

Alice R. Walker

Wayne State University Chemistry
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Github: Walker Lab

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

Associate Professor at Wayne State University (Detroit, MI), August 2026-present.
Carl R. Johnson Early Career Endowed Chair at Wayne State University (Detroit, MI), August 2024-August 2026.
Assistant Professor at Wayne State University (Detroit, MI), August 2021-August 2026.
Postdoctoral Scholar at Stanford Linear Accelerator Lab/Stanford University (Stanford, CA), May 2018-July 2021
Adviser: Prof. Todd J. Martínez

Awards and Honors

Election to the Junior Academy of Scholars at Wayne State University (2026)
OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award, ACS COMP (Fall 2026)
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)
Chancellor's Scholarship, University of Michigan-Dearborn (2005-9)
Honor's Program, University of Michigan-Dearborn (2005-11)

Research Grants and External Support

- [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
- [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: 9/10/2024-9/9/2029.

Theses Directed

Graduate Students:

Vishaka Pathirana, PhD, 2026
Solomon Yamoah Effah (2021-present)

Widana Kaushalya (2021-present)
Victoria Mfon Sunday (2022-present)
Anita Adams (2022-present)
Pramoda Gamage (2023-present)
Janya Subasinghe (2023-present)
Dylan Yost-Slinker (2025-present)
Sandeepa Fernando (2026-present)

Postdoctoral Researchers:

Mark A. Hix (2022-present)
Christina McCulley (2021-2023)

Funded Undergraduate Student Researchers:

Ashlyn Murphy, BS, 2022
Nathaniel Turner, BS, 2023
John Muller, BS, 2024
Morgan Grougan, BS, 2026

Undergraduate Student Theses Directed:

Grant Porter, Undergraduate, 2023
Joel Daniel, Undergraduate, 2023
Nathan Shultz, Undergraduate, 2023
Mahmood Alsughayer, Undergraduate, 2024
Gordon Stroster, Undergraduate, 2024
Zakaria Khan (co-directed), Undergraduate, 2024
Abdulaziz Alenezi, Undergraduate, 2025
Benjamin Delozier, Undergraduate, 2025
Austin Frederick, Undergraduate, 2025
Ally Scott, Undergraduate, 2025
Cooper Lundh, Undergraduate, 2026
Ortheo Mara, Undergraduate, 2026

Peer Reviewed Publications

Single stars (*) indicate corresponding authorship. Daggers (†) indicate equal authorship. **Bold** indicates undergraduate or high school author.

36. Anita Houston Adams, Mark A. Hix, and Alice R. Walker*. Simulations of solvent effects on excited state dynamics of p-dapa, a red single benzene-based fluorophore. *The Journal of Chemical Physics*, 165(2):024303, 07 2026
35. Morgan Grougan, Janya Subasinghe, Mark A. Hix, and Alice R. Walker*. Librarian of Alexandria: A modular chemical data extraction pipeline to compare LLM performance. *Journal of Chemical Information and Modeling*, 66(12):6921–6932, 2026. PMID: 42262247 Preprint DOI: 10.26434/chemrxiv-2025-fb8hj
34. Andrea L. Batchev, Widana Kaushalya, Chashitha Padukka, Janya Subasinghe, Alice R. Walker*, and Matthew J. Allen*. Cyclen tetra-amide ligands as a privileged class of ligands for studying second-sphere coordination environments. *Chemistry – A European Journal*, n/a(n/a):e71136
33. Premashis Manna*, Mark A. Hix, Srijit Mukherjee, Alice R. Walker, and Ralph Jimenez*. Dark-state-mediated photobleaching in mCherry-based red fluorescent proteins. *The Journal of Physical Chemistry Letters*, 17(12):3596–3604, 2026. PMID: 41838933
32. Jiusheng Lin, Oksana Gerlits, Daniel W. Kneller, Kevin L. Weiss, Leighton Coates, Jennifer L. Clarke, Mark A. Hix, Solomon Y. Effah, Andrey Kovalevsky*, Alice R. Walker, and Mark A. Wilson*. Environmental contributions to proton sharing in protein low-barrier hydrogen bonds. *Biochemistry*, 65(6):764–778, 2026. PMID: 41656622. Featured on Cover.
31. Mfon V. Sunday, Ke Ji, Derik A. Adams, Weicheng Peng, Sheel C. Dodani*, and Alice R. Walker*. Physical mechanisms of an unconventional green fluorescent protein indicator for chloride. *The Journal of Physical Chemistry B*, 130(11):3065–3075, 2026. PMID: 41784459
30. Lina Yang, Vishaka Pathiranaage, Shihao Zhou, Xiaoting Sun, Hanbin Zhang, Cuixin Lai, Chenlei Gu, Fedor V. Subach, Mikhail Drobizhev, Alice R. Walker*, and Kiryl D. Piatkevich*. Sensitive red fluorescent indicators for real-time visualization of potassium ion dynamics in vivo. *PLOS Biology*, 23(9):1–36, 09 2025

