

Education

- PhD student, Physics** **August, 2017-Current**
Department of Physics and Institute for Physical Science and Technology,
University of Maryland, College Park
Advisor: Prof. Pratyush Tiwary
Coadvisor in Physics Department: Prof. Christopher Jarzynski
- Master of Science, Physics** **July, 2013**
Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

Master's Thesis: "Study of spin, electronic, and lattice structures of a Quasi-Topological-Insulator alloy thin film"
Advisor: Prof. Shu-Jung Tang
- Bachelor of Science, Physics** **June, 2011**
Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

Experience

- Graduate Research at Maryland** **2017.8 -**
Advisor: Prof. Pratyush Tiwary
- Studying dynamic disorder, resonant activation, and nucleation with metadynamics.
 - Develop useful distance metric between two molecular configurations based on kinetic map, commute map, diffusion map, spectral gap optimization method, and machine learning.
 - Applying Recurrent neural network to study memory effect and dynamics of nucleation process.
- Soft Matter Physics Laboratory** **2014.11 - 2017.6**
Advisor: Prof. Tzay-Ming Hong
- MD simulation with large-scale atomic/molecular massively parallel simulator (LAMMPS).
 - Used LAMMPS to study twisting dynamics of a cylindrical shell and crumpling paper.
 - Customized the force field in LAMMPS in order to include changeable plasticity.
 - Developed imaging tools and conducted post-analysis on LAMMPS output data in Python.
 - Analyzed acoustic emission data using C/C++ and MATLAB.
 - Designed a fracture machine with force-sensing functionality.
 - Analyzed the Akaike information criterion of single/double power-law models using R language.
 - Generated, modified, and analyzed the sandpile model using Mathematica.
- Military Service** **2013.10 - 2014.11**
- Graduate and Undergraduate Research** **2011.09 - 2013.07**
Advisor: Prof. Shu-Jung Tang
- Conducted an experiment using angle-resolved photoemission spectroscopy (ARPES).
 - Measured low-energy electron diffraction (LEED) on the single-layered binary alloy.
 - Measured Fermi surface on the AuPb binary alloy at U90 21B1 beamline, NSRRC, Taiwan.
 - Conducted an experiment of spin-resolved ARPES (SARPES) at Photon Factory, KEK, Japan
 - Used Igor Pro to analyze the data collected by ARPES, LEED, and SARPES.
 - Taught Undergraduate Quantum Physics for one year.

Poster

Title: “Dynamic disorder and rare event kinetics”, Sun-Ting Tsai and Pratyush Tiwary at Gordon Research Conference, 2018 Water and Aqueous Solutions (July 22, 2018 - July 27, 2018)

Publication

“Towards automated sampling of polymorph nucleation and free energies with SGOOP and metadynamics”, [Sun-Ting Tsai](#), Pratyush Tiwary (2020) (under review)

“SGOOP-d: Estimating kinetic distances and reaction coordinate dimensionality for rare event systems from biased/unbiased simulations”, [Sun-Ting Tsai](#), Zachary Smith, Pratyush Tiwary (2020) (under review)

“Learning Molecular Dynamics with Simple Language Model built upon Long Short-Term Memory Neural Network”, [Sun-Ting Tsai](#), En-Jui Kuo, Pratyush Tiwary, Nat. Commu. **11** 5115 (2020)

“Mechanism of Evolution Shared by Gene and Language”, Li-Min Wang, Hsing-Yi Lai, [Sun-Ting Tsai](#), Shan-Jyun Wu, Meng-Xue Tsai, Daw-Wei Wang, Yi-Ching Su, Chen Siang Ng, and Tzay-Ming Hong, Preprint at arXiv:2012.14309 (2020) (under preparation)

“On the distance between A and B in molecular configuration space”, [Sun-Ting Tsai](#) and Pratyush Tiwary (2020) Molecular Simulation. 1-8 (2020)

“Crumple-Origami Transition for Twisting Cylindrical Shells”, Li-Min Wang, [Sun-Ting Tsai](#), Chih-yu Lee, Pai-Yi Hsiao, Jia-Wei Deng, Hung-Chieh Fan Chiang, Yicheng Fei, Tzay-Ming Hong, Phys. Rev. E **101** (5), 053001 (2020)

“Reaction coordinates and rate constants for liquid droplet nucleation: quantifying the interplay between driving force and memory”, [Sun-Ting Tsai](#), Zachary Smith and Pratyush Tiwary, J. Chem. Phys. **151** (15), 154106 (2019)

“Kinetics of Ligand-Protein Dissociation from All-Atom Simulations: Are We There Yet?”, João Marcelo Ribeiro, [Sun-Ting Tsai](#), Debabrata Pramanik, Yihang Wang, Pratyush Tiwary, Biochemistry **58** (3), 156-165 (2018)

“Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional probability factorization”, Zachary Smith, [Sun-Ting Tsai](#), Debabrata Pramanik, Pratyush Tiwary, J. Chem. Phys. **149** (23), 234105 (2018)

“Acoustic Emission from Breaking Bamboo Chopsticks”, [Sun-Ting Tsai](#), Panpan Huang, Li-Min Wang, Zhengning Yang, Chin-De Chang, Tzay-Ming Hong, Phys. Rev. Lett. **116**, 035501 (2016)

“Power-law Ansatz in Complex Systems: Excessive Loss of Information”, [Sun-Ting Tsai](#), Chin-De Chang, Ching-Hao Chang, Meng-Xue Tsai, Nan-Jung Hsu, Tzay-Ming Hong, Phys. Rev. E **92**, 062925 (2015)

“Significantly Enhanced Giant Rashba Splitting in a Thin Film of Binary Alloy”, Wei-Chuan Chen, Tay-Rong Chang, [Sun-Ting Tsai](#), S Yamamoto, Je-Ming Kuo, Cheng-Maw Cheng, Ku-Ding Tsuei, Koichiro Yaji, Hsin Lin, H-T Jeng, Chung-Yu Mou, Iwao Matsuda and S-J Tang, New J. Phys. **17**, 083015 (2015).