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 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) and the GW Approximation.
- Interests lie in strongly correlated materials (SCMs) useful for semiconductors, high-T_c superconductivity, magnetism, Mott transitions, spintronics, 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
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

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.

Grant writing

- Took a leadership role in coordinating the efforts of the group in preparing and securing allocation of XSEDE computing resources in Stampede2 and Bridges super-computing clusters. (2018, 2019, 2020)
- Successfully secured grant for DOE-EPSCOR Project :*"Searching optimal strongly correlated materials for neuromorphic computing."* (2019)

Mentorship

- Mentored a post-doc in the group on the usage of the DMFTwDFT framework to treat strongly correlated materials.

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 Jan, 2014 –Dec, 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.

Skills

- **First principles *ab-initio* calculations** :
  ◦ Proficient in the development and usage 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 electronic, vibrational, magnetic, mechanical, elastic, thermal and optical properties of bulk material and heterostructures.
- **Experienced in the development and usage of materials research methods and tools** :
  ◦ ELSI Interface - *A unified software interface designed for electronic structure codes to connect with various high-performance eigensolvers and density matrix solvers.*
  ◦ 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.* ***(in-house code)***
  ◦ Wannier90 - *Basis transformation through Maximally Localized Wannier Functions.*
  ◦ Impurity Solvers and Quantum Monte Carlo Methods - *Solving the Anderson Impurity model with the CTQMC method.*
  ◦ Tightbinding Hamiltonians - *Employing Tightbinding Hamiltonians to study strongly correlated material.*
  ◦ PyProcar - *A robust, open-source Python library used for pre- and post-processing of the electronic structure data coming from DFT calculations.* ***(in-house code)***
  ◦ PyChemia - *An open-source Python library for materials structural search.* ***(in-house code)***
  ◦ MechElastic - *An open-source Python library to calculate elastic properties of materials.* ***(in-house code)***
  ◦ AFLOW - *A materials database and search framework.*
  ◦ VTST Tools - *A code for finding saddle points and evaluating transition state theory (TST) rate constants.*
  ◦ DiSPy - *A utility for applying the distortion symmetry method (DSM) to the calculation of minimum energy pathways using the nudged elastic band (NEB) algorithm.*
  ◦ SOD (Site Occupation Disorder) *-A package of tools for the computer modelling of periodic systems with site disorder, using the supercell ensemble method.*
  ◦ Molecular Dynamics Simulations - *MDWC (A command line open-source Python program for constrained molecular dynamics simulations. -* ***in-house code****), VMD, qAgate, Jmol.*
  ◦ Pymatgen (Python Materials Genomics) - *A robust, open-source Python library for materials analysis.*
  ◦ phonopy - *An open source package for phonon calculations at harmonic and quasi-harmonic levels.*
  ◦ Graphical tools - *VESTA (Visualization for Electronic Structure Analysis), 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** : 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
- **Libraries** : BLAS, LAPACK, SCALAPACK, FFTW, GSL
- **Graphics and Publishing** : Latex, Markdown, Adobe Photoshop, Adobe Premiere, Adobe After Effects, Adobe Illustrator
- **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, Scientific grant writing (NSF and DOE)

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.,** Singh, V., Bhat, S. S., Park, H. & Romero, A. H. *Stability and diffusion of oxygen vacancies in $LaNiO_3$: a DMFT study* 2022. arXiv: 2212.07348 [cond-mat.str-el].
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* **261,** 107778 (2021).
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).
4. **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).
5. 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

6. Lang, L., Tavadze, P., Tellez, A., Bousquet, E., Xu, H., Muñoz, F., Vasquez, N., **Herath, U.** & Romero, A. H. Expanding PyProcar for new features, maintainability, and reliability. *Submitted to Computer Physics Communications* (2023).
7. Bhat, S. S., Singh, V., **Herath, U.,** Varughese, B., Sankaranarayanan, S. K. R. S., Park, H. & Romero, A. H. Dynamical correlations leading to site and orbital selective Mott insulator transition in hydrogen doped SmNiO3. *Submitted to Physical Review Letters* (2023).
8. Biliroglu, M., Seyitliyev, D., Kotyrov, M., Abdelsamei, M., Qin, X., Findik, G., Alma, G. A., **Herath, U.,** Lei, L., Chai, J., Mehta, Y., Swan, A., Temnov, V., Blum, V., So, F. & Gundogdu, K. Two-Step Phase Transition in Superfluorescence of Lead-Halide Perovskites. *Submitted to Science* (2023).
9. **Herath, U.,** Bhat, S., Singh, V., Park, H. & Romero, A. H. Investigating strongly correlated alloys via Dynamical Mean Field Theory.

Peer Review Contributions

- Computer Physics Communications 2022

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**, Pedram Tavadze, He Xu, Eric Bousquet, Sobhit Singh, Reese Boucher, Logan Lang, Freddy Farah, Francisco Muñoz and Aldo H Romero
  "Recent Developments in PyProcar: A Python library for electronic structure pre/post-processing"
  APS March Meeting, Mar 15-19, 2021 (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)
- **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"
  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 1-4, 2020, University of California, Merced (VIRTUAL TALK)
- **Uthpala Herath**, Hyowon Park and Aldo H. Romero
  "An ab-initio DFT+DMFT study of the effect of oxygen vacancies on structural, electronic and magnetic properties of rare-earth nickelate perovskites ($RNiO_3$)"
  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)

Teaching Experience

- **Postdoctoral Mentor**, Department of Mechanical Engineering and Materials Science, Duke University 2022
  Assisted in graduate level computational materials science course for Dr. Volker Blum (postdoc PI).
- **Volunteer Instructor**, Department of Physics and Astronomy at West Virginia University 2017-2022
  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.

Contribution to code development

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

- **FHI-aims**
  "All-electron electronic structure theory with numeric atom-centered orbitals."
  `https://fhi-aims.org`
- **ELSI Interface**
  "A unified software interface designed for electronic structure codes to connect with various high-performance eigensolvers and density matrix solvers."
  `https://gitlab.com/elsi_project/elsi_interface`
- **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

- **Quantum Multiscale Hackaton 2023** : Sept 10 –16, 2023
  Rutgers University
- **Quantum Monte Carlo Virtual Workshop 2021** : Oct 5 –November 23, 2021
  ORNL
- **Comscope Summer School 2021** : June 21 –24, 2021
  BNL
- **PRACE Seasonal School on Modeling Materials using HPC and AI/ML** : June 15 –18, 2021
- **Bridging first-principles calculations and effective Hamiltonians** : June 7 –16
  IIT Genova, Italy
- **20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods** : Feb 23 –25, 2021
  ICTP
- **BerkeleyGW Tutorial Workshop** : Jan 4 –6, 2021
- **2nd Berkeley Excited States Conference (BESC2021)** : Jan 7 –8, 2021
- **Texas A&M University Summer School On Computational Materials Science Across Scales** : June 29 –July 10, 2020
- **School on Wannier90 v3.0: new features and applications** : March 25 –27, 2020
- **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 Mechanic** : 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

- Council Member - Duke University Postdoc Association (DUPA) July, 2022 –Current

  - DUPA was established to address the needs and concerns of Duke postdocs and celebrate their accomplishments. As a member of the council and the DUPA social committee I am involved in organizing events that bring postdocs together.
- 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

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- **Prof. Francisco Muñoz**
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