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Tesia D. Janicki

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EDUCATION

PHD, MAJOR IN CHEMISTRY Summer 2022 (anticipated)

University of Wisconsin - Madison (UW)

NSF GRFP Fellow

Advisor: JR Schmidt

(1) Developed a GPU-accelerated plugin for OpenMM to implement custom anisotropic force expressions and co-developed an anisotropic first-principles interatomic potential for benzene

(2) Collaborated with an interdisciplinary team (UW MRSEC) and created dynamic and kinetic models of metal oxide solid-phase epitaxy using both molecular dynamics and enhanced sampling methods in masked 3D geometries and polymorphic crystals

BS, MAJORS IN CHEMISTRY & PHYSICS, MINOR IN GENDER STUDIES 2016

University of Notre Dame (ND)

Triota Honor Society; Advisor: Steven Corcelli

Simulated 1CKA protein structure relaxation and computed vibrational spectra to rationalize structure stability

AWARDS & HONORS

GRADUATE RESEARCH FELLOWSHIP PROGRAM (GRFP) FELLOW 2018-present
National Science Foundation

DEPT OF CHEMISTRY MENTOR AWARD 2021
Graduate Student Faculty Liaison Committee (GSFLC), UW

1ST PLACE POSTER 2021
Computing in Engineering Forum, Grainger Institute for Engineering (GIE), UW

MOST INFORMATIVE OUTREACH VIDEO 2021
UW Materials Research Science & Engineering Center (MRSEC)

3RD PLACE POSTER, Computing in Engineering Forum, GIE, UW 2020

CONFERENCE TRAVEL GRANT, UW Student Research Grants Competition 2019

BEST POSTER, Midwest Theoretical Chemistry Conference 2019

TRAVEL GRANT, Association for Women in Science Notre Dame Chapter (AWIS-ND) 2018

CATALYST MENTOR AWARD, Dept of Chemistry, UW (1) 2017 (2) 2018 (3) 2019 (4) 2020

CLARE BOOTHE LUCE FOUNDATION GRANT, College of Science, ND 2015

MARSHALL FIXMAN SUMMER THEORY PROGRAM 2014
Dept of Chemistry, Colorado State University
Advisor: Branka Ladanyi

SUMMER UNDERGRADUATE RESEARCH FELLOWSHIPS, ND 2013

FIRST YEAR IGNITION FELLOWSHIP, ND 2013

PUBLICATIONS

- 1 R. Adhikary, J. Zimmermann, J. Liu, R. P. Forrest, **T. D. Janicki**, P. E. Dawson, S. A. Corcelli, and F. E. Romesberg, "Evidence of an Unusual N-H—N Hydrogen Bond in Proteins" (communication) *J. Am. Chem. Soc.* 136, 13474 (2014).
- 2 M. S. Beasley*, M. A. Lumley*, **T. D. Janicki***, R. L. Fernandez*, T. M. Tuchoski, L. H. Manger, L. D. Whitmire, N. C. Thomas, A. J. Lawson, and A. R. Buller. "Student-Led Climate Assessment Promotes a Healthier Graduate School Environment" *J. Chem. Educ.* 97, 643-650 (2020).
**These authors contributed equally to this work*
- 3 R. Liu, O. Elleuch, Z. Wan, P. Zuo, **T. D. Janicki**, A. D. Alfieri, S. E. Babcock, D. E. Savage, J. R. Schmidt, P. G. Evans, and T. F. Kuech. "Phase Selection and Structure of Low-Defect-Density γ - Al_2O_3 Created by Epitaxial Crystallization of Amorphous Al_2O_3 " *ACS Appl. Mater. Interfaces* 12, 57598-57608 (2020).
- 4 **T. D. Janicki**, Z. Wan, R. Liu, P. G. Evans, and J. R. Schmidt. "Guiding nanoscale crystallization of amorphous solids: interfaces, stress, and precrystalline structure" *revisions submitted to J. Chem. Phys.* 17 June 2022.
- 5 **T. D. Janicki**, J. R. Schmidt, and M. J. Van Vleet. "Multipolar Anisotropic Slater-Type Intermolecular Force Field (MASTIFF) Benzene" *to be submitted to J. Phys. Chem A by August 2022.*
- 6 **T. D. Janicki**, R. Liu, Z. Wan, J. Sun, P. Gopalan, P. G. Evans, and J. R. Schmidt. "Epitaxially controlled 3D geometries in strontium titanate" *in preparation.*

PRESENTATIONS

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| GIE COMPUTING IN ENGINEERING FORUM , <i>Poster</i> | 2021 |
| "GPU-Accelerated OpenMM Plugin Enables Anisotropic Benzene Model" | |
| AMERICAN CHEMICAL SOCIETY (ACS) GREAT LAKES REGIONAL MEETING , <i>Talk</i> | 2021 |
| "Student-Led Climate Assessment Promotes a Healthier Graduate School Environment" | |
| ACS NATIONAL MEETING , <i>Poster, Live session</i> | Spring 2021 |
| "Modeling polymorphic crystallization pathways of aluminum oxide (Al_2O_3)" | |
| ACS DIVISION OF CHEMICAL HEALTH AND SAFETY (DCHS) JOURNAL CLUB , <i>Invited Talk</i> | 2021 |
| "Student-Led Climate Assessment Promotes a Healthier Graduate School Environment" | |
| UW PHYSICAL CHEMISTRY STUDENT SEMINAR , <i>Talk</i> | 2020 |
| "Ahead of the (Free Energy) Curve: Enhanced Sampling Applied to Polymorphic Material Crystallization" | |
| GIE COMPUTING IN ENGINEERING FORUM , <i>Poster</i> | 2020 |
| "Modeling crystallization pathways of polymorphic materials" | |
| ACS NATIONAL MEETING - SAN DIEGO , <i>Poster</i> | Fall 2019 |
| "Modeling crystallization pathways of polymorphic materials: Enhanced sampling techniques and method development" | |
| MIDWEST THEORETICAL CHEMISTRY CONFERENCE (MWTCC) , <i>Poster</i> | 2019 |
| "Modeling crystallization pathways of polymorphic materials: Enhanced sampling techniques and method development" | |

