Alice R. Walker

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Education

March 2018	**Ph.D.** in Physical Chemistry, University of North Texas
Dissertation:	Computational Simulations of Cancer and Disease-Related Enzymatic Systems using Molecular Dynamics and Combined Quantum Methods
September 2013-August 2016	**Ph.D. Candidate** in Physical Chemistry, Wayne State University
May 2011	**B.S.** in Chemistry with distinction, University of Michigan-Dearborn

Awards and Honors

Promise in COMP Award, 258th ACS National Meeting, San Diego, CA (2019)
Robert Wade Brown Award, University of North Texas (2018)
Chemical Computing Group Excellence Award, 255th ACS National Meeting, New Orleans, LA (2018)
American Society for Mass Spectrometry Sanibel Conference Travel Award, St. Petersburg, FL (2018)
Award for Best Poster, 6th EU-US Conference on Repair of Endogenous DNA Damage, University of Udine (2017)
College of Science Travel Grant, University of North Texas (2017)
Ed and Julie Hodges Memorial Scholarship, University of North Texas (2017)
ANTON Molecular Dynamics Simulations Computing Award, PSCA15038 (2015)
Chemistry-Biology Interface (CBI) Fellowship, Chemistry Division (2015-16)
Honor Citation for Teaching Services in Chemistry, Wayne State University (2013)
Chancellor's Scholarship, University of Michigan-Dearborn (2005-9)
Honor's Program, University of Michigan-Dearborn (2005-11)

Research & Professional Experience

Assistant Professor at Wayne State University (Detroit, MI), August 2021-present.

Postdoctoral Scholar at Stanford Linear Accelerator Lab/Stanford University (Stanford, CA), May 2018-July 2021
Adviser: Prof. Todd J. Martínez

Graduate Research Assistant at University of North Texas (Denton, TX), Sept. 2016-May 2018
Graduate Research Assistant at Wayne State University (Detroit, MI), Sept. 2013-August 2016
Adviser: Prof. G. Andrés Cisneros

Analytical Chemist at RTI Laboratories (Livonia, MI), Sept. 2011-May 2013

Undergraduate Research at University of Michigan-Dearborn (Dearborn, MI), June 2009-Nov. 2010
Adviser: Prof. Daniel B. Lawson

Peer Reviewed Publications

12. Alice R. Walker, Boning Wu, Jan Meisner, Michael D. Fayer, and Todd J. Martínez. Proton transfer from a photoacid to a water wire: First principles simulations and fast fluorescence spectroscopy. *J. Phys. Chem. B*, 125(45):12539–12551, November 2021. Featured on Supplemental Cover.
11. Madison B. Berger, Alice R. Walker, Erik Antonio Vázquez-Montelongo, and G. Andrés Cisneros. Computational investigations of selected enzymes from two iron and α-ketoglutarate-dependent families. *Physical Chemistry Chemical Physics*, 23:22227–22240, 2021
10. Joseph E. Thomaz, Alice R. Walker, Stephen J. Van Wyck, Jan Meisner, Todd J. Martínez, and Michael D. Fayer. Proton transfer dynamics in the aprotic proton accepting solvent 1-methylimidazole. *Journal of Physical Chemistry B*, 124(36):7897–7908, September 2020
9. Alice R. Walker, Nikhil Baddam, and G. Andrés Cisneros. Unfolding pathways of hen egg-white lysozyme in ethanol. *The Journal of Physical Chemistry B*, 123(15):3267–3271, **2019**
8. Hailey L. Gahlon, Alice R. Walker, G. Andrés Cisneros, Meindert H. Lamers, and David S. Rueda. Reduced structural flexibility for an exonuclease deficient DNA polymerase III mutant. *Physical Chemistry Chemical Physics*, 20(40):26892–26902, **2018**
7. Nicole Antczak, Alice R. Walker, Hannah R. Stern, Emmett M. Leddin, Carl Palad, Timothy A. Coulther, Rebecca J. Swett, G. Andrés Cisneros, and Penny J. Beuning. Characterization of nine cancer-associated variants in human DNA polymerase κ. *Chemical Research in Toxicology*, 31(8):697–711, 8 **2018**
6. Pramodha S. Liyanage, Alice R. Walker, Alfonso Brenlla, G. Andrés Cisneros, Louis J. Romano, and David Rueda. Bulky lesion bypass requires Dpo4 binding in distinct conformations. *Scientific Reports*, 7(1):17383–, **2017**
5. Alice R. Walker and G. Andrés Cisneros. Computational simulations of DNA polymerases: Detailed insights on structure/function/mechanism from native proteins to cancer variants. *Chemical Research in Toxicology*, 30(11):1922–1935, 11 **2017**
4. Alice R. Walker, Pavel Silvestrov, Tina A. Müller, Robert H. Podolsky, Gregory Dyson, Robert P. Hausinger, and G. Andrés Cisneros. ALKBH7 variant related to prostate cancer exhibits altered substrate binding. *PLOS Computational Biology*, 13(2):1–13, 2 **2017**
3. Alice R. Walker, Robin Bonomi, Vadim Popov, Juri G. Gelovani, and G. Andrés Cisneros. Investigating carbohydrate based ligands for galectin-3 with docking and molecular dynamics studies. *Journal of Molecular Graphics and Modelling*, 71:211 – 217, **2017**
2. Eric G. Kratz, Alice R. Walker, Louis Lagardére, Filippo Lipparini, Jean Philip Piquemal, and G. Andrés Cisneros. LICHEM: A QM/MM program for simulations with multipolar and polarizable force fields. *Journal of Computational Chemistry*, 37(11):1019–29, 1 **2016**
1. Daniel B. Lawson and Alice Walker. Cycloaddition of ethene on a series of single-walled carbon nanotubes. *Computational and Theoretical Chemistry*, 981:31 – 37, **2012**

