## BIMAL K C

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### EDUCATION Ph.D. in Computational Science (CPS)

University of Texas at El Paso (UTEP), El Paso, TX **Expected: Fall 2024** Dissertation title: "Thermal Anharmonicity of Transition Metals: A case study of Tantalum"

MS in Physics

UTEP, El Paso, TX
Awarded: Dec 2019
Tribhuvan University (TU), Kathmandu, Nepal
Awarded: Dec 2016

BS in Physics

TU, Kathmandu, Nepal Awarded: Jan 2013

RESEARCH INTEREST Phase stability & thermodynamics Atomistic modelling & simulations

Phonon & Anharmonicity Computational Physics

ACADEMIC EXPERIENCES Graduate Teaching Assistant
Department of Physics, UTEP

Aug 2024 - Present

• Physics Instructor - Conduct workshop for undergraduate Introductory Mechanics course(including teaching, designing quizzes, & grading).

Graduate Research Associate
Department of Physics, UTEP

Aug 2023 - Aug 2024

- Use of classical (LAMMPS) & quantum Molecular Dynamics (QMD) calculations of vibrational spectra of solids as a function of temperature.
- Study material behavior using *ab-initio* calculation (QMD, DFT, VASP, Quantum Espresso, QHA).
- Reproduce the accurate thermal pressure and equation of states (EOS) in transition metals by including the effect of temperature on the phonon density of state (DOS).

Visiting Summer Research Student
The University of California at Berkeley

Jun 2023 - Jul 2023

• Studied the magnetic Order-Dependent Properties of FeV and Fe<sub>3</sub>V Alloys using density functional theory (VASP).

Graduate Teaching Assistant Computational Science Program, UTEP

Aug 2019 - May 2023

• Math Tutor - Assisted students in undergraduate Math classes (Discrete Mathematics, Differential Equations, Matrix Algebra, & Calculus - up to Calculus III) including concept clarification & problem-solving strategies.

 Teaching Assistant - Assisted professors with grading papers, & conduct weekly workshops for assigned undergraduate/graduate Physics, Mathematics & Computer Science courses.

Graduate Teaching Assistant Department of Physics, UTEP

Aug 2017 - July 2019

- Physics Instructor Taught undergraduate Introductory Electromagnetism, Introductory Mechanics, & undergraduate general Physics Lab (Electronics & Mechanics).
- Teaching Assistant Assisted professors with teaching classes, grading papers, & conducted workshops for assigned undergraduate/graduate Physics courses.

Senior Laboratory Instructor
Department of Physics, UTEP

Jan 2018 - May 2019

 Assisted teaching assistants for undergraduate Electronics & Mechanics weekly laboratory sessions.

#### **PUBLICATONS**

- C. Diaz-Caraveo, B. K. C., & J. A. Muñoz; Lattice Dynamics & Free Energies of Fe-V Alloys with Thermal & Chemical Disorder. Journal of Physics: Condensed Matter (2024). https://doi.org/10.1088/1361-648X/ad66a5.
- Homero Reyes-Pulido, Bimal K C, Ravhi S. Kumar, Russell J. Hemley, Jorge A. Muñoz; Thermally frustrated phase transition at high pressure in B2-ordered FeV. AIP Advances, 14 (7): 075108 (2024). https://doi.org/10.1063/5.0219881.
- S. Deng, B. K C, & V. Kreinovich; Why Optimization Is Faster than Solving Systems of Equations: A Qualitative Explanation. Uncertainty, Constraints, and Decision Making. Cham: Springer Nature Switzerland (2023). 341-344.
- B. K. C., "Quasi-Harmonic & Anharmonic Entropies in Transition Metals" (2019). Open Access Theses & Dissertations. 2866. https://scholarworks.utep.edu/open\_etd/2866.

