Davis Unruh

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EDUCATION

University of California Davis   Davis, CA

PhD in Physics, Condensed Matter Theory   Expected August 2021
- Honors: Ray and Constance Chandler Fellowship, 2016

Bowdoin College   Brunswick, ME

BA, *magna cum laude,* Physics   May 2016
- Honors: Sarah and James Bowdoin Scholar (Dean's List): 2013, 2015; Faculty Scholar, 2012

RESEARCH EXPERIENCE

UC Davis Physics, Condensed Matter Theory   Davis, CA

Graduate Research Assistant with Prof. Gergely T. Zimányi   January 2018 - Present
- Modeled performance degradation of silicon heterojunction (Si-HJ) solar cells from femtoseconds to gigaseconds by tracking the dynamics of the creation of structural defects, which in turn create electronic defects. The structural evolution was modeled by molecular dynamics. By using a machine-learning based interatomic Gaussian approximation potential (GAP), we were able to achieve energy minimization on the level of DFT while using only classical molecular dynamics. I developed additional methods based on DFT and accelerated super-basin kinetic Monte Carlo.
- Currently training a Machine-Learning based Gaussian Approximation Potential (GAP) to model Si-H interactions, to extend the above work to modelling hydrogen migration at interfaces in Si-HJT solar cells, the predicted mechanism behind long-term open-circuit voltage degradation
- Conducted computational research on electron transport in nanoparticle solar cells, particularly the impacts of epitaxial fusion of nanoparticles, disorder and extended lattice defects, primarily using an extended kinetic Monte Carlo algorithm approach
- Carried out extensive research to discover and to explore Mott-Hubbard physics in nanoparticle solids, focusing on Metal-Insulator Transitions driven by interactions, disorder and their interplay

UC Davis Physics, Condensed Matter Experiment   Davis, CA

Graduate Research Assistant with Prof. Eduardo da Silva Neto   2017
- Performed research on cuprates using Resonant Inelastic X-ray Scattering (RIXS) spectroscopy
- Developed routines for processing and analyzing raw spectroscopic data, and created a computational toolset for calibrating detector error out of RIXS data sets to facilitate accurate comparison

NASA Goddard Space Flight Center   Greenbelt, MD

Undergraduate Physics Intern   Summer 2015
- Developed image analysis routines for Wide Field Infrared Survey Telescope (WFIRST) IR detectors
- Created MATLAB GUI for application of routines to detector data
- Presented results at WFIRST Cycle 6 Design Meeting and NASA GSFC Summer Poster Session

University of Utah Physics and Astronomy REU   Salt Lake City, UT

Cosmic Ray Group Undergraduate Student Researcher   Summer 2014
- Computationally gathered and analyzed data from air fluorescence telescopes to measure the VAOD (Vertical Aerosol Optical Depth) at the Cosmic Ray Group's Telescope Array site.

PUBLICATIONS

D. Unruh, A. Camjayi, C. Hansen, J. Bobadilla, M. J. Rozenberg, and G. T. Zimányi – *Disordered Mott–Hubbard Physics in Nanoparticle Solids: Transitions Driven by Disorder, Interactions, and Their Interplay*. Nano Letters **20**, 8569–8575 (2020).

X. Chu, H. Heidari, A. Abelson, **D. Unruh**, C. Hansen, C. Qian, G. T. Zimányi, M. Law, A. J. Moulé – *Structural characterization of a polycrystalline epitaxially-fused colloidal quantum dot superlattice by electron tomography*. J. Mater. Chem. A **8**, 18254-18265 (2020).

E. H. da Silva Neto, M. Minola, B. Yu, W. Tabis, M. Bluschke, **D. Unruh**, H. Suzuki, Y. Li, G. Yu, D. Betto, K. Kummer, F. Yakhou, N. B. Brookes, M. Le Tacon, M. Greven, B. Keimer, A. Damascelli – *Coupling between dynamic magnetic and charge-order correlations in the cuprates superconductor* $Nd_{2-x}Ce_xCuO_4$. Phys. Rev. B **98**, 161114 (2018).

