presentations

- **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)
- **Uthpala Herath**, Pedram Tavadze, Xu He, Eric Bousquet, Sobhit Singh, Francisco Muñoz, and Aldo H. Romero
  "Recent developments in PyProcar: A Python library for electronic structure pre/post-processing"
  Carolina Science Symposium, Nov 12-13, 2020 (VIRTUAL TALK)
- **Uthpala Herath**, Pedram Tavadze, Xu He, Eric Bousquet, Sobhit Singh, Francisco Muñoz, and Aldo H. Romero
  "PyProcar: A Python library for electronic structure pre/post-processing"
  Electronic Structure Workshop, June, 2020, University of California, Merced (VIRTUAL TALK)
- **Uthpala Herath**, Pedram Tavadze, Xu He, Eric Bousquet, Sobhit Singh, Francisco Muñoz, and Aldo H. Romero
  "PyProcar: A Python library for electronic structure pre/post-processing"
  APS March Meeting, March 4-8, 2019, Boston, MA (TALK)
- **Uthpala Herath**, Hyowon Park and Aldo H. Romero
  "Development of computational methods for the characterization of novel strongly correlated materials"
  International Summer School on Computational Quantum Materials, June 2018, Sherbrooke, Québec, Canada (POSTER)
- **Uthpala Herath** and Weichao Tu
  "The Effect of Magnetic Field Line Curvature Scattering on the Rapid Loss of Ring Current Ions"
  Geospace Environment Modeling (GEM) conference, July 2017, Portsmouth, VA (POSTER)

Contribution to code development

See full list on `https://uthpalaherath.github.io/projects`.

- **PyProcar**
  "PyProcar is a robust, open-source Python library used for pre- and post-processing of the electronic structure data coming from DFT calculations."
  `https://github.com/romerogroup/pyprocar`
- **DMFTwDFT**
  "An open-source computational package (and a library) combining DMFT with various DFT codes interfaced through the Wannier90 package."
  `https://github.com/DMFTwDFT-project/DMFTwDFT`
- **MechElastic**
  "An open-source Python library to calculate elastic properties of materials."
  `https://github.com/romerogroup/mechelastic`
- **PyChemia**
  "PyChemia is an open-source Python library for materials structural search."
  `https://github.com/MaterialsDiscovery/PyChemia`
- **mdwc**
  "The molecular dynamics with constraints (mdwc3) package is a command line open-source Python program for constrained molecular dynamics simulations."
  `https://github.com/romerogroup/mdwc3`
- **pymatgen**
  "Pymatgen (Python Materials Genomics) is a robust, open-source Python library for materials analysis."
  `https://github.com/materialsproject/pymatgen`

Workshops attended

- **BerkeleyGW Tutorial Workshop** Jan 4 –6, 2021
  Virtual
- **2nd Berkeley Excited States Conference (BESC2021)** Jan 7 –8, 2021
  Virtual
- **Texas A&M University Summer School On Computational Materials Science Across Scales** June 29 –July 10, 2020
  Virtual
- **School on Wannier90 v3.0: new features and applications** March 25 –27, 2020
  Virtual
- **School on Stochastic Approaches to Electronic Structure Calculations** July 29th –August 2nd, 2019
  University of Pittsburgh, PA
- **3rd Summer School on Materials Growth and Design: Exotic Magnetic States in Quantum Mechanics** June 17 –June 22, 2018
  Johns Hopkins University, Baltimore, MD
- **International Summer workshop on Computational Quantum Materials** May 27 –June 8, 2018
  Sherbrook, Québec, Canada
- **CISM Space Weather Summer School** July 11 –July 22, 2016
  Boulder, CO

Extracurricular Activities

- Judge - Virtual Summer Undergraduate Research Symposium, WVU July, 2020

  -Volunteered as a graduate student judge at the 2020 Virtual Summer Undergraduate Research Symposium organized by the Office of Undergraduate Research in the Mathematics and Physics Category

- Coordinator - Condensed Matter Seminar, Department of Physics and Astronomy, WVU 2018–Current

  -Coordinated the Condensed Matter Seminar sessions at the Department of Physics and Astronomy, West Virginia University.

- Outreach Volunteer - Physics and Astronomy Graduate Student Organization, WVU (PAGSO) 2015–Current

  -Conducted physics outreach programs to enlighten the public on science in West Virginia.

- Member - Sri Lankan Student's Organization, WVU (SLSA) 2018–Current

  -SLSA is a student body of Sri Lankan students at West Virginia University aiming to share the Sri Lankan cultural and heritage experience with the rest of the world.
  -Took a leading role in organizing a vigil in memory of the Easter Sunday terrorist attacks that occured in Sri Lanka in April, 2019.

- President - Astronomy Society of University of Peradeniya 2013–2014

  - Organized "Water Rocket Challenge 2014"; the first-ever water rocket competition held at University of Peradeniya
  - Conducted regular astronomy lectures, planetary and deep sky observation sessions and workshops in the university as well as in local schools aiming to promote astronomy among students and the general public.
  - Volunteered for United Nations World Space Week- Sri Lanka (2014)

- Junior Editor - Physical Society of University of Peradeniya 2012–2013

  -Compiled academic articles for the "Echo" magazine which is the annual scientific journal issued by the society

- Faculty Representative - The Ceylon Drama Society of University of Peradeniya 2011–2012

  -Represented the Faculty of Science in the Ceylon Drama Society of the University of Peradeniya, Sri Lanka.

- Volunteer - Let Them Smile 2010–2014

  -Volunteered in "Let Them Smile", an annual charity event organized by the undergraduates of the Faculty of Science of University of Peradeniya, Sri Lanka to facilitate the education of under privileged students in rural schools around the country.
  URL: `https://www.facebook.com/letsmile14`

- Volunteer Software Developer - Department of Agriculture, Sri Lanka 2012

  -Took part in an auxiliary research project conducted by the Sri Lanka Department of Agriculture to develop a system for plant disease diagnosis. This would allow farmers around the island to use a software framework to self-diagnose and treat plant diseases. Assisted in computational aspects of this system.

References

- **Dr. Aldo H. Romero**
  Department of Physics and Astronomy
  West Virginia University
  aldo.romero@mail.wvu.edu
  +1 (304) 293-6317

- **Dr. T. Ranawaka**
  Department of Physics
  Faculty of Science
  University of Peradeniya
  Peradeniya (20400), Sri Lanka
  tpranawa@gmail.com
  +94 812394612

- **Prof. P. Samarasekara**
  Department of Physics
  Faculty of Science
  University of Peradeniya
  Peradeniya (20400), Sri Lanka
  pubudus@pdn.ac.lk
  +94 812394610

- **Dr. Weichao Tu**
  Department of Physics and Astronomy
  West Virginia University
  wetu@mail.wvu.edu
  +1 (304) 293-3349

- **Mr. S. Gunasekara**
  Senior Research Scientist
  Space Applications Division
  Arthur C. Clarke Institute for Modern Technologies
  Moratuwa (10400), Sri Lanka
  saraj@accmt.ac.lk
  +94 714415243