29. Cheng Chen[†], Vishaka Pathirana[†], Whitney S. Y. Ong, Sheel C. Dodani, [Alice R. Walker*](#), and Chong Fang*. A twisted chromophore powers a turn-on fluorescent protein chloride sensor. *Proceedings of the National Academy of Sciences*, 122(32):e2508094122, 2025
28. Hawau Abdulsalam, Mark A. Hix, Livia Philip, Kartikey Singh, [Alice R. Walker*](#), and Hien M. Nguyen*. From docking and molecular dynamics to experimental discovery: Exploring the hydrophobic landscapes of heparanase to design potent inhibitors. *Journal of Chemical Information and Modeling*, 65(13):6899–6912, 2025. PMID: 40586429
27. Michael Hotor, Joseph Wakpal, Solomon Y. Effah, Nur-E Alom, [Alice R. Walker*](#), and Hien M. Nguyen*. Could hydrophobicity of sulfated pseudo-trisaccharides derived from repurposing aminoglycoside tobramycin modulate the enzymatic activity of heparanase? *Journal of Medicinal Chemistry*, 68(12):12708–12732, 2025. PMID: 40500735
26. Mark A. Hix and [Alice R. Walker*](#). Adaptive restraints to accelerate geometry optimizations of large biomolecular systems. *Journal of Computational Chemistry*, 46(12):e70127, 2025
25. Mark A. Hix, A. G. Pramoda Sahankumari, Ashok S. Bhagwat, and [Alice R. Walker*](#). DNA hairpin base-flipping dynamics drives APOBEC3A recognition and selectivity. *Physical Chemistry Chemical Physics*, 27:11551–11557, 2025
24. Solomon Y. Effah, Mark A. Hix, and [Alice R. Walker*](#). Strategic design of fluorescent perylene-modified nucleic acid monomers: Position-, phosphorylation-, and linker-dependent control of electron transfer. *Journal of Chemical Information and Modeling*, 65(6):2940–2949, 2025
23. Cuixin Lai, Lina Yang[†], Vishaka Pathirana[†], 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. *Communications Biology*, 7(1):1375, October 2024
22. Elisa Pieri, [Alice R. Walker](#), Mingning Zhu, and Todd J. Martínez*. Conical intersection accessibility dictates brightness in red fluorescent proteins. *Journal of the American Chemical Society*, 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. *Journal of Physical Chemistry 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. *Journal of Physical Chemistry 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. *Journal of Chemical Information and Modelling*, 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. *Journal of Physical Chemistry C*, 127(33):16654–16667, August 2023
16. Joseph Wakpal, Vishaka Pathirana[†], [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 Pathirana[†], 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. *Journal of Physical Chemistry 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:

- 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. Preprint: 10.26434/chemrxiv-2023-sdrw7
- Cheng Chen, Jiawei Liu, Ivan M. Myasnyanko, Daniil I. Rudik, Anita Houston Adams, [Alice R. Walker](#), Mikhail S. Baranov, and Chong Fang.* Meta effect enables redder and larger Stokes shift chromophores by enhanced aromaticity reversal. Preprint: 10.26434/chemrxiv-2025-56x1p
- Jasmine Tutol, Vishaka Pathirana, [Alice R. Walker](#), and Sheel C. Dodani.* An all-optical approach to probe chloride transport with a bright ChlorON. Preprint: <https://www.biorxiv.org/content/10.64898/2026.03.09.710669v1>
- Hannah L. Palomino, Sophia Liu, Mark A. Hix, [Alice R. Walker](#)*, and Nicolai Lehnert.* Minima remodeling converts enzymes into efficient heterogeneous biocatalysts in organic solvents. Submitted.
- Anita Houston Adams and [Alice R. Walker](#).* Excited state QM/MM simulations of far red fluorescent proteins show diverging electronic and physical structure correlated with red shifts. Submitted.
Preprint: <https://chemrxiv.org/doi/full/10.26434/chemrxiv.15004889/v1>