L. Qu, **D. Unruh**, G. T. Zimányi – *Percolative Charge Transport in Binary Nanocrystal Solids*. Phys. Rev. B (accepted for publication). arXiv:2011.11244.

C. Hansen, **D. Unruh**, M. Alba, C. Qian, A. Abelson, M. Law, G. T. Zimányi – *Hierarchical carrier transport simulator for defected nanoparticle solids*. Scientific Reports (accepted for publication). arXiv:2009.01319v1.

D. Unruh, R. V. Meidanshahi, C. Hansen, S. Manzoor, S. M. Goodnick, M. I. Bertoni, G. T. Zimányi – *From Femtoseconds to Gigaseconds: The SolDeg Platform for the Performance Degradation Analysis of Silicon Heterojunction Solar Cells*. arXiv: 2012.01703; submitted to ACS Appl. Mater. Interfaces.

D. Unruh, R. V. Meidanshahi, S. M. Goodnick, G. T. Zimányi, G. Csányi – *Training a Machine-Learning Driven Gaussian Approximation Potential for Si-H Interactions*. In preparation.

S. Manzoor, **D. Unruh**, C. Hansen, R. V. Meidanshahi, S. M. Goodnick, M. I. Bertoni, G. T. Zimányi – *Hydrogen Driven Performance Degradation in Silicon Heterojunctions*. In preparation.

PRESENTATIONS

"Performance degradation in aSi/cSi Heterjunction Solar Cells by Glassy Dynamics." Poster presentation at the June 2020 Institute of Electrical and Electronics Engineers (IEEE) Photovoltaic Specialists Conference (PVSC).

"Persistent Coulomb Blockade Across the Metal-Insulator Transition in Nanoparticle Solids." Oral presentation at the 2020 APS March Meeting in Session M62: Electron Transport in Nanostructures II.

"Performance Degradation in aSi/cSi Heterojunction Solar Cells by Glassy Dynamics." Poster presentation at the August 2019 National Renewable Energy Laboratory (NREL) Silicon Workshop.

"A Computational Measurement of VAOD for Cosmic Ray Air Showers." Oral presentation at the October 2014 APS 4-Corners Meeting.

COMPUTER AND RESEARCH SKILLS

- Molecular dynamics, machine-learning, DFT, kinetic Monte Carlo, ensemble Monte Carlo, and data analysis
- Skilled in Python, C++, Julia, Java, bash, Linux terminal, LAMMPS, Quantum Espresso, MATLAB
- Proficient in resonant inelastic x-ray scattering spectroscopy, gamma ray spectroscopy, standard advanced undergraduate physics lab techniques

COLLABORATIVE EXPERIENCE

Participated in four substantive collaborations

- With profs. Adam Moule (UC Davis) and Matt Law (UC Irvine) on nanoparticle tomography;
- With prof. Csanyi (U. of Cambridge, UK) developing machine learning-driven GAP potentials;
- With profs. Mariana Bertoni and Stephen Goodnick (both ASU), on heterojunction solar cell performance degradation;
- With profs. Matt Law (UC Irvine), H. Zheng (UC Berkeley), A. Kummel (UCSD), R. Wu (UC Irvine) V. Klimov (LANL), and D. Yu and A. Moule (both UC Davis): on "Designer Mesoscale Quantum Dot Solids" – a large all-UC collaboration of 8 research groups

TEACHING EXPERIENCE

UC Davis Physics Department   Davis, CA
Teaching Assistant   2016 – Present

- Instructor for discussion sections and labs for the 2 primary UC Davis introductory physics series
- Grader/ TA for Graduate Condensed Matter Physics, and Undergraduate Quantum Mechanics

Bowdoin Baldwin Center for Learning and Teaching   Brunswick, ME
Quantitative Reasoning Tutor   2015 - 2016

- Individual tutor for math and economics courses; worked with 16-20 students/week

DEPARTMENT SERVICE

UC Davis Physics Department Grad Curriculum (Policy) Committee   2020 - Present
Graduate Student Representative