BIMAL K C, MS, Ph.D. candidate (ABD)

CONTACT INFORMATION

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EDUCATION

Ph.D. in Computational Science (CPS) Expected May 2024
The University of Texas at El Paso
Dissertation: "*Phonon Anharmonicity of Transition Metals*"
Committee: Ramon J. Ravelo (Chair), Jorge A. Muñoz (Co-Chair), Sreeprasad T Sreenivasan, Arturo Bronson

MS in Physics Awarded: Dec 2019
The University of Texas at El Paso
Thesis: "*Quasi-harmonic and Anharmonic Entropies in Transition Metals*"
Advisor: Ramon J. Ravelo, Ph.D.

MS in Physics Awarded: Dec 2016
Amrit Science College, Tribhuvan University, Kathmandu, Nepal
Thesis: "*First Principles Study of NaCl • • • A-B (A-B= C2H4, CH3, NH3, H2O, H2, HF, HNa, HLi,FNa, FLi, NaCl) Complexes.*"
Advisor: Rajendra Parajuli, Ph.D

BS in Physics Awarded: Jan 2013
Tri-Chandra Campus, Tribhuvan University, Kathmandu, Nepal

EXPERTISE

Computational Science (CPS):

- Atomistic modeling and simulations, High-Performance Computing (HPC), Quantum Computing, Mathematical and Statistical Modeling, etc.

Data Science and Statistics:

- Data Mining, Machine Learning, Computational Statistics, Statistical Process Control, etc.

Computer Science:

- Serial And Parallel Programming, Distributed Data Storage and Processing, Functional and Object-Oriented Programming, etc.

RESEARCH INTEREST

- Theoretical computer science emphasizing modeling, simulation, and visualization for understanding real-world phenomena and computation fundamentals.
- Use of classical and ab- initio calculations of vibrational spectra of solids as a function of temperature.
- Understanding material behavior using density functional theory (using Molecular Dynamics, VASP, Quantum Espresso) and Quasiharmonic Approximation (QHA).
- Phase stability of the material and their alloys, phonons, and phonon entropy, Machine learning, Atomistic simulations of materials at extreme environment.

SOFTWARE SKILLS

Statistical Programming and Scientific Computing:
- R, Python, Matlab, Mathematica, Gaussian, VASP, MD, QMD, etc.

Programming:
- C(including OpenMPI, CUDA), Python, UNIX

Scientific Typesetting:
- LaTeX, BibTeX, Microsoft Office Package, Adobe Package, etc

Operating Systems:
- Microsoft Windows, Linux, and UNIX

GRANTS, AWARDS, & SCHOLARSHIPS

- **Best Oral Presentation Award**, New Mexico State University (NMSU)-NeSA 15th International Conference (March 2024).
- **Graduate Research Award**, Graduate School, UTEP (Fall 202, Spring 2024, Summer 2024).
- **Forum on Graduate Student Affairs (FGSA) URM March meeting award** (Feb 2021).
- **Reading is Fundamental (RIF) award**, College of Science, UTEP (Nov. 2020).
- **Academic and Research Excellence Outstanding Graduate Student Physics**,UTEP, Dec. 2019.
- **C. Sharp Cook Graduate Scholarship**, UTEP (Oct. 2019).
- **Outstanding achievement: Better Rated by Students**, Physics, UTEP (May 2019).
- **Graduate Assistantship**, College of Science, UTEP (Aug 2017-Present).

PROFESSIONAL TRAINING & WORKSHOPS

Sustainable Horizons Institute (SHI) Sustainable Research Pathways, Jan 2023
Berkeley National Laboratory (DOE)
Berkeley, California

PDB3 AWS Python Developer Bootcamp Sep 2022 – Dec 2022
TAKEO TECH LLC
Manhattan, New York

MEMBERSHIP /AFFILIATIONS

- American Physical Society (APS)
- American Mathematical Society (AMS)
- Vice President, Nepalese Student Association, UTEP Sep 2019 - Jun 2021

ACADEMIC EXPERIENCES

Graduate Research Associate Aug 2023 - Present
Computational Science Program, UTEP

Visiting Summer Research Student June 2023 - July 2023
The University of California at Berkeley
Department of Material Science and Engineering

Graduate Teaching Assistant, UTEP August 2019 - May 2023

Computational Science Program, UTEP
Department of Physics, UTEP August 2017 - May 2019

- Tutor at Math Resource Center for Students (MaRCS) - Assist students in basic Math classes (Discrete Mathematics, Differential Equations, Matrix Algebra, and Calculus - up to Calculus III.
- Instructor for Introductory Electromagnetism and General Physics: Engage students in discussion and activity on related topics.
- Graduate Teaching Assistant: Assisting professors with teaching classes, grading papers, and conducting workshops for assigned undergraduate/graduate Mathematics, and Computer Science courses.

Teaching Assistant Instructor Jan 2018 - May 2019
Department of Physics, UTEP

- Lab instructor: Assisting teaching assistants for undergraduate Electronics Laboratory sessions.

CONFERENCE PRESENTATIONS

1. "*First Principle Investigation of Magnetic, Elastic, and Thermodynamic Properties of Ordered D03 Fe_3V*", New Mexico State University (NMSU) Nepalese Student Association (NeSA) 15th International Conference, Las Cruces, NM (March 16, 2024).
2. "*Free Energy of the Order-disorder Phase Transition in FeV from Molecular Dynamics*", APS March Meeting, Minneapolis, MN (March 3 - 8, 2024).
3. "*Harmonic Ensemble Lattice Dynamics of Crystals with Thermal and Configurational Disorder*", 30th Joint NMSU/UTEP Workshop on Mathematics, Computer Science, and Computational Sciences, University of Texas at El Paso, El Paso, TXM (October 28, 2023).
4. "*Why Optimization is Faster than Solving Systems of Equations: A Qualitative Explanation*", 27th Joint NMSU/UTEP Workshop on Mathematics, Computer Science, and Computational Sciences, New Mexico State University, Las Cruces, NM (April 2, 2022).
5. "*Anharmonicity in the Vibrational Entropy of Transition Metals*", APS March Meeting, online (March 16, 2021).
6. "*Classical Molecular Dynamical Simulations of Melting Curve of Copper*",10th International Conference, 2018, New Mexico State University, Las Cruces, NM (March 31, 2018).

PAPER PUBLICATONS

1. S. Deng, B. K C, & V. Kreinovich (2023). *Why Optimization Is Faster than Solving Systems of Equations: A Qualitative Explanation.* In Uncertainty, Constraints, and Decision Making (pp. 341-344). Cham: Springer Nature Switzerland.

THESIS PUBLICATIONS

2. B. K C, "*Quasi-Harmonic and Anharmonic Entropies in Transition Metals*" (2019). Open Access Theses & Dissertations. 2866. https://scholarworks.utep.edu/open_etd/2866

CONFERENCE PUBLICATIONS

3. J. A. Muñoz, H. R. Pulido, B. K C, R. Hemley, R. Kumar, "*Finite-temperature lattice dynamics of FeV at high pressure from first principles*". Bulletin of the American Physical Society, 2023.
4. B. K C, C Garcia, R Ravelo, "*Phonon Anharmonicity in the Vibrational Entropy of Transition Metals*". Bulletin of the American Physical Society, 2021.
5. B. K C, "*Classical Molecular Dynamical Simulations of Melting Curve of Copper*", 10.13140/RG.2.2.31333.14567, 2018.

PAPERS IN PREPARATION

6. C. Diaz-Caraveo, B. K C, and J. A. Muñoz, "*Lattice dynamics and free energies of Fe-V alloys with thermal and chemical disorder*"(submitted).
7. B. K C, J. A. Munoz, R. Ravelo, "*Anharmonic Vibrational Entropy in Elemental Tantalum at High Temperature*"(preprint).
8. B. K C, R. Parajuli,"*FIRST PRINCIPLES STUDY OF NaCl $\bullet\bullet\bullet$A-B (A-B= C_2H_4, CH_3, NH_3, H_2O, H_2, HF, HNa, HLi, FNa, FLi, NaCl) COMPLEXES*".
9. C. Garcia, B. K C, R. Ravelo, "*Comparative Study of Analytical Models of the Gruneisen Parameter of Metals as a Function of Pressure.*".
10. H. R. Pulido, B. K C, R. Kumar, R. J. Hemley, and J. A. Muñoz, "*Frustrated dynamical instability in body-centered cubic FeV to 80 GPa*".
11. C. Diaz-Caraveo, D. A. Juareza, B. K C, E. O. Oyetunji, and J. A. Muñoz "*Effect of short-range order on the mechanical and thermal properties of shape-memory alloy NiTi.*"