TECHNICAL SKILLS

- Comprehensive programming experience with proficiency in C, C++, Fortran and Python
- Incorporating parallel computing algorithms: OpenMP, MPI, and GPU (CUDA)
- Software management and version control (github)
- Extensive use of high-performance and high-throughput computing resources
- Interfacial/epitaxial systems modeling and characterization
- Force field development and validation
- Molecular simulation with proficiency in GROMACS, LAMMPS, and OpenMM
- Enhanced sampling simulation (PLUMED)
- Statistical mechanics
- Electronic structure theory

LEADERSHIP AT UW-MADISON

EXECUTIVE COMMITTEE, UW MRSEC	2021-present
GRADUATE STUDENT CLIMATE SURVEY TEAM CO-LEAD, Dept of Chemistry, UW	2019-2020
STUDENT SEMINAR COORDINATOR, Physical Chemistry Path, UW	2019-2020
WELLNESS SUBCOMMITTEE CHAIR, GSFLC, UW	2018-2019
TREASURER, GSFLC, UW	2018-2019
LEAD HOST, Dept of Chemistry Graduate Student Recruiting, UW	2019
WORKSHOP COMMITTEE CHAIR, 2018 Women in Science Conference (AWIS-ND)	2018
ACS "PREPARING FOR LIFE AFTER GRADUATE SCHOOL" COORDINATOR, GSFLC, UW	2018
PHYSICAL CHEMISTRY REPRESENTATIVE, GSFLC, UW	2017-2018

PROFESSIONAL SERVICE & OUTREACH AT UW-MADISON

AP CHEMISTRY VISITING SPEAKER, Hartford Union High School, Hartford, WI	2021
ENGINEERING OUTREACH VIDEO DEVELOPMENT, UW MRSEC Determining Distances with Diffracton (feat. Dogs)	2021
FACULTY MENTOR TRAINING ACTION TEAM, Dept of Chemistry, UW	2020-2021
GRADUATE STUDENT CLIMATE SURVEY TEAM, Dept of Chemistry, UW	2017-2021
WELLNESS & PROFESSIONAL DEVELOPMENT COMMITTEE, Dept of Chemistry, UW	2019-2020
WELLNESS SUBCOMMITTEE, GSFLC, UW	2019-2020
ACTIVITY FACILITATOR, WI Science Fest and Engineering Expo	2018-present
SCORE AND TIME KEEPER, Regional ScienceBowl Competition	2020
CONTENT CONSULTANT, UW MRSEC Content input for educational game "Lost at the Forever Mine"	2018

TEACHING & MENTORING EXPERIENCE AT UW-MADISON

UNDERGRADUATE MENTOR , <i>Dept of Chemistry, UW</i>	2019-present
CHEMISTRY GRADER , <i>Dept of Chemistry, UW</i> CHEM 565/665: Biophysical Chemistry	2021-2022
GRADUATE MENTOR , <i>Chemistry Opportunities - CHOPs, Dept of Chemistry, UW</i>	2017-2021
GRADUATE MENTOR , <i>Catalyst, Dept of Chemistry, UW</i>	2017-2021
RESEARCH EXPERIENCE FOR TEACHERS (RET) MENTOR , <i>UW MRSEC</i>	2018
CHEMISTRY TUTOR , <i>Dept of Chemistry, UW</i> General Chemistry (all levels), Biophysical Chemistry	2017-2021
TEACHING ASSISTANT , <i>Dept of Chemistry, UW</i> CHEM 115 & 116: Chemical Principles I & II (both lab & lecture)	2016-2017

TEACHING EDUCATION & PROFESSIONAL DEVELOPMENT

TELLURIDE SCHOOL ON THEORETICAL CHEMISTRY , <i>Telluride Science Research Center</i>	Fall 2021
MANY-BODY INTERACTIONS: FROM QUANTUM MECHANICS TO FORCE FIELDS WORKSHOP , <i>Telluride Science Research Center</i>	Summer 2020
BREAKTHROUGH RESEARCH AND EDUCATION WORKSHOP (BREW) , <i>UW MRSEC</i>	Annual 2018-21
ANTIRACIST BOOK CLUB , <i>Dept of Chemistry, UW</i>	Fall 2020 - Present
BLACK, BROWN AND BRUISED - TALKING ABOUT RACE AND STEM EDUCATION , <i>Delta Program</i>	Spring 2021
EQUITY AND INCLUSION IN THE COLLEGE CLASSROOM , <i>Delta Program</i>	Spring 2020
REDUCING MATH ANXIETY AMONG YOUR STUDENTS WORKSHOP , <i>CIRTL</i>	Fall 2020
RESEARCH MENTOR TRAINING , <i>Delta Program</i>	Summer 2019
BREAKING THE BIAS HABIT: A WORKSHOP TO PROMOTE A DIVERSE, WELCOMING, AND INCLUSIVE RESEARCH GROUP , <i>WISELI</i>	Fall 2018
MENTOR TRAINING , <i>Catalyst, National Research Mentor Network</i>	Fall 2017

REFERENCES

JR SCHMIDT

Professor
UW Dept of Chemistry
Primary Research Advisor
schmidt@chem.wisc.edu

PAUL EVANS

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UW Materials Science & Engineering
IRG2 Leader, Thesis Committee
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SUE BABCOCK

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