BIMAL K C

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EDUCATION

Ph.D. in Computational Science (CPS)
University of Texas at El Paso (UTEP), El Paso, TX **Awarded: Dec 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

Atomistic modelling and simulations
Phonon and Anharmonicity
Phase stability and thermodynamics
Modeling Material behavior at extreme environment
Lattice dynamics and Free energy
Equation of state and thermodynamics
Electronic structure and magnetism

EXPERTISE

Density functional theory(DFT), Quantum molecular dynamics(QMD), Classical molecular dynamics (MD), High-Performance Computing (HPC), Quantum Computing, Serial and Parallel Programming, LAMMPS, Quantum Espresso(QE), and VASP.

ACADEMIC EXPERIENCES

Volunteer Research Scientist
Department of Physics, UTEP Jan 2025 - Present

- Current Project: *"Temperature-dependence of phonons in transition metals."*

Graduate Teaching Assistant
Department of Physics, UTEP Aug 2024 - Dec 2024

- Physics Instructor - Conducted workshop for undergraduate Introductory Mechanics course (including teaching, designing quizzes, and grading).

Graduate Research Associate
Department of Physics, UTEP Aug 2023 - Aug 2024

- Use of classical (LAMMPS) and 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_3V 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, and Calculus - up to Calculus III) including concept clarification and problem-solving strategies.
- Teaching Assistant - Assisted professors with grading papers, and conduct weekly workshops for assigned undergraduate/graduate Physics, Mathematics and Computer Science courses.

Graduate Teaching Assistant
Department of Physics, UTEP Aug 2017 - July 2019

- Physics Instructor - Taught undergraduate Introductory Physics (Electromagnetism, Introductory Mechanics, including teaching and grading).
- Taught undergraduate general Physics Lab (Electronics and Mechanics, including lab equipment setup, guiding students through experiments, and explaining theoretical concepts).
- Teaching Assistant - Assisted professors with teaching classes, grading papers, and 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 and Mechanics laboratory sessions, providing support with laboratory training and experimental setup.

PUBLICATONS

- **B. K C**, R. Parajuli; "*First Principles Study of NaCl···A-B Type (A-B = Acceptor) Complexes*". Journal of Institute of Science and Technology, 30(1), 65–72. https://doi.org/10.3126/jist.v30i1.68199.
- **B. K C**, "*Thermal Anharmonicity of Transition Metals: A Case Study of Tantalum*" (2024). Open Access Theses & Dissertations. 4261. https://scholarworks.utep.edu/open_etd/4261
- 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**, 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.*"

CONFERENCE/ WORKSHOP PRESENTATIONS

- "*First Principle Investigation of Magnetic, Elastic, & Thermodynamic Properties of Ordered D03 Fe_3V*", 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

- **Academic and Research Excellence Outstanding Graduate Student Computational Science**, UTEP (Dec 2024).
- **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 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).

TECHNICAL SKILLS

R, Python, MATLAB, Mathematica, Ovito, Gaussian, C(including OpenMPI), Java, SQL, Linux, and UNIX, etc.