

EDUCATION:

2018 Jun – 2023 Dec	University of California, Merced, CA, USA PhD in Physics (Supervisor: Prof. David Strubbe) Thesis: “Understanding the Structure, Electronic, Phononic, Optical, and Mechanical Properties of Low-Dimensional Materials”
2018 Jan – 2018 May	Missouri State University, Springfield, MO, USA Master’s Program in Material Science Studied for a semester and later transferred to UC Merced for PhD program
2012 Aug – 2016 Aug	Kathmandu University, Dhulikhel, Kavre, Nepal Thesis: “Numerical analysis of effects of void factor, inlet temperature, initial fluid flow-rate, and particle size for solar thermal energy storage in packed pebble bed” Supervisor: Dr. Ujjwal Man Joshi

RESEARCH/WORK EXPERIENCE:

2024 January onwards	Postdoctoral Research Associate: Los Alamos National Laboratory <u>Experiments:</u> Fabrication of magneto-thermoelectric MEMS platforms, quantum materials synthesis (HfTe5), contacts and device processing in a cleanroom at Sandia National Lab, quantum materials theory using density functional theory and GW-BSE, strain-tuned transport and Raman properties, high magnetic field experimentation, cryogenic experiment setup, experiment remote control setup, ultrafast optical characterization, and class3B/4 laser operation and alignments. <u>Simulations:</u> Understand the bandstructure of topological materials, Polarized Raman simulation under strain, temperature dependent Raman, Thermodynamic properties (Grüneisen parameters, heat capacity, phonon lifetimes, phonon scattering mechanism, and thermal conductivity).
2018 Summer & Fall and 2019 Fall onwards	Supervisor: Professor David Strubbe, UC Merced <u>Ni doped MoS₂:</u> Studied possible favorable site for Ni in bulk and monolayer phases, electronic and mechanical properties, IR and Raman spectra, structural relaxation, topological invariants, new structure analysis. <u>New Phase in TMD:</u> Discovered the new phase in TMD and worked the structural identification, and experimental synthesis route, characterization technique, and possible application unique to this phase. <u>Perovskites (1D, 2D and 1.5D):</u> Studied the excited state properties, optical absorption, self-trapped excitons mechanism, symmetry analysis of the structure, transport properties like electrical and thermal conductivities, dielectric tensor, electron-phonon coupling, vibrational modes, polarized Raman and IR. <u>Code development:</u> Polarized Raman spectra from Quantum ESPRESSO, and Excited State Forces in BerkeleyGW.
2022 September – 2023 August	Supervisor: Dr. Michael T. Pettes, Los Alamos National Laboratory Simulating polarized Raman, elastic coefficients, strained Raman and Bandstructure

2019 Spring	<p>calculation of HfTe_5 using DFT. Experimental work on polarized Raman Spectroscopy and micro-electromechanical system fabrication for magneto-thermal transport measurements in a cleanroom.</p> <p>Supervisor: Professor Sarah Kurtz, UC Merced</p> <p>Theoretical Study on Temperature Coefficient for Open Circuit Voltage</p> <p>Modelled the Shockley-Queisser Limit in python and studied the open circuit voltage as a function of temperature over different band gap material.</p>
2018 January – 2019 May	<p>Teaching Assistant: Calculus I and II</p> <p>Attend lectures, Instruction of 1-3 section of lab per week, Hold 2 office hours per week, Supervise ASE meeting, Read and evaluate up to 2 weekly quizzes, proctor all examinations, Perform individual/group tutoring, Maintain/submit student records.</p>
2015 August – 2017 December	<p>Research Assistant in Chemical Engineering Lab, Kathmandu University</p> <p>Supervisor: Dr. Bhim Kafle</p> <p>Worked in Kathmandu University Solar Energy Laboratory to design a dye-sensitized solar cell and installed the first Solar Simulator in Nepal. I conducted solar cell efficiency measurements and provided training to other students.</p>

TECHNICAL SKILLS:

