

Kuntal Talit, Ph. D.

Postdoctoral Research Associate, University of California, Merced

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Education

University of California, Merced

Ph.D. in Physics

01/2017 – 08/2022

Advisor: Prof. David A. Strubbe

MS in Physics

01/2017 – 12/2019

Indian Institute of Engineering Science and Technology, India

M. Tech. in Materials Engineering

07/2009 – 06/2011

M.Sc. in Applied Physics

07/2007 – 06/2009

Employment

Postdoctoral Research Associate

11/2022 – Present

Department of Chemical & Materials Engineering

University of California, Merced

Advisor: Prof. Elizabeth Nowadnick

Mainframe Application Developer

06/2011 – 07/2016

IBM India, Bangalore

Research Experience

Postdoctoral Research Associate - Nowadnick Group

11/2022 – Present

Chemical & Materials Engineering, University of California, Merced.

- Developing **TritonDFT**, an agentic AI platform that automates end-to-end first-principles workflows, including structure acquisition, VASP and Quantum ESPRESSO input generation, remote HPC configuration, Slurm job submission and monitoring, error diagnosis, and results analysis.
- Developing an LLM-based literature agent to retrieve, analyze, and synthesize research papers, identify relevant materials and computational methods, and translate published findings into actionable DFT research directions.
- Currently investigating topological quantum materials within the multi-campus UC-LEAP collaboration, generating reproducible first-principles datasets to study the relationships among crystal structure, defects, magnetism, and topological behavior.
- Developed Python- and SQL-based computational workflows using Materials Project and OQMD data for high-throughput materials simulations and AI-guided materials discovery.
- Led first-principles studies of Ca- and Ti-doped hexagonal TbInO₃, establishing how doping modifies local structure, defect energetics, charge localization, electronic structure, band gaps, and dielectric response; this work contributed to two publications.

- Investigated anion substitution and point defects in titanate and vanadate pyrochlores and spinel oxides, evaluating site preference, charge compensation, conductivity, stability, and dopant-induced electronic behavior.
- Collaborated with experimental researchers at Stanford, Cornell, Harvard, and national laboratories to connect first-principles predictions with synthesis and characterization of doped TbInO_3 project.

Research Assistant - Strubbe Ab Initio Laboratory (SAIL)

01/2017 – 08/2022

Dept. of Physics, University of California, Merced.

- Ph. D. dissertation: "Investigation of local strain, symmetry, and elastic properties of methylammonium lead iodide (MAPI) hybrid perovskite using density functional theory."
- Developed a method to calculate vibrational mode symmetry in approximately symmetric materials.
- Implemented feature updates in Quantum ESPRESSO, enhancing its computational capabilities.
- Quantified localized strains in MAPI through theoretical Raman and IR spectroscopy.
- Automated computational workflows using Shell and Python scripts, reducing solution time by 50x.
- Performed structural optimization, electronic structure, DFPT phonon, Raman/IR spectroscopy, elastic tensor, and stress-dependent calculations for hybrid perovskites.
- Optimized Quantum ESPRESSO parallelization and compute node configurations on HPC systems.
- Led a multidisciplinary Lawrence Livermore National Laboratory data-science project involving exploratory data analysis, feature engineering, random forests, support-vector machines (80% accuracy), and a three-dimensional convolutional neural network for molecular binding prediction.

Graduate Researcher - Martini Research Group

08/2016 – 01/2017

Advisor: Prof. Ashlie Martini

Dept. of Mechanical Engineering, University of California, Merced

- Investigated the role of humidity on friction within MoS_2 sliding interfaces. Used molecular dynamics (MD) simulations in LAMMPS to study MoS_2 layer interactions using REAX, REBO, and LJ interatomic potentials.

Graduate Researcher - IACS Kolkata, India

06/2010 – 06/2011

Advisors: Prof. Gour P. Das and Prof. N. R. Bandyopadhyay

- M. Tech. thesis: Ground state properties of homo- and hetero- clusters of group-IV elements.

Graduate Researcher - IEST, Shibpur, India

01/2009 – 06/2009

Advisor: Prof. S. Minhaz Hossain

- M.Sc. thesis: Experimental studies on critical opalescence in binary fluid.

