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Summary

Experienced Computational Materials Scientist with a strong foundation in leveraging High-Performance Computing (HPC) and High-Throughput Computing (HTC) for pioneering materials research. Specializes in strongly correlated materials, developing advanced beyond-DFT quantum many-body Green's functions methods, including Dynamical Mean Field Theory (DMFT) and the GW Approximation (GWA), to explore materials critical to semiconductors, spintronics, neuromorphic computing, optics, photovoltaics, and energy applications. Proficient in leading the design, characterization, and collaborative advancement of novel material solutions, aiming to drive innovation and sustainability in technology.

Education

Doctor of Philosophy (Physics) Aug, 2017 – May, 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) Aug, 2015 – Aug, 2017
Department of Physics and Astronomy, West Virginia University, USA

Bachelor of Science (Physics major and Mathematics minor) Jul, 2010 – Dec, 2014
Department of Physics, Faculty of Science, University of Peradeniya, Sri Lanka

Experience

Duke University May, 2022 – Present
Postdoctoral Associate (Computational Materials Science) Blum Group

Electronic structure method development

- Pioneered the integration of relativistic spin-orbit coupling to Periodic GWA in `FHI-aims` revolutionizing the exploration of novel semiconductors and renewable energy materials with heavy elements.
- Developed a novel Δ-SCF method within `FHI-aims` and `ELSI` to study particle excitations, enabling the detection of superfluorescence phenomena. This method, developed in collaboration with experimental researchers, holds promising applications in quantum optics and nano-medicine, culminating in a high-impact submission to Nature Photonics.
- Led a global collaborative effort to establish stability, usability, and performance of `FHI-aims` and `ELSI` improving code reliability and efficiency. Orchestrated the comprehensive enhancement of `ELSI` by implementing a CI pipeline with Docker and integrating cutting-edge eigen solvers and density matrix solvers.
- Played a key role in the organizing committee of the `FHI-aims` Developers' and Users' Meeting in Hamburg, Germany (2023). This leadership position underscored the commitment to fostering a vibrant community of developers and users, enhancing collaboration and knowledge exchange.
- Successfully secured a collaborative grant of 46,000 node-hours (equivalent to over $125,000) on the NSF-funded TACC Frontera supercomputing cluster supporting the project, *"Research and development of methods for many-body electronic structure theory and applications in FHI-aims"*, demonstrating proficiency in grant writing, team-work, resource management, and project planning.

Other experience

- As a council member of the Duke University Postdoctoral Associate (DUPA), organized and led events bringing postdocs from different backgrounds together fostering interdisciplinary research collaborations.

West Virginia University Aug, 2017 – May, 2022

Graduate Research Assistant (Computational Condensed Matter Physics) Romero Group

Strongly Correlated Materials Research

- Developed the `DMFTwDFT` framework, significantly lowering the barrier to entry for researchers studying strongly correlated materials. Interfaced popular DFT codes (VASP, Quantum Espresso, Siesta), fostering a global community of users. Maintained a code repository with 65+ stars and 15+ forks and a user forum with 35+ global users, with a publication cited 20+ times.
- Conducted electronic structure calculations to unveil the electronic properties of transition and rare-earth correlated nickelate perovskites, leveraging `DMFTwDFT`.
- Investigated symmetrically induced oxygen vacancies based on site occupation disorder in strongly correlated rare-earth nickelate perovskites, identifying potential for neuromorphic computing and micro-electronics applications. This included studying minimum energy pathways for oxygen vacancy diffusion using the Nudged Elastic Band (NEB) algorithm within DMFT and developing an Artificial Neural Network (ANN) based atomic interaction potential.
- Implemented an innovative approach for analyzing alloying and defects in strongly correlated materials, utilizing a novel interface between the Virtual Crystal Approximation (VCA) and Dynamical Mean Field Theory (DMFT), substantially reducing the computational resources needed to investigate these complex systems.
- Carried out molecular dynamics simulations of strongly correlated nickelate perovskites utilizing the open-source code `MDWC` to investigate their behavior on longer time scales.

Contribution to materials research frameworks

- Developed the electronic structure pre/post-processing tool `PyProcar`, maintaining a code repository with 160+ stars, 70+ forks, and a global user forum of 260+ users, with a publication cited 225+ times.
- Developed `MechElastic`, an open-source Python library for calculating elastic properties of materials. The tool, available on PyPI, includes EOS analysis and an Abinit interface with pressure corrections for VASP, maintaining a repository with 40+ stars, 20+ forks, and a user forum of 45+ global users, with a publication cited 55+ times.
- Developed `MDWC`; a command line open-source Python program for constrained molecular dynamics simulations and `PyChemia`; an open-source Python library for materials structural search through debugging, simulation, and testing.

Other experience

- Mentored a postdoc and graduate students on electronic structure calculations and computational tools, demonstrating a commitment to developing the next generation of scientists.
- Successfully secured an interdisciplinary research grant for DOE-EPSCOR Project: *"Applications of Nickelate perovskites for neuromorphic computing from electronic structure and Machine Learning"* (2019), as well as allocations on NSF-funded XSEDE supercomputing resources (2018-2021) amounting to over 30 million core-hours (equivalent to over $350,000), showcasing collaborative grant writing expertise and the ability to secure funding for cutting-edge research projects.
- Volunteered in physics outreach programs enhancing public literacy in science across West Virginia, demonstrating skills in public communication, educational outreach, and community service.

West Virginia University Jan, 2016 – May, 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 Jan, 2013 – Dec, 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

- **Postdoctoral Mentor**, Department of Mechanical Engineering and Materials Science, Duke University May, 2022 - Present
  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 May, 2017 - Apr, 2022
  Occasionally covered for Dr. Aldo Romero's (dissertation advisor) graduate level Quantum Mechanics class.
- **Graduate Teaching Assistant**, Department of Physics and Astronomy at West Virginia University Aug, 2015 - May, 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 Dec, 2014 - May, 2015
  Conducted lab and tutorial sessions for STEM undergraduate students. Graded exams and homework.

Skills

- **First principles (*ab-initio*) electronic structure calculations**:
  ◦ Expertise in developing and applying electronic structure codes including *FHI-aims*, *VASP*, *Siesta*, *Abinit*, *Elk*, *Quantum Espresso* for Density Functional Theory (DFT), DFT+U, Hybrid functionals, GWA, and DMFT calculations
  ◦ Skilled in the analysis of electronic, vibrational, magnetic, mechanical, elastic, thermal and optical properties of bulk/2D material and heterostructures
  ◦ Advanced proficiency in studying strongly correlated materials using DMFT
- **Development and application of 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.*
  ◦ ELSI - *A unified software interface designed for electronic structure codes to connect with various high-performance eigensolvers and density matrix solvers.*
  ◦ 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.*
  ◦ Phonopy - *An open source package for phonon calculations at harmonic and quasi-harmonic levels.*
  ◦ 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.*
  ◦ Pymatgen (Python Materials Genomics) - *A robust, open-source Python library for materials analysis.*
  ◦ 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.*
  ◦ Vacancy, defect and alloying methods - *Virtual Crystal Approximation (VCA), Coherent Potential Approximation (CPA), SPRKKR.*
  ◦ Molecular Dynamics Simulations - *MDWC (A command line open-source Python program for constrained molecular dynamics simulations.), VMD, qAgate, Jmol.*
  ◦ Graphical visualization - *VESTA (Visualization for Electronic Structure Analysis), gnuplot, Xmgrace, xcrysden.*
- **Programming languages and platforms**: Python, Matlab, Fortran, C/C++, Bash, Java, SQL, MongoDB, GPU programming (CUDA)
- **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 and Unit testing
- **Graphics and Publishing**: Latex, Markdown, Adobe Creative Suite (Photoshop, Premiere, After Effects, Illustrator), Microsoft Office
- **Grant writing**: Successfully secured grants exceeding $475,000 for innovative research through collaborative efforts, crafting compelling narratives for proposals across multiple funding agencies including National Science Foundation (NSF) and Department of Energy (DOE)
- **Soft skills**: Demonstrated abilities in creative problem-solving, leadership, organization, communication, teamwork, flexibility, networking, time and resource management, and mentorship
- **Languages**: English (Native or bilingual proficiency), Sinhala (Native or bilingual proficiency), Tamil (Elementary proficiency)

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. 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. *Computer Physics Communications* **297,** 109063 (2024).
6. 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 $SmNiO_3$. *Phys. Rev. B* **109,** 205124 (20 May 2024).
7. 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?hl=en&user=aWQymokAAAAJ`

Publications in progress

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 Nature Photonics* (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, March 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, November 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)

Projects

Projects I have developed or contributed to are listed below.

- **FHI-aims**
  "All-electron electronic structure theory with numeric atom-centered orbitals."
  `https://fhi-aims.org`
- **ELSI**
  "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

- **TACC AI For Science Bootcamp** : August 7 –8, 2024
  TACC, Austin, TX (Virtual)

- **NIH-OITE Management Short Course** : June 13 –14, 2024
  NIEHS, Durham, NC

- **Quantum Multiscale Hackathon** : September 10 –16, 2023
  Rutgers University, New Brunswick, NJ

- **Quantum Monte Carlo Virtual Workshop** : October 5 –November 23, 2021
  ORNL, Oak Ridge, TN (Virtual)

- **Comscope Summer School** : June 21 –24, 2021
  BNL, Upton, NY (Virtual)

- **PRACE Seasonal School on Modeling Materials using HPC and AI/ML** : June 15 –18, 2021
  Centre of Operations, Slovak Academy of Sciences, Bratislava, Slovakia (Virtual)

- **Bridging first-principles calculations and effective Hamiltonians** : June 7 –16
  IIT Genova, Italy (Virtual)

- **20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods** : February 23 –25, 2021
  The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (Virtual)

- **2nd Berkeley Excited States Conference (BESC2021)** : January 7 –8, 2021
  Berkeley, CA (Virtual)

- **BerkeleyGW Tutorial Workshop** : January 4 –6, 2021
  Berkeley, CA (Virtual)

- **Summer School on Computational Materials Science Across Scales** : June 29 –July 10, 2020
  Texas A&M University, College Station, TX (Virtual)

- **School on Wannier90 v3.0: new features and applications** : March 25 –27, 2020
  University of Oxford, Oxford, United Kingdom (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

- **CISM Space Weather Summer School** : July 11 –July 22, 2016
  Boulder, CO

Extracurricular Activities

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

  - 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 May, 2018 – May, 2022

  -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) Aug, 2015 – May, 2022

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

- Member - Sri Lankan Student's Organization, WVU (SLSA) Jan, 2018 – May, 2022

  -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 Jan, 2014 – Dec, 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 Jan, 2013 – Dec, 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 Jan, 2012 – Dec, 2012

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

- Volunteer - Let Them Smile Aug, 2010 – Dec, 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 Jan, 2010 – Dec, 2010

  -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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