# UNDER REVIEW/ WORKING PAPERS

- B. K C, R. Parajuli, "First Principle Study of NaCl • A-B (A-B= C<sub>2</sub>H<sub>4</sub>,NH<sub>3</sub>, H<sub>2</sub>O, H<sub>2</sub>, HF, HNa, HLi, FNa, FLi, NaCl) Complexes", (Under Review), The Journal of Chemical Physics.
- B. K C, J. A. Muñoz, R. Ravelo, "Anharmonic Vibrational Entropy in Elemental Tantalum at High Temperature".
- C. Garcia, B. K. C., R. Ravelo, "Comparative Study of Analytical Models of the Gruneisen Parameter of Metals as a Function of Pressure".
- C. Diaz-Caraveo, D. A. Juarez, B. K. C., E. O. Oyetunji, & J. A. Muñoz "Effect of short-range order on the mechanical & thermal properties of shape-memory alloy NiTi."
- B. Ayirizia, B. K. C., & J. A. Muñoz "Magnetic Order-Dependent Properties of FeV and Fe<sub>3</sub> V Alloys: Computational Insights from Density Functional Theory."

# CONFERENCE/ WORKSHOP PRESENTATIONS

• "First Principle Investigation of Magnetic, Elastic, & Thermodynamic Properties of Ordered D03 Fe<sub>3</sub>V", New Mexico State University (NMSU) Nepalese Student Association (NeSA) 15th International Conference, Las Cruces, NM (Mar 16, 2024).

- "Free Energy of the Order-disorder Phase Transition in FeV from Molecular Dynamics", APS March Meeting, Minneapolis, MN (Mar 3 8, 2024).
- "Harmonic Ensemble Lattice Dynamics of Crystals with Thermal & Configurational Disorder", 30th Joint NMSU/UTEP Workshop on Mathematics, Computer Science, & Computational Sciences, University of Texas at El Paso, El Paso, TXM (Oct 28, 2023).
- "Why Optimization is Faster than Solving Systems of Equations: A Qualitative Explanation", 27th Joint NMSU/UTEP Workshop on Mathematics, Computer Science, & Computational Sciences, New Mexico State University, Las Cruces, NM (Apr 2, 2022).
- "Anharmonicity in the Vibrational Entropy of Transition Metals", APS March Meeting, online (Mar 16, 2021).
- "Classical Molecular Dynamical Simulations of Melting Curve of Copper",10th International Conference, 2018, New Mexico State University, Las Cruces, NM (Mar 31, 2018).

# GRANTS, AWARDS, & SCHOLARSHIPS

- Graduate Research Award, Graduate School, UTEP (Aug 2023- Aug 2024).
- Best Oral Presentation Award, New Mexico State University (NMSU)-NeSA 15th International Conference (Mar 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 & 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).

## EXPERTISE

### Computational Science

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

## Data Science & Statistics

• Data Mining, Cluster analysis, Machine Learning, Computational Statistics, Statistical Process Control, etc.

#### Computer Science

• Serial & Parallel Programming, Distributed Data Storage & Processing, Functional & Object-Oriented Programming, etc.

# SOFTWARE SKILLS

#### Statistical Programming & Scientific Computing:

• R, Python, Matlab, Mathematica, Gaussian, C(including OpenMPI), etc.

#### Scientific Typesetting:

• LATEX, BIBTEX, Microsoft Office Package, Adobe Package, etc

## Operating Systems:

• Microsoft Windows, Linux, & UNIX

PROFESSIONAL Grant Writing Skills Series Session TRAINING

UTEP, EL Paso, TX

&

WORKSHOPS

Sustainable Horizons Institute (SHI) Sustainable Research-

-Pathways, Berkeley National Laboratory (DOE)

Berkeley, CA

PDB3 AWS Python Developer Bootcamp

TAKEO TECH LLC, Manhattan, NY

Sep 2022 - Dec 2022

Feb 13, 2024

Jan 10 - 13, 2023

**SERVICE** COURI Annual Symposium at UTEP

Judge Apr 27, 2024

Nepalese Student Association at UTEP

Vice President Sep 2019 - Jun 2021

REFERENCES Available upon request.