Teaching and Mentoring Experience

Teaching Assistant, University of California Merced

Aug. 2016 - May. 2018

- PHYS-009: Introductory Physics II for Physical Science and Engineering Majors.
 - Conducted a weekly classroom session and a lab, where I designed problem sets for classroom practice, aiding students in understanding and solving their homework. Each lab session began with a focused 15-20 minute overview of the relevant theory and methods. Additionally, I was responsible for grading homework and lab work, providing timely feedback to support students' learning and progress.
- ME-021: Fortran and Matlab programming.
 - Facilitated two lab sessions weekly, thoroughly covering the theoretical aspects alongside coding examples. The entire course, including homework assignments, was managed via CatCourses, an online educational platform. Conducted plagiarism checks on each coding assignment to ensure originality and graded them based on their adherence to academic integrity guidelines.
- During my PhD, I mentored an undergraduate student from the University of Texas at El Paso during a summer research internship and guided junior graduate students on project-specific computational research tasks.
- Currently mentoring two graduate students in Quantum ESPRESSO, VASP, fundamental and practical aspects of DFT, and the use of our in-house TritonDFT agentic AI platform for routine computational workflows.

Technical Skills

- **Electronic structure and atomistic simulation:** VASP, Quantum ESPRESSO, LAMMPS, spin-polarized DFT, DFT+ U , spin-orbit coupling, hybrid-functional benchmarking, density of states, band structures, charge localization, dielectric response, DFPT phonons, elastic properties, classical molecular dynamics, substitutional doping, point defects, defect formation energies, phase stability, and finite-size corrections.
- **Scientific computing and machine learning:** Python, NumPy, SciPy, pandas, scikit-learn, TensorFlow, matplotlib, pymatgen, FORTRAN, MATLAB, SQL, Bash, Git, and $\text{\LaTeX}$; random forests, support-vector machines, and convolutional neural networks.
- **Workflow automation and HPC:** End-to-end automated DFT workflows, LLM-assisted input generation and validation, SSH-based remote execution, Slurm job preparation and monitoring, provenance and reproducibility, and computing on NERSC, SDSC Expanse, and UC Merced clusters.
- **AI-assisted development:** GitHub Copilot, Claude, ChatGPT/Codex, Ollama, and Nemotron for scientific-software development and autonomous simulation workflows.

Fellowships & Awards

- NASA-funded Merced Nanomaterials Center for Energy and Sensing (MACES) Summer Research Fellowship; 2022 MACES Grad-Slam finalist. 2018, 2021, 2022

- Dan David Solar Fellowship, University of California, Merced. 2018
- 2nd prize for poster competition at APS Bridge Program and National Mentoring Community Conference, Stanford University & Google HQ. 2018
- Certificate of appreciation from ESI and IBM for ability to quickly learn and deliver during command center support. 2013
- Outstanding Contributor Award at IBM India. 2012

Publication

- "Structural and electronic properties of Ti- and Ca-doped hexagonal TbInO₃"
Kuntal Talit, Nabaraj Pokhrel, Yang Zhang, Johanna Nordlander, Margaret A. Anderson, Eli Gerber, Eun-Ah Kim, Julia A. Mundy, Ismail El Baggari, and Elizabeth A. Nowadnick
[Physical Review Materials](#), 9, 114401 (2025)
- "Signatures of quantum spin liquid state and unconventional transport in thin film TbInO₃"
J. Nordlander, M. A. Anderson, T. Chiang, A. Kaczmarek, N. Pokhrel, K. Talit, S. Doyle, E. Mercer, C. Tzschaschel, J.-H. Son, H. El-Sharif, C. M. Brooks, E.-A. Kim, A. de la Torre, I. E. Baggari, E. A. Nowadnick, K. Nowack, J. T. Heron, and J. A. Mundy.
[Nature Communications](#), 16, 9469 (2025)
- "Stress effects on Raman spectroscopy of cubic hybrid perovskite: A probe of local strain"
Kuntal Talit and David A. Strubbe
[The Journal of Physical Chemistry C](#) 2020, 124, 50, 27287–27299

Manuscripts in Preparation (available in arXiv)

- "TritonDFT: Automating DFT with a Multi-Agent Framework"
Zhengding Hu, Kuntal Talit, Zhen Wang, Haseeb Ahmad, Yichen Lin, Prabhleen Kaur, Christopher Lane, Elizabeth A. Peterson, Zhiting Hu, Elizabeth A. Nowadnick, and Yufei Ding
Manuscript in preparation (2026) — [arXiv:2412.17771v1](#) [[cond-mat.mtrl-sci](#)]
- "Quantifying Hidden Symmetry in the Tetragonal CH₃NH₃PbI₃ Perovskite"
Kuntal Talit and David A. Strubbe
To be submitted to J. Phys. Chem. Lett. (2025) - [arXiv:2301.11281v1](#) [[cond-mat.mtrl-sci](#)]
- "Resolving Discrepancies in Mechanical Properties of CH₃NH₃PbI₃ Perovskites"
Kuntal Talit and David A. Strubbe
To be submitted to Phys. Rev. Mater. (2025) - [arXiv:2412.17771](#) [[cond-mat.mtrl-sci](#)]

