Alice R. Walker

Wayne State University Chemistry
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Websites: Google Scholar, ResearchGate

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

Professional Experience

Carl R. Johnson Early Career Endowed Chair at Wayne State University (Detroit, MI), August 2024-present.
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

Awards and Honors

Maximizing Investigators' Research Award (MIRA), National Institutes of Health (2024)
American Society of Photobiology Junior Faculty Travel Award, Chicago, IL (2024)
Carl R. Johnson Early Career Endowed Chair, Wayne State University (2024)
NSF Career Award, National Science Foundation (2024)
Ebbing Faculty Development Award, Wayne State University (2022)
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)

Research Grants and External Support

1. **[Active]** National Science Foundation (CHE2338804): CAREER: Computational Design of Fluorescent Proteins with Multiscale Excited State QM/MM Methods
Total Award: $690,816.00 Role: Sole PI Period: 4/1/2024-3/31/2029

2. **[Active]** National Institutes of Health (1R35GM154949-01): Computational rational design of carbohydrate and nucleic acid drug scaffolds with multiscale dynamics and AI.
Total Award: $1,811,366.00 Role: Sole PI Period: Recommended for award by Sept 30, 2024.

Students Supervised

Graduate Students:
Solomon Yamoah Effah (2021-present)
Widana Kaushalya (2021-present)
Vishaka Pathiranage (2021-present)
Victoria Mfon Sunday (2022-present)
Anita Adams (2022-present)
Pramoda Gamage (2023-present)
Janya Subasingsinghe (2023-present)

Undergraduate Students:
Ashlyn Murphy (2021-2022), UCSD
Nathaniel Turner (2021-2023)
Morgan Grougan (2022-present)

Peer Reviewed Publications

Starred entries (**) denote papers where ARW is a corresponding author.
Single stars (*) indicate equal authorship.

22. Elisa Pieri, Alice R. Walker, Mingning Zhu, and Todd J. Martínez. Conical intersection accessibility dictates brightness in red fluorescent proteins. *J. Am. Chem. Soc.*, 146(26):17646–17658, July 2024
21. ** Gibson Kirui, Widana Kaushalya, S. Sameera Perera, Alice R. Walker, and Cláudio N. Verani. Influence of peripheral and ancillary changes on the electron transport of HS3d5 FeIII metallosurfactants - substituents, chain length, subphase polarity, and junction electrodes. *J. Phys. Chem. C*, 128(25):10668–10681, June 2024
20. ** Christina H. McCulley and Alice R. Walker. Dimer interface destabilization of photodissociative Dronpa driven by asymmetric monomer dynamics. *J. Phys. Chem. B*, 127(43):9248–9257, November 2023
19. Yasmin Shamsudin, Alice R. Walker, Chey M. Jones, Todd J. Martínez, and Steven G. Boxer. Simulation-guided engineering of split GFPs with efficient β-strand photodissociation. *Nature Communications*, 14(1):7401, 2023
18. ** Mark A. Hix and Alice R. Walker. AutoParams: An automated web-based tool to generate force field parameters for molecular dynamics simulations. *J. Chem. Inf. Model.*, 63(20):6293–6301, October 2023
17. ** Abigail Cousino, Lanka D. Wickramasinghe, Widana Kaushalya, S. Sameera Perera, Habib Baydoun, Alice R. Walker, and Cláudio N. Verani. Studies on monolayer formation and electron transport in Au|LB|Au junctions containing 3d4 MnIII metallosurfactants. *J. Phys. Chem. C*, 127(33):16654–16667, August 2023
16. ** Joseph Wakpal, Vishaka Pathiranage, Alice R. Walker, and Hien M. Nguyen. Rational design and expedient synthesis of heparan sulfate mimetics from natural aminoglycosides for structure and activity relationship studies. *Angewandte Chemie International Edition*, 62(32):e202304325, 2023
15. ** Whitney S. Y. Ong, Ke Ji, Vishaka Pathiranage, Caden Maydew, Kiheon Baek, Rhiza Lyne E. Villones, Gabriele Meloni, Alice R. Walker, and Sheel C. Dodani. Rational design of the β-bulge gate in a green fluorescent protein accelerates the kinetics of sulfate sensing. *Angewandte Chemie International Edition*, 62(26):e202302304, 2023
14. ** Ashlyn R. Murphy, Mark A. Hix, and Alice R. Walker. Exploring the effects of mutagenesis on FusionRed by using excited-state QM/MM dynamics and classical force field simulations. *ChemBioChem*, 24(12):e202200799, 2023. Featured on Cover.

13.** Solomon Yamoah Effah, W. K. D. N. Kaushalya, Mark A. Hix, and Alice R. Walker. Computational investigations of the excited state dynamics and quenching mechanisms of polycyclic aromatic hydrocarbon DNA adducts in solution. *Electronic Structure*, 2022

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

Preprints and manuscripts under review:

- ** Cheng Chen*, Vishaka Pathiranage*, Whitney S. Ong, Sheel Dodani, Alice R. Walker, and Chong Fang. A twisted chromophore that powers a fluorescent protein chloride sensor. https://chemrxiv.org/engage/chemrxiv details/669ce9ee5101a2ffa8388287

- ** Cuixin Lai, Lina Yang*, Vishaka Pathiranage*, Ruizhao Wang, Fedor V. Subach, Alice R. Walker, and Kiryl D. Piatkevich. Genetically encoded green fluorescent sensor for probing sulfate transport activity of solute carrier family 26 member a2 (Slc26a2) protein. Under review.

- ** Widana Kaushalya and Alice R. Walker. Simulations of DNA-coordinated light emission vs. intramolecular electron transfer: electron donor-acceptor systems with benzo[a]pyrene derivatives. https://chemrxiv.org/eng details/64ea410c3fdae147fae2cd1b

- ** Mark A. Hix and Alice R. Walker. Adaptive restraints to accelerate geometry optimizations of large biomolecular systems. https://chemrxiv.org/engage/chemrxiv/article-details/6490b93ba2c387fa9a94f607 Source code: https://github.com/arwalkerlab/TeraChemAdaptiveRestraints/

- ** Mark A. Hix, Pramoda Gamage, Ashok S. Bhagwat, and Alice R. Walker. DNA hairpin base-flipping dynamics drives APOBEC3A recognition and selectivity. Under review.

Prior to faculty appointment:

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**

Teaching and Mentoring Experience

College Courses taught at Wayne State University (Detroit, MI) September 2021-present

- Structure and Function of Biomolecules (5600/7600)
- Computational Chemistry (6440/7440)

Quantum Molecular Design Summer School Instructor at Stanford University (Stanford, CA), August 2019
Protein Subgroup Leader, Martínez Group at Stanford University (Stanford, CA) June 2018-July 2021
BUILD Program Coordinator and Lecturer at Wayne State University (Detroit, MI), July 2015/July 2016
Graduate Teaching Assistant at Wayne State University (Detroit, MI), Sept. 2013-Aug. 2015
Student Teacher at Southfield-Lathrup High School (Southfield, MI), Jan. 2011-April 2011

Invited Seminars at Universities

12. Bowling Green University, Bowling Green, OH, 2024
11. NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai, China, 2024
10. University of Texas-Dallas, Dallas, TX, 2024
9. University of Texas-Arlington, Arlington, TX, 2024
8. Heinrich Heine University Düsseldorf, Düsseldorf, Germany, 2024
7. Youngstown State University, Youngstown, OH, 2023
6. Chico State, Chico, CA, 2023
5. Aquinas College, Grand Rapids, MI, 2023
4. Instituto Tecnológico de Celaya, Celaya, Mexico. December 3, 2021.
3. Department of Physics, Wayne State University, Detroit, MI. November 9, 2021.
2. Autonomous University of Zacatecas, Zacatecas, Mexico. October 22, 2021.
1. University of Michigan-Dearborn Colloquium, Dearborn, MI. September 10, 2021.

Conference and Workshop Presentations

25. "Rapid molecular dynamics and docking simulations of functionalized carbohydrate-based ligands." **Invited Talk**. ACS Fall 2024, Denver, CO. 2024.
24. "Excited state dynamics simulations of fluorescent proteins." **Invited Talk**. 42nd Biannual Meeting of the American Society for Photobiology, Chicago, IL. July 2024.
23. "Large-scale quantum mechanics simulations of extended electronic effects in ICH Ralstonia." **Invited Talk**. 7th Ringberg Workshop in Structural Biology. Bavaria, Germany. February 2024.

22. "Rapid molecular dynamics and docking simulations of functionalized carbohydrate-based ligands for promising cancer targets heparanase and galectin-3." **Invited Talk**. ACS Fall 2023, San Francisco, CA. 2023.
21. "Excited state dynamics simulations of fluorescent proteins."**Invited Talk**. CERM Session: Cellular signaling and respiration. ACS Regional Meeting, Dearborn, MI. 2023.
20. "Molecular simulation: Principles and application." **Invited Talk**. COMP Undergraduate Symposium, ACS Spring 2023, Indianapolis, IN. 2023.
19. **Invited Talk**. 40 years of exploring potential energy surfaces: a symposium honoring H. Bernhard Schlegel, ACS Fall 2022, Chicaco, IL. 2022.
18. **Poster**. American Conference in Theoretical Chemistry. Olympic Valley, CA, 2022.
17. "*Ab initio* simulations of proton transfer from a photoacid to water." **Talk**. Fusion of Classical- and Quantum-Mechanical Molecular Simulations Session. Pacifichem 2021 Virtual Congress, Honolulu, HI. December 16, 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.

Prior to faculty appointment:

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.

University, Campus and Departmental Service

NOBCChE Coadviser (2023-present)
ChatGPT Committee Chair (2023)
MARC Mentor (2022-present)
C&IT Liasion Team (2021-present)
WSU Research Technology Advisory Council (2022-present)
Gopal Symposium Planning Committee (2021-present)
Seminar Committee (2021-2022)
Faculty Hiring Rubric Committee (2021-2022)
Graduate Admissions Committee (2021-2024)

Public and Professional Service

Journal referee (20 reviews per year) (including Electronic Structure, Chemical Science, Computational and Structural Biochemistry, ChemBioChem, J Comp Biophys Chem, Angewandtie Chemie Int Ed, Journal of Physical Chemistry Letters, Journal of Cheminformatics, Journal of Chemical Information and Modeling)
Project SEED Mentor (American Chemical Society)
Reviewer for Department of Energy, Basic Energy Sciences FOA for Accelerated, Inclusive Research
Early Career Reviewer for National Institutes of Health (MSFB)
Ad Hoc Reviewer for National Institutes of Health (MBBC-10, SBIR/STTR)
MARC Mentor (WSU), 2021-present
Volunteer for career planning assistance (2021-present)
Poster Judge for undergraduate posters at ANACHEM Symposium (2021)
ACS Graduate School Fair at ACS Spring 2022 in San Diego, CA (2022)
WSU ACS Pride Month Event Speaker (June 26, 2022)
ACTC Session Chair (July 2022)
Organizer for Regional ACS Midwest 2-day symposium (October 2022-May 2023)
Poster Judge for Wayne State University Chemistry Graduate Research Symposium (2022)
Girl Scouts Women in Science Day (January 2023)
WSU ACS Pride Month Event Panelist (June 26, 2023)
MARC LGBTQIA+ Panelist (December 1, 2023)

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)

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