Experimental Skills:	<p>Design: Proficiency in Tanner L-Edit for multi-layer nano-device design</p> <p>Fabrication: Expertise in various fabrication techniques including SiN MEMS, JEOL e-beam lithography, chemical vapor deposition, atomic layer deposition, sputtering, wet etching, plasma etching and cleaning. Experience with cleanroom processes for nanofabrication.</p> <p>Characterization and Testing: Skilled in using SEM, profilometers, and Keyence digital microscope for material characterization. Proficient in sensitive electrical and thermal measurements of nanostructures. Experience of measuring transport properties of materials in high (and pulsed) magnetic fields. Familiarity with in-situ stress cells (Razorbill).</p> <p>Optical Spectroscopy: Proficiency in operating and maintaining ultrafast optical spectroscopic systems. Experience with micro-Raman/photoluminescence systems (Horiba LarRAM HR Evolution) with cryogenic systems (He_4, He_3, dilution, and adiabatic demagnetization cryostats). Competence in handling complex ultrafast amplified Class 3B/4 laser systems with alignment using polarization optics.</p> <p>Programming and Data Analysis: Proficiency in computer programming using LabVIEW and Python for computer-controlled data acquisition and analysis. Experience in data acquisition using low-level precision instruments, including Keithley and Stanford Research instruments (Lock-In Amplifiers, Photon Counters, Voltage and Current Sources).</p>
Material Simulations	<p>Ground State: Experience in transition metal doping on 2D materials, phase diagram, transport properties, stress-strain analysis, new phase and symmetry analysis, topological phase analysis, electronic structures, piezoelectric, ferroelectric, magnetization, spintronics, polarized Raman and IR spectroscopy using density functional theory in Quantum Espresso or VASP, Wannier90, EPW and BoltzTraP.</p> <p>Excited State: Experience in excited state studies on materials using Green's function and Bethe-Salpeter equation (GW-BSE) to explore the electronic structure and dynamics of excitons and self-trapped excitons, absorption and photoluminescence spectra, and GW level excited state forces for excitons structures and force field generations.</p>

	<p>Excited State Forces: Using novel and more accurate GW-BSE method to calculate excited state forces and hence understand light matter interaction upon absorption, exciton structures, and excited state structures.</p> <p>Molecular Dynamics: Using LAMMPS, studied the Ni doping in understanding the friction and wear in MoS₂. ReaxFF Reactive Force Field for Ni-doped MoS₂.</p> <p>Machine Learning: Raman spectra under strain and high throughput superconducting material search.</p>
Language/ Script	Python, MATLAB, C, Bash Script
Tools and IDE's	Quantum Espresso, BerkeleyGW, EPW, VASP, AiiDA, ASE, TORA, BoltzTrap, Z2Pack, Wannier90, WannierTools, RESPACK, LATEX, Spyder, Gnuplot, Origin, Google Sketchup, GIMP, Ovito, Vesta, Xcrysden, Blender, ISOTROPY
Libraries Database	Scikit-learn, TensorFlow, NumPy, Matplotlib, Pandas, SciPy, Seaborn, Plotly

PUBLICATIONS:

