

<b>EDUCATION</b>	<b>Ph.D. in Computational Science (CPS)</b> 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 Tribhuvan University (TU), Kathmandu, Nepal Awarded: Dec 2019 Awarded: Dec 2016
	<b>BS in Physics</b> TU, Kathmandu, Nepal Awarded: Jan 2013
<b>RESEARCH INTEREST</b>	Atomistic modeling and simulations Phonon and Anharmonicity Phase stability and thermodynamics Modelling Material behavior at extreme environment Lattice dynamics and Free energy Equation of state (EOS) and thermodynamics
<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>ACADEMIC EXPERIENCES</b>	<i>Graduate Teaching Assistant</i> Department of Physics, UTEP Aug 2024 - Present <ul style="list-style-type: none"><li>• Physics Instructor - Conduct workshop (three sessions per week) for undergraduate Introductory Mechanics course (including teaching, designing quizzes, and grading).</li></ul>
	<i>Graduate Research Associate</i> Department of Physics, UTEP Aug 2023 - Aug 2024 <ul style="list-style-type: none"><li>• Use of classical (LAMMPS) and quantum Molecular Dynamics (QMD) calculations of vibrational spectra of solids as a function of temperature.</li><li>• Study material behavior using <i>ab-initio</i> calculation (QMD, DFT, VASP, Quantum Espresso, QHA).</li><li>• 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).</li></ul>
	<i>Visiting Summer Research Student</i> The University of California at Berkeley Jun 2023 - Jul 2023 <ul style="list-style-type: none"><li>• Studied the magnetic Order-Dependent Properties of FeV and Fe<sub>3</sub>V Alloys using density functional theory (VASP).</li></ul>

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, four sessions per week- including teaching and grading).
- Laboratory Instructor: Taught undergraduate general Physics Lab (Electronics and 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, 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 (two sessions per week), providing support with laboratory training and experimental setup.

## 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](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*".

**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 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, Gaussian, C(including OpenMPI), Linux, and UNIX, etc.

**SERVICE**

COURI Annual Symposium at UTEP  
Judge

Apr 27, 2024

Nepalese Student Association at UTEP  
Vice President

Sep 2019 - Jun 2021

## REFERENCES

**Ramon Ravelo, Ph.D.(Dissertation Chair)**

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**Jorge A. Muñoz, Ph.D.(Dissertation Co-chair)**

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**Sreeprasad T. Sreenivasan , Ph.D.(Dissertation Committee Member)**

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