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 Lagardère, 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)
- Undergraduate Research (5999): 15 students total

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

22. Wayne State University, Department of Pharmaceutical Sciences, Detroit, MI, 2025
21. K College, Kalamazoo, MI, 2025
20. Ohio State, Columbus, OH, 2025
19. North Carolina State, Raleigh, NC, 2025
18. Duke University, Durham, NC, 2025
17. The University of North Carolina at Chapel Hill, Chapel Hill, NC, 2025
16. Akron University, Akron, OH, 2025
15. Oakland University, Oakland, MI, 2025
14. Texas Tech, Lubbock, TX, 2025
13. Georgia State University, Atlanta, GA, 2025
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

35. Fluorescent Proteins and Biological Sensors VIII. **Invited Poster**. HHMI Janelia Research Campus, 2026.4 Scheduled.
34. Multiscale Simulations of Fluorescent Proteins for Rational Design. **Invited Talk**. 21st International Conference on Retinal Proteins, Università di Siena, Siena, Italy, 2026. Scheduled.
33. "Simulations of fluorescent biomolecules for rational design." **Invited Talk**. ACS Fall, Chicago, IL, 2026. Scheduled.
32. "Simulations of biomolecules in complex environments for rational design with excited state dynamics and machine learning." **Invited poster**. ACS Fall, Chicago, IL, 2026. Scheduled.
31. "Simulations of Fluorescent Biomolecules for Rational Design." **Invited Talk**. Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, MN, 2026.
30. Spring ACS 2026. **Invited Talk**. Presidential Symposium: Human, Computer and Artificial Intelligence, Atlanta, GA, 2026.

29. Anachem Symposium. **Invited Talk**. Machine Learning for Analytical Chemistry in the Classroom. Livonia, MI, Anachem 2026.
28. "Excited state simulations of p-DAPA and mGrape fluorophores in explicit solvent." **Invited Talk**. ACS Fall Washington, DC, 2025.
27. "Engineering fluorescent proteins as anion-sensitive scaffolds." **Invited Talk**. RosettaCon, Suncadia, WA, 2025.
26. "Engineering fluorescent proteins as anion-sensitive scaffolds." **Invited Talk**. Design of Light-Responsive and Light-Emitting Proteins Workshop, Telluride, CO. 2025.
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, Chicago, 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. Pacificchem 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

Graduate Recruiting Chair (2026-2027)

Faculty Council (2026-2029)

NOBCCHE Coadviser (2023-present)

ChatGPT Committee Chair (2023)

MARC Mentor (2022-2025)

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) **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)

Selected Public and Professional Service

Journal Referee (~20 reviews per year) (including Electronic Structure, PhotochemPhotobio, PCCP, Chemical Science, Computational and Structural Biochemistry, ChemBioChem, J Comp Biophys Chem, Angewandte Chemie Int Ed, Journal of Physical Chemistry Letters, Journal of Cheminformatics, Journal of Chemical Information and Modeling, Journal of the American Chemical Society)

Reviewer for Department of Energy, Basic Energy Sciences FOA for Accelerated, Inclusive Research

Ad Hoc Reviewer for National Science Foundation

Reviewer for American Chemical Society Petroleum Research Fund, New Directions Grant

Early Career Reviewer for National Institutes of Health (MSFB)

Ad Hoc Reviewer for National Institutes of Health (MBBC-10, SBIR/STTR, MRAB ESI MIRA, MBBC)

Reviewer for US-Egypt Science and Technology Joint Fund

Committee Member in Chemistry and Materials for PASC 2026, Bern, Switzerland (2026)

Panel Moderator for Michigan Drug Discovery & Development Symposium, Ann Arbor, MI (2026)

Poster Judge for Phys Division, Fall ACS, Washington, DC (2025)

Poster Judge for RosettaCon, Suncadia, WA (2025)

Project SEED Mentor (American Chemical Society)

Co-organizer for Midwest Theoretical Chemistry Conference, 2025

Girl Scouts Women in Science Day (January 2023)

Organizer for Regional ACS Midwest 2-day