1. Jun B. Park, **Rijan Karkee**, Michael T. Pettes*, “Improved thermoelectric performance in Cr-doped Bi₂Te₃ nanoribbon”, *Materials Today Quantum (under review)*, (2025).
2. Micah P. Vallin, **Rijan Karkee**, Hisato Yamaguchi, Chanhoo Lee, Ramon M. Martinez, Saryu J. Fensin, Jun Beom Park, Richard Z. Zhang, and Michael T. Pettes*, “Thermal conductivity of graphene coated copper under uniaxial tensile mechanical strain”, *Nanoscale Advances* 7, 3655-363 (2025).
3. Micah P. Vallin, **Rijan Karkee**, Theresa M. Kucinski, Huan Zhao, Han Htoon, Chanhoo Lee, Ramon M. Martinez, Saryu J. Fensin, Richard Z. Zhang, and Michael T. Pettes*, "SnSe₂ thermal conductivity from optothermal Raman and Stokes/anti-Stokes thermometry," *Nanotechnology* 36(9), 095401 (2024). <https://doi.org/10.1088/1361-6528/ad99df>, LA-UR-24-30121
4. Theresa M. Kucinski, Rohan Dhall, Benjamin H. Savitzky, Colin Ophus, **Rijan Karkee**, Avanish Mishra, Enkeleda Dervishi, Jun Hoon Kang, Chul-Ho Lee, Jinkyoungh Yoo, and Michael T. Pettes*, "Direct measurement of the thermal expansion coefficient of epitaxial WSe₂ by four-dimensional scanning transmission electron microscopy," *ACS Nano* 18(27), 17725–17734 (2024). <https://doi.org/10.1021/acsnano.4c02996>, LA-UR-23-30920
5. Jun Beom Park, Wei Wu, Jason Yingzhi Wu, **Rijan Karkee**, Theresa Marie Kucinski, Karen C. Bustillo, Matthew M. Schneider, David A. Strubbe, Colin Ophus, and Michael Thompson Pettes*, "Carrier type switching in bismuth telluride nanoribbons through *in-situ* organic molecule coating," *Nano Letters* 23(24), 11395–11401 (2023). <https://doi.org/10.1021/acs.nanolett.3c02000>, LA-UR-23-26384
6. **Rijan Karkee** and David A. Strubbe*, “Panoply of doping-induced reconstructions and electronic phases in Ni-doped 1T-MoS₂,” *Journal of Physical Chemistry Letters* 15, 2, 565-574 (2024). <https://doi.org/10.1021/acs.jpclett.3c03175>
7. Sujin Lee, **Rijan Karkee**, Azza Ben-Akacha, Derek Luong, J. S. Raaj Vellore Winfred, Xinsong Lin, David A. Strubbe*, Biwu Ma*, “One-dimensional organic metal halide nanoribbons with dual emission,” *Chemical Communication*, 59, 3711-3714 (2023). DOI: 10.1039/D3CC00044C
8. Luke M. McClintock, Long Yuan, Ziyi Song, Michael T. Pettes, Dmitry Yarotski, **Rijan Karkee**, David A. Strubbe, Liang Z. Tan, Azza Ben-Akacha, Biwu Ma, Yunshu Shi, Valentin Taufour, Dong Yu*, “Surface effects on anisotropic phonoluminescence in one-dimensional organic metal halide hybrids,” *Small Structures* **2200387** (2023). <https://doi.org/10.1002/sstr.202200378>
9. **Rijan Karkee**, Enrique Guerrero, David A. Strubbe*, “Enhanced interlayer interactions in Ni-doped MoS₂ and structural and electronic signatures of doping site,” *Physical Review Materials* 5, 7 (2021). <https://doi.org/10.1103/PhysRevMaterials.5.074006>

10. Enrique Guerrero, **Rijan Karkee**, David A. Strubbe*, “Phase Stability and Raman/IR Signatures of Ni-Doped MoS₂ from Density Functional Theory Studies,” *Journal of Physical Chemistry C* 125, 24, 13401-13412 (2021). <https://doi.org/10.1021/acs.jpcc.1c02974>
11. **Rijan Karkee**, David A. Strubbe*, “Low-energy nine -layer rhombohedral stacking of transition metal dichalcogenides,” *arXiv:2404.17575* (2024).
12. Bijaya Basnet, Mahesh Nepal, Gaurab J. Thapa, Madhav Kafle, Ram P. Kharel, **Rijan Karkee**, Tara P. Dhakal, Bhim P. Kafle*, “Theoretical model for determining the thickness and optical constants of transparent conducting oxide thin films from the measured reflectance spectra,” *Surface and Interface Analysis* 0, 1-12 (2024)
13. **Rijan Karkee**, Azza Ben-Akacha, Biwu Ma, Michael T. Pettes, David A. Strubbe*, “Anisotropy and exciton-self trapping in the 1D organic metal halide hybrids,” *in preparation* (2025).
14. **Rijan Karkee**, Jinyu Liu, Luis Jauregui, David A. Strubbe, Michael T. Pettes*, “Polarized Raman spectroscopy of HfTe5 under strain from DFT and experiment,” *in preparation* (2025).
15. **Rijan Karkee*** and Sumit Khadka, “Closer approximation to optimize solar panels performance with cleaning cycle: a follow-up,” *Open Journal of Energy Efficiency* 8, 04, 166 (2019).
16. **Rijan Karkee***, Sumit Khadka, Gaurav Luitel, Mausham Devkota, Bibek Khadka, Shushilata Sapkota, Puja Bhetwal, “Comparing and optimizing of solar insolation on yearly, monthly and seasonally basis for solar devices performance in Nepal,” *International Journal of New Technology and Research* 3, 1, 26-33 (2017).
17. **Rijan Karkee***, Sumit Khadka, Saurav Gautam, “Introducing a modified water powered funicular technology and its prospective in Nepal,” *International Journal of Science and Technology* 4, 8, 412-419 (2015).