Manuscripts in preparation:

- Alice R. Walker, T.J. Lane, Henry van den Bedem and Todd J. Martínez. "Theoretical insights into the excitation mechanism of fatty acid photodecarboxylase."
- Yasmin Shamsudin, Alice R. Walker, Chey Jones, Todd J. Martínez, and Steven G. Boxer. "Simulation-guided engineering of rapidly dissociating β-strands from split green fluorescent protein."
- Elisa Pieri*, Alice R. Walker*, Nancy Zhu, Todd J. Martínez. "Computational study of relationship between quantum yield, structure and energy of red fluorescent protein variants."

Teaching and Mentoring Experience

Quantum Molecular Design Summer School Instructor at Stanford University (Stanford, CA), August 2019

Designed a curriculum for an interdisciplinary group of graduate students and postdoctoral researchers to explore how to structure theory-experiment collaborations in the context of excited state QM/MM simulations of proteins.

- Taught and created a curriculum in the context of a hands-on tutorial to explore the excited state dynamics of photoactive yellow protein in explicit solvent.
- Organized and facilitated a set of relevant lectures from graduate students and postdocs.

Protein Subgroup Leader, Martínez Group at Stanford University (Stanford, CA) June 2018-July 2021
Leader for protein related research in the Martinez group. Act as a research coordinator and prepare monthly targeted meetings for group members working on simulations of photoswitchable and fluorescent proteins, including discussion of relevant computational techniques and presentations of current work.

BUILD Program Coordinator and Lecturer at Wayne State University (Detroit, MI), July 2015/July 2016
Co-created and co-implemented, with another graduate student, a two-week chemistry curriculum aimed at advancing and supporting incoming underrepresented minority undergraduate students majoring in scientific fields.

- Lessons focused on active learning, integration of laboratory and interactive lecture, and completion of a group oral presentation on literature research.
- BUILD is part of an interdisciplinary program at multiple local universities, and funded by the NIH.

Graduate Teaching Assistant at Wayne State University (Detroit, MI), Sept. 2013-Aug. 2015
Assisted with teaching for Chemistry Skills and Reasoning, General Chemistry I Laboratory, General Chemistry II: Analytical Chemistry, and General Chemistry II: Analytical Chemistry Laboratory.

Student Teacher at Southfield-Lathrup High School (Southfield, MI), Jan. 2011-April 2011
Created and implemented consistent lesson plans throughout the semester for four chemistry classes and one English class, as well as a variety of classroom materials and activities for students, including demonstrations and laboratories.

Highlighted Presentations

20. "Theoretical biochemistry: discovery and prediction through simulations of complex and excited state systems." **Invited talk**. Instituto Tecnológico de Celaya, Celaya, Mexico. December 3, 2021.
19. "Theoretical biochemistry: discovery and prediction through simulations of complex and excited state systems." **Invited talk**. Department of Physics, Wayne State University, Detroit, MI. November 9, 2021.
18. "Theoretical biochemistry: discovery and prediction through simulations of complex and excited state systems." **Invited talk**. Autonomous University of Zacatexas, Zacatecas, Mexico. October 22, 2021.
17. "Theoretical biochemistry: discovery and prediction through simulations of complex and excited state systems." **Invited talk**. University of Michigan-Dearborn Colloquium, Dearborn, MI. September 10, 2021.
16. "Mentorship and outreach: women working together in science." **Invited talk**. Women Make COMP: Inspiring the next generation of women in computational chemistry, ACS Fall 2021, Atlanta, GA. August 24, 2021.

