

<b>EDUCATION</b>	<b>Ph.D. in Computational Science (CPS)</b> The University of Texas at El Paso (UTEP), El Paso, TX Dissertation title: <i>“Thermal Anharmonicity of Transition Metals : A case study of Tantalum”</i> Awarded: Dec 2024
	<b>MS in Physics</b> UTEP, El Paso, TX Awarded: Dec 2019
	<b>BS in Physics</b> Tribhuvan University (TU), Kathmandu, Nepal Awarded: Dec 2016
	<b>BS in Physics</b> TU, Kathmandu, Nepal Awarded: Jan 2013
<b>RESEARCH INTEREST</b>	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
<b>EXPERTISE</b>	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.
<b>PROFESSIONAL POSITIONS</b>	<i>Professor of Physics</i> Department of Science and Agriculture Central Texas College (CTC),Killeen, TX Sep 2025 - Present
<b>ACADEMIC EXPERIENCES</b>	<i>Research Scientist</i> Department of Physics, UTEP El Paso, TX Jan 2025 - Aug 2025 (Full-time) Sep 2025 - Dec 2025 (Part-time) <ul style="list-style-type: none"><li>• Investigated lattice dynamics, phonon behavior, and thermal properties of metals and alloys under a wide range of temperature and pressure conditions using atomistic simulations.</li><li>• Modeled free energies, phase stability, and thermodynamic properties of materials beyond the quasiharmonic approximation, incorporating anharmonic effects.</li><li>• Developed and applied advanced computational methods, including Molecular Dynamics and machine-learning–based interatomic potentials, to study materials with near first-principles accuracy.</li></ul> <i>Graduate Teaching Assistant</i> Department of Physics, UTEP Aug 2024 - Dec 2024 <ul style="list-style-type: none"><li>• Physics Instructor - Conducted workshop (three sessions per week) for undergraduate Introductory Mechanics course (including teaching, designing quizzes, &amp; grading).</li></ul>

*Graduate Research Associate*  
Department of Physics, UTEP

Aug 2023 - Aug 2024

- Used classical (LAMMPS) & quantum Molecular Dynamics (QMD) calculations of vibrational spectra of solids as a function of temperature.
- Studied material behavior using *ab-initio* calculation (QMD, DFT, VASP, Quantum Espresso, QHA).
- Reproduced 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).
- Built HPE workflows for material modelling using Python, Bash environment.
- Machine learning assisted analysis of material datasets.

*Graduate Teaching Assistant*  
Computational Science Program, UTEP

Aug 2019 - May 2023

- Teaching Assistant - Assisted professors with grading papers, & conduct weekly workshops for assigned undergraduate/graduate Computer Science (Statistical Data Mining (using R and Python) and Statistical Programming in R) courses.
- 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.

*Graduate Teaching Assistant*  
Department of Physics, UTEP

Aug 2017 - July 2019

- Physics Instructor - Taught undergraduate Introductory Physics (Electromagnetism, Introductory Mechanics, four sessions per week- including teaching & grading).
- Taught undergraduate general Physics Lab (Electronics & Mechanics, 3 sessions per week- including lab equipment setup, guiding students through experiments, and explaining theoretical concepts).
- 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 laboratory sessions (two sessions per week), providing support with laboratory training and experimental setup.

## **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 & 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).

## PUBLICATIONS

- **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](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. <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](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<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).

## TEACHING EXPERIENCE

**PHYS 2425 University Physics I:** Fundamental principles of physics (Introductory calculus-based Classical Mechanics and Thermodynamics). Fall 2025.

**PHYS 1401 College Physics I:** Fundamental principles of physics (Introductory algebra-based Classical Mechanics and Thermodynamics). Fall 2025.

**PHYS 1415 Physical Science:** Conceptual Physical Science for first-year college non-science majors. Fall 2025.

## SOFTWARE SKILLS

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

## SERVICE

Nepalese Student Association at UTEP  
Vice President

Sep 2019 - Jun 2021