Kuntal Talit

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EXPERIENCE

- **Research Assistant - Strubbe Ab Initio Laboratory (SAIL)** Jun. 2017 - Present
  Dept. of Physics, University of California Merced
- **Teaching Assistant, University of California Merced** Aug. 2016 - May. 2018
  - PHYS-009: Introductory Physics II for Physical Science and Engineering Majors.
  - ME-021: Fortran and Matlab programming.
- **Application Developer, IBM India Pvt. Ltd.** Jun. 2011 - Jul. 2016
  - Mainframe Technology: Worked on mainframe development, QA testing and Support Projects which includes JCL, COBOL, DB2, SQL, VSAM and CICS.
  - Worked on ticket management system and automated business processes using DB2 SQL and JCL.
  - Worked for health care domain for Express Scripts Inc (ESI-AMS) and integration Project for ESI and MEDCO, general insurance project for ACE Insurance and IBM internal project (IBM IGA-FMS).

SKILLS

- Python
- Fortran
- C++
- Shell Scripting
- DB2 SQL
- Matlab
- HPC Applications
- Quantum ESPRESSO
- BerkeleyGW
- LAMMPS
- XCrySDen
- Materials Studio
- Virtual NanoLab
- Data Analysis
- Machine Learning
- COBOL
- JCL
- MS Office

EDUCATION

- **University of California Merced, Merced, CA**
  - Ph.D. candidate in Physics. Jan 2017-present
  - Ph.D. program in Mechanical Engineering. Aug 2016-Jan 2017
- **Indian Institute of Engineering Science and Technology, Shibpur, India**
  - Master of Technology, Materials Engineering. July 2009-June 2011
  - Master of Science, Applied Physics. July 2007-June 2009

Publication & Presentation

- "Stress effects on Raman spectroscopy of cubic hybrid perovskite: A probe of local strain," https://doi.org/10.1021/acs.jpcc.0c07389, Kuntal Talit and David A. Strubbe — Dec. 2020
- "Raman Spectroscopy as a probe of local strain in perovskite solar cells" (contributed talk), Kuntal Talit and David A. Strubbe, APS March Meeting, Boston, MA — 2019
- "Raman spectra as a probe of localized strain in perovskite solar cells" (poster, 2nd prize), Kuntal Talit and David A. Strubbe, APS Bridge Program, Stanford University & Google HQ — 2018
- "Density-functional theory calculations of hybrid perovskites for photovoltaics" (poster), Kuntal Talit and David A. Strubbe, APS Far West, UC Merced — 2017

Fellowships & Awards

- MACES Summer Research Fellowship — 2018
- Dan David Solar Fellowship — 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

Relevant coursework

- Quantum mechanics
- Condensed matter physics
- Materials simulation
- Transport phenomena
- Electrodynamics
- Statistical mechanics
- Electronic devices circuits
- Atomic and molecular physics
- Numerical methods and computer applications

Academic Research

- **Density-functional theory calculations of hybrid perovskite for photovoltaics** — 2017-current
  Ph. D. Project, Advisor: Prof. David A. Strubbe
  University of California, Merced

  Studying Methylammonium Lead Iodide (MAPI) structures to find the root cause behind light induced

degradation. Working on structural optimization, calculation of band-structure, phonon modes, IR and Raman spectra, structural changes with strain analysis using Raman spectra, Gruneisen parameter etc. using DFT (Density Functional Theory) and DFPT (Density Functional Perturbation Theory).

- **Role of humidity on friction within MoS_2 sliding interfaces** 2016-2017
  Project Advisors: Prof. Ashlie Martini and Prof. Lilian P. Davila
  University of California, Merced

  Studied frictional behavior of MoS_2 layers using molecular dynamics (MD) simulation as implemented in LAMMPS code. Simulated deck-of-card movements between layers, calculated coefficient of friction. Studied frictional behavior for different humidity conditions using REAX, REBO and LJ interatomic potential but could not make the system stable at 300k.

- **Ground state properties of homo- and hetero- clusters of group-IV elements** 2010-2011
  M. Tech Thesis, Advisors: Prof. G.P Das and Prof. N.R. Bandyopadhyay
  Indian Association for the Cultivation of Science (IACS), Kolkata, India

  Studied different group-IV clusters using DFT as implemented in CASTEP, DMoL3 packages of Material Studio software. Calculated binding energy, HIMO-LUMO gaps etc. for Si_n and C_n clusters and for mixed Si_nC_m clusters. Studied the structural transitions of these clusters based on the number of atoms in the clusters.

- **Experimental Studies on Critical Opalescence in Binary Fluid** Jan 2009-June 2009
  M. Sc Thesis, Advisor: Dr. S. Minhaz Hossain
  Indian Institute of Engineering Science And Technology (IIEST), Shibpur, India

  Designed a simple experiment to review and analyze the phenomenon of critical opalescence in binary fluid (Hexane and Methanol). Measured critical temperature for the system. Analyzed the nature of correlation function and correlation length and its divergence at critical temperature. Able to measure critical exponents which are universal constants using my simple experimental set up which costs less than $20.

Workshops Attended

- **UC Merced Virtual Bootcamp: Machine Learning (virtual)** Oct. 19-22nd, 2020
  X, the moonshot factory in association with UC Merced.

- **SDSC Summer Institute 2020 (virtual)** Aug. 3-7th 2020
  High Performance Computing and Data Science.

- **BerkeleyGW - A Massively Parallel GW/BSE Code** 10-12th Jan 2018, Oakland, CA
  Hands on training and workshop which includes lectures on theory, application and computational details of GW and Bethe-Salpeter calculation for quasiparticles and optical properties of solids, molecules and nanosystems.

- **CASTEP - A plane wave based DFT code package** 5-7th Jan 2011, Delhi, India
  Hands on training and workshop on computational methods for experimental spectroscopy using CASTEP.