Invited Talks

- **Accelerating Research with Autonomous AI Agents**, Invited Talk, Mathematical Biology SMART Team/Directed Study Group, University of California, Merced, April 1, 2026.
- **Engineering Function Through Imperfection: A First-Principles Perspective**, Invited Seminar, California State University, Fresno, January 23, 2026.

- **Listening to the Lattice: DFT Insights into Stress, Raman Signatures, and Defect Physics**, Invited Seminar, Materials and Biomaterials Science and Engineering, University of California, Merced, December 8, 2025.

Conference Presentations

- "TritonDFT: An Expert-Informed Agentic Framework and Benchmark for Automated DFT Workflows" (**Poster**) 2026
AI Science at Scale Annual Meeting, UC-LEAP Project, Santa Fe, New Mexico.
- "TritonDFT: Empowering Materials Discovery with Multi-Agent Automation" (**Poster**) 2026
School of Engineering Industry Day, University of California, Merced.
- "Electronic Effects of Anion Substitution in Titanate and Vanadate Pyrochlores from First Principles" 2026
American Physical Society March Meeting, Denver, Colorado, March 2026. (**Contributed talk**)
- "First-Principles Investigation of Anion Substitution in Vanadate and Titanate Pyrochlores" 2025
APS March Meeting, Anaheim, California, March 2025. (**Contributed talk**)
- "Structural and Electronic Properties of Ti- and Ca-Doped Hexagonal TbInO_3 " 2024
K. Talit, N. Pokhrel, Y. Zhang, J. Nordlander, I. El Baggari, J. Mundy, and E. Nowadnick, Materials Research Society Spring Meeting (**contributed talk**)
- "Quantifying Hidden Symmetry in the Tetragonal $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite" 2023
K. Talit and D. Strubbe, APS March Meeting (**contributed talk**)
- "Resolving Discrepancies in Mechanical Properties of Hybrid Perovskites: A DFT Study" 2022
K. Talit and D. Strubbe, APS March Meeting (**contributed talk**)
- "Interplay of Structural Changes, Symmetry, and Vibrations in Orthorhombic and Tetragonal Hybrid Perovskites Under Stress" 2021
K. Talit and D. Strubbe, Molecular Foundry User Meeting, Lawrence Berkeley National Laboratory (LBNL) (**contributed talk**)
- "Interplay of Structural Changes, Symmetry, and Vibrations in Orthorhombic and Tetragonal Hybrid Perovskites Under Stress" 2021
K. Talit and D. Strubbe, APS March Meeting (**contributed talk, online due to COVID-19**)
- "The Effect of Strain on Vibrations in Cubic CsPbI_3 Perovskite" 2021
Nicholas Lopez, K. Talit, and D. Strubbe, APS March Meeting (**poster**)
- "Stress Effects on Vibrational Spectra of Orthorhombic and Tetragonal Hybrid Perovskites" 2020
K. Talit and D. Strubbe, Molecular Foundry User Meeting, LBNL (**poster**)
- "Stress Effects on Vibrational Spectra of Orthorhombic and Tetragonal Hybrid Perovskites" 2020
K. Talit and D. Strubbe, Workshop in Electronic Structure Methods, UC Merced (**poster**)
- "Stress Effects on Vibrational Spectra of Orthorhombic and Tetragonal Hybrid Perovskites" 2020
K. Talit and D. Strubbe, APS March Meeting (**contributed talk, cancelled**), Denver, CO

- "Raman Spectroscopy as a Probe of Local Strain in Perovskite Solar Cells" 2019
K. Talit and D. Strubbe, APS March Meeting, Boston, MA (**contributed talk**)
- "Stress Effects on Vibrational Spectra of Cubic Hybrid Perovskite: A Probe of Local Strain" 2019
K. Talit and D. Strubbe, Molecular Foundry User Meeting, LBNL (**poster**)
- "Raman Spectra as a Probe of Localized Strain in Perovskite Solar Cells" 2018
K. Talit and D. Strubbe, APS Bridge Program and National Mentoring Community Conference, Stanford University & Google HQ (**poster**)