BIMAL K C, MS, Ph.D. candidate (ABD)

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INFORMATION E-mail: bkc@miners.utep.edu

LinkedIn: in/kcbimal

EDUCATION Ph.D. in Computational Science

University of Texas at El Paso (UTEP), El Paso, TX Expected: Fall 2024

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

ACADEMIC INTEREST & EXPERTISE

Computational Science (CPS):

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

Data Science & Statistics:

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

Computer Science:

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

ACADEMIC EXPERIENCES Graduate Research Associate
Department of Physics, UTEP

Aug 2023 - Present

Visiting Summer Research Student

The University of California at Berkeley Jun 2023 - Jul 2023

Graduate Teaching Assistant, UTEP

Computational Science Program, UTEP Jun 2022 - Aug 2022 Department of Physics, UTEP Aug 2017 - May 2019

- Tutor Algebra & Calculus at Math Resource Center for Students (MaRCS).
- Teaching Instructor Introductory Electromagnetism & General Physics Lab.

Lab Instructor for TA's- Introductory Electromagnetism Lab

Department of Physics, UTEP Jan 2018 - May 2019

RESEARCH INTEREST

 \bullet Theoretical computer science emphasizing modeling, simulation, & visualization for understanding real-world phenomena & computation fundamentals.

- Develop a mathematical models using appropriate numerical methods, implement them in the form of a computer program, and visualize the numerical results.
- Use of classical & ab- initio calculations of vibrational spectra of solids as a function of temperature.
- Understanding material behavior using ab-initio calculation (QMD, DFT, VASP, Quantum Espresso, QHA).
- Phase stability of the material & their alloys, phonons, & phonon entropy, Machine learning, Atomistic simulations of materials at extreme environment.

PUBLICATONS

- 1. 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.
- 2. 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.
- 3. 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.
- 4. 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

- 5. B. K. C., R. Parajuli, "First Principle Study of NaCl $\bullet \bullet \bullet A$ -B (A-B= C_2H_4 , NH₃, H_2O , H_2 , HF, HNa, HLi, FNa, FLi, NaCl) Complexes", (Under Review), The Journal of Chemical Physics.
- 6. B. K.C., J. A. Muñoz, R. Ravelo, "Anharmonic Vibrational Entropy in Elemental Tantalum at High Temperature".
- 7. C. Garcia, B. K. C., R. Ravelo, "Comparative Study of Analytical Models of the Gruneisen Parameter of Metals as a Function of Pressure.".
- 8. 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."
- 9. B. Ayirizia, B. K. C., & J. A. Muñoz "Magnetic Order-Dependent Properties of FeV and Fe₃V Alloys: Computational Insights from Density Functional Theory."

CONFERENCE PRESENTATIONS

- "First Principle Investigation of Magnetic, Elastic, & Thermodynamic Properties of Ordered D03 Fe₃V", New Mexico State University (NMSU) Nepalese Student Association (NeSA) 15th International Conference, Las Cruces, NM (Mar 16, 2024).
- 11. "Free Energy of the Order-disorder Phase Transition in FeV from Molecular Dynamics", APS March Meeting, Minneapolis, MN (Mar 3 8, 2024).
- 12. "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).

- 13. "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).
- 14. "Anharmonicity in the Vibrational Entropy of Transition Metals", APS March Meeting, online (Mar 16, 2021).
- 15. "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- Present).
- 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).
- Graduate Assistantship, College of Science, UTEP (Aug 2017-May 2023).

SOFTWARE SKILLS

Statistical Programming & Scientific Computing:

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

Scientific Typesetting:

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

Operating Systems:

• Microsoft Windows, Linux, & UNIX

PROFESSIONAL TRAINING

PROFESSIONAL Sustainable Horizons Institute (SHI) Sustainable Research Pathways,

& Berkeley National L. Berkeley, California

Berkeley National Laboratory (DOE)

WORKSHOPS

PDB3 AWS Python Developer Bootcamp

Sep 2022 - Dec 2022

Jan 2023

TAKEO TECH LLC Manhattan, New York