15. "Awarded Long Talk for Outstanding Lightning Talk: Simulations of crystal structure packing effect on green fluorescent protein variant isomerization." Alice R. Walker, Chey Jones, Nanna List, Todd J. Martínez. **Talk**. Virtual Conference on Theoretical Chemistry, July 2020.
14. "Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations." Alice R. Walker, T.J. Lane, Henry van den Bedem, Todd J. Martínez. **Talk**. Division of Computers in Chemistry: Women Make COMP, 258th ACS National Meeting, San Diego, CA. August 26, 2019.
13. "Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations." Alice R. Walker, T.J. Lane, Henry van den Bedem, Todd J. Martínez. **Talk**. Northern California Theoretical Chemistry Meeting, Berkeley, CA. May 19, 2019.
12. "Mechanistic insights into photodecarboxylation of fatty acids from classical and QM/MM simulations." Alice R. Walker, T.J. Lane, Henry van den Bedem, Todd J. Martínez. **Poster**. D. E. Shaw Research Graduate and Postdoc Women's Forum, New York, NY. May 9, 2019.
11. "Effects of a single point mutation and mismatched base on DNA polymerase III holoenzyme proofreading." Alice R. Walker, Hailey Gahlon, David Rueda, G. Andrés Cisneros. **Talk**. Division of Computers in Chemistry: Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation, 255th ACS National Meeting, New Orleans, LA. March 20, 2018.
10. "Unfolding of hen egg white lysozyme in high alcohol solutions: Insights from molecular dynamics and IMS-MS." Alice R. Walker, Daniel W. Woodall, Ellen Inutan, Nikhil Baddam, G. Andrés Cisneros, Sarah Trimpin. **Poster**. Division of Computers in Chemistry Poster Session, 255th ACS National Meeting, New Orleans, LA. March 20, 2018.
9. "Hot Topic Talk: Unfolding of hen egg white lysozyme in high alcohol solutions: Insights from molecular dynamics and IMS-MS." Alice R. Walker, Daniel W. Woodall, Ellen Inutan, Nikhil Baddam, G. Andrés Cisneros, Sarah Trimpin. **Talk and Poster**. 30th ASMS Sanibel Conference on Mass Spectrometry, St Petersburg, FL. January 27, 2018.
8. "ALKBH7 variant related to prostate cancer exhibits altered substrate binding." Alice R. Walker, Pavel Silvestrov, Tina A. Müller, Robert H. Podolsky, Gregory Dyson, Robert P. Hausinger, G. Andrés Cisneros. **Poster**. 6th EU-US Conference on Repair of Endogenous DNA Damage, University of Udine, Udine, Italy. September 26/27, 2017.
7. "ALKBH7 variant related to prostate cancer exhibits altered substrate binding." Alice R. Walker, Pavel Silvestrov, Tina A. Müller, Robert H. Podolsky, Gregory Dyson, Robert P. Hausinger, G. Andrés Cisneros. **Poster**. Division of Computers in Chemistry Poster Session, 253rd ACS National Meeting, San Francisco, CA. April 4, 2017.
6. "ALKBH7 variant related to prostate cancer exhibits altered substrate binding." Alice R. Walker, Pavel Silvestrov, Tina A. Müller, Robert H. Podolsky, Gregory Dyson, Robert P. Hausinger, G. Andrés Cisneros. **Poster**. Graduate Student Research Symposium, Texas Women's University, Denton, TX. March 31, 2017.
5. "GPU-enabled binding free energy calculations of potential ligands for pancreatic cancer imaging." Alice R. Walker, Robin Bonomi, Juri Gelovani, G. Andrés Cisneros. **Poster**. Division of Computers in Chemistry Poster Session, 251st ACS National Meeting, San Diego, CA. March 16, 2016.
4. "Computational studies on potential PET imaging ligands for Galectin-3 in pancreatic cancer tumors." Alice R. Walker, Robin Bonomi, Juri Gelovani, G. Andrés Cisneros. **Poster**. Division of Computers in Chemistry Poster Session, 250th ACS National Meeting, Boston, MA. August 18, 2015.
3. "Computational Studies on Potential Ligands for Imaging Cancer Tumors and Examination of Dealkylation Mechanism of AlkBH2." Alice R. Walker, G. Andrés Cisneros. **Talk**. Second year seminar at Wayne State University. February 25, 2015.
2. "Computational Studies of Inhibitors for Galectin-3." Alice R. Walker, G. Andrés Cisneros. **Poster**. Wayne State University 16th Annual Chemistry Graduate Research Symposium, Detroit, MI. October 11 2014.

1. "Binding of Ethene to Carbon Nanotubes." Alice R. Walker, Daniel B. Lawson. **Talk**. 20th Annual Argonne Undergraduate Research Symposium, Argonne, IL. November 13, 2009.

Service

divSTEM Mentorship Group Leader (July 2020-July 2021)
Facilitating the mentorship wing of the Martínez lab diversity outreach initiative with regular meetings, literature review and actively participating in mentorship opportunities at Stanford.
Physical Chemistry Faculty Hiring Committee, at University of North Texas (Spring 2018)
UNT Chemistry Graduate Social Group, at University of North Texas (January 2016-April 2018)
Phoenix Mentoring Project, Mentor (June 2007-June 2010)
Women in Learning and Leadership, Member (2005-2011)

Professional Organizations & Development

Association for Women in Science (November 2018-present)
Software Summer School at Virginia Tech (June 2015)
NVDIA CUDA qwiklabs (April 2015)
American Chemical Society, Member (January 2015-present)
AGEP Seminar Series (January 2015-September 2016)
STEM Pedagogy Seminar Series (September 2014-September 2016)
BEST Professional Development Program (September 2014-September 2016)

Last updated: December 8, 2021