

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 teaching 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:	
	<ul style="list-style-type: none"> • R, Python, Matlab, Mathematica, Gaussian, VASP, MD, QMD, etc. 	
	Programming:	
	<ul style="list-style-type: none"> • C(including OpenMPI, CUDA), Python, UNIX 	
GRANTS, AWARDS, & SCHOLARSHIPS	Scientific Typesetting:	
	<ul style="list-style-type: none"> • L^AT_EX, B_IB_TE_X, Microsoft Office Package, Adobe Package, etc 	
	Operating Systems:	
	<ul style="list-style-type: none"> • Microsoft Windows, Linux, and UNIX 	
GRANTS, AWARDS, & SCHOLARSHIPS	<ul style="list-style-type: none"> • Best Oral Presentation Award, New Mexico State University (NMSU)-NeSA 15th International Conference (March 2024). 	
	<ul style="list-style-type: none"> • Graduate Research Award, Graduate School, UTEP (Fall 202, Spring 2024, Summer 2024). 	
	<ul style="list-style-type: none"> • Forum on Graduate Student Affairs (FGSA) URM March meeting award (Feb 2021). 	
	<ul style="list-style-type: none"> • Reading is Fundamental (RIF) award, College of Science, UTEP (Nov. 2020). 	
	<ul style="list-style-type: none"> • Academic and Research Excellence Outstanding Graduate Student Physics, UTEP, Dec. 2019. 	
	<ul style="list-style-type: none"> • C. Sharp Cook Graduate Scholarship, UTEP (Oct. 2019). 	
	<ul style="list-style-type: none"> • Outstanding achievement: Better Rated by Students, Physics, UTEP (May 2019). 	
PROFESSIONAL TRAINING & WORKSHOPS	<ul style="list-style-type: none"> • 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	
MEMBERSHIP /AFFILIATIONS	PDB3 AWS Python Developer Bootcamp Sep 2022 – Dec 2022 TAKEO TECH LLC Manhattan, New York	
	<ul style="list-style-type: none"> • American Physical Society (APS) • American Mathematical Society (AMS) • Vice President, Nepalese Student Association, UTEP Sep 2019 - Jun 2021 	
ACADEMIC EXPERIENCES	<i>Graduate Research Associate</i> Aug 2023 - Present Computational Science Program, UTEP	
	<i>Visiting Summer Research Student</i> June 2023 - July 2023 The University of California at Berkeley Department of Material Science and Engineering	
	<i>Graduate Teaching Assistant</i> , 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
Department of Physics, UTEP

Jan 2018 - May 2019

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

CONFERENCE PRESENTATIONS

1. “*First Principle Investigation of Magnetic, Elastic, and Thermodynamic Properties of Ordered $D03\text{ Fe}_3\text{V}$* ”, 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 PUBLICATIONS

1. S., Deng, K C, Bimal, & 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. K C, Bimal, ” *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. Munoz, H. Reyes 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. Munoz, “*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 •••A-B (A-B= C₂H₄, CH₃, NH₃, H₂O, H₂, 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. Juarez, 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.*”