CONFERENCE PRESENTATIONS:

- R. Karkee, D. A. Strubbe, “Anisotropy and exciton self-trapping in the 1D perovskite C₄N₂H₁₄PbBr₄ from first principles”, March Meeting, American Physical Society, Las Vegas, USA, 2023
- R. Karkee, D. A. Strubbe, “Panoply of doping-induced reconstructions and electronic phases in Ni-doped 1T-MoS₂”, March Meeting, American Physical Society, Chicago, USA, 2022
- R. Karkee, E. Guerrero and D. A. Strubbe, “Structural studies of Ni-doped MoS₂ monolayers and polytypes using density functional theory (DFT)”, March Meeting, American Physical Society, virtual, 2021
- Molecular Foundry User Meeting, “Structural studies of Ni-doped MoS₂ monolayers and polytypes using density functional theory (DFT)”, Lawrence Berkeley National Laboratory, Poster Presentation, 2020
- Virtual Electronic Structure Methods, “Structural studies of Ni-doped MoS₂ monolayers and polytypes using density functional theory (DFT)”, UC Merced, Poster Presentation, 2020
- R. Karkee, P. Subedi, A. Poudel, S. Thapa and B. Kafle, “Performance Test of Dye Sensitized Solar Cell with Solar Cell Simulator”, 3rd National Symposium on Nanotechnology and Material Processing, Dhulikhel, Nepal, 2017

TRAINING, WORKSHOPS & INDEPENDENT STUDY:

- Virtual school on many body calculations using EPW and BerkeleyGW, 2023
- MagLab Summer School, University of Florida, 2023
- Wannier 2022 Summer School, virtual, May 16- 20, 2022
- 8th BerkeleyGW Tutorial Workshop and 3rd Berkeley Excited State Conference, virtual, 2022
- Python for Data Science, IBM (online)
- Machine Learning Tutorial with Python
- Deep Learning with TensorFlow, Keras and Python

- Data Analysis and Modern Visualization, APS March Meeting, virtual, 2021
- 7th BerkeleyGW Tutorial Workshop and 2nd Berkeley Excited State Conference, virtual, 2021
- ICTP/CERN Experimental Physics Masterclass, Kathmandu University, Dhulikhel, Nepal, 2014

SCHOLARSHIPS/FELLOWSHIPS:

- Merced nAnomaterials Center for Energy Sensing (MACES) Summer Fellowship, (NASA funded program) (2019, 2021)
- Physics Departmental Fellowship, University of California Merced (2022)
- Wells Mountain Initiative Scholarship (2012-2016)
- Abi Kattel Memorial Scholarship (2012)
- United States Education Foundation Nepal's Opportunity Funds Scholar (2011)

ORGANIZATIONAL ACTIVITIES:

- Mentored high school students in a project aimed at optimizing the tilt angle for solar panels and water heaters through Incubate Nepal (2021)
- Co-founded STEM Foundation Nepal (2017) to foster interest in STEM fields among Nepalese high school students and provide exposure to international platform.
- Served as an executive member of Kathmandu University Robotics Club (2015) where I played a key role in establishing and promoting hands-on robotics training for students from diverse backgrounds.