

Uthpala Herath

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SUMMARY

Uthpala is a PhD candidate in Computational Condensed Matter Physics at the Department of Physics and Astronomy at West Virginia University. His main research interests include the study of strongly correlated materials using Density Functional Theory (DFT) and Dynamical Mean Field Theory (DMFT). He is also involved in code development to facilitate electronic structure calculation and analysis.

EDUCATION

- | | |
|---|------------------|
| Doctor of Philosophy (Physics) | 2017–2021 (Exp.) |
| Department of Physics and Astronomy, West Virginia University, Morgantown, WV 26508, USA | |
| Thesis: <i>“Development of computational methods for electronic structural characterization of strongly correlated materials: from different ab-initio perspectives.”</i> | |
| 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) | 2010–2014 |
| Department of Physics, Faculty of Science, University of Peradeniya, Peradeniya, Sri Lanka | |

RESEARCH EXPERIENCE

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|---|---------------|
| West Virginia University | 2017 –current |
| Graduate Research Assistant (Computational Condensed Matter Physics) | |
| <ul style="list-style-type: none">– The study of strongly correlated materials using beyond-DFT methods such as Dynamical Mean Field Theory.– A computational approach to study properties of strongly correlated materials using a combination of Density Functional Theory (DFT) and Dynamical Mean Field Theory (DMFT)– Studied the effect of oxygen vacancies in strongly correlated rare earth nickelates using DFT+DMFT.– Studied alloying/ defects in strongly correlated materials using virtual crystal approximation within DMFT.– DMFTwDFT– Development of DMFTwDFT; an open-source, user-friendly framework to calculate electronic, vibrational and elastic properties in strongly correlated materials (SCM) using beyond-DFT methods such as DFT+U, DFT+Hybrids and DFT+DMFT (Dynamical Mean Field Theory) with a variety of different DFT codes.– PyProcar– Development of PyProcar; a robust, open-source Python library used for pre- and post-processing of the electronic structure data coming from DFT calculations.– PyProcar provides a set of functions that manage data obtained from the PROCAR format. Basically, the PROCAR format is a projection of the Kohn-Sham states over atomic orbitals. That projection is performed to every k-point in the considered mesh, every energy band and every atom. PyProcar is capable of performing a | |

multitude of tasks including plotting plain and spin/atom/orbital projected band structures and Fermi surfaces- both in 2D and 3D, Fermi velocity plots, unfolding bands of a super cell, comparing band structures from multiple DFT calculations, plotting partial density of states and generating a k-path for a given crystal structure.

West Virginia University

2016 –2017

Graduate Research Assistant (Computational Space Physics))

- 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 is determined which is incorporated into the RAM-SCB model.

Arthur C. Clarke Institute of Modern Technologies, Sri Lanka

2014

Intern- Space Applications Division

- Identification of Blue Stragglers in the globular cluster M53 using CCD photometry
- 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”
- The traits, synthesis methods, functionalization and applications of Nano Magnets were investigated.

SKILLS

- High Performance Computing
- Density Functional Theory calculations with VASP, Siesta, Elk, Abinit, Quantum Espresso
- Calculations and analysis with the packages DMFTwDFT, PyProcar and Mechelastic.
- VMD, VESTA, qAgate, jmol
- Parallelization of programs using OpenMP and MPI
- C, C++, Fortran, Bash, Python, Java, Matlab, SQL, git
- Linux, Latex, Adobe Photoshop, Adobe Premiere, Adobe After Effects
- Sun/Oracle Certified Programmer for the Java SE Platform

TEACHING

- **Graduate Teaching Assistant** at the Department of Physics and Astronomy at West Virginia University 2015-2017
Conducted lab and tutorial sessions on electrostatics, electromagnetism and optics for physics undergraduate students in Physics 112. Graded exams and homework.
- **Graduate Teaching Assistant** at the Department of Physics, Faculty of Science at University of Peradeniya, Sri Lanka 2014-2015
Conducted lab and tutorial sessions for physics undergraduate students. Graded exams and homework.

SCHOLARSHIPS AND AWARDS

- **Robert T. Bruhn Physics Research Award at West Virginia University** 2020
Funding to support the research effort of a graduate or undergraduate student in the Department of Physics and Astronomy in nanotechnology and material science.
- **Office of the Provost Graduate Student Travel Award** 2018
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
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).

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)

PROJECTS

See full list of projects 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.
- **DMFTwDFT**
An open-source computational package (and a library) combining DMFT with various DFT codes interfaced through the Wannier90 package.
- **MechElastic**
A Python library to calculate elastic properties of materials.

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
 University of Pittsburgh, PA, July 29th –August 2nd 2019
- 3rd Summer School on Materials Growth and Design: Exotic Magnetic States in Quantum Mechanics
 Johns Hopkins University, MD, July 2018
- International Summer workshop on Computational Quantum Materials
 Sherbrook, Québec, Canada, June 2018
- CISM Space Weather Summer School
 Boulder, CO, July 2016

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.
- 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 for 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
“Let Them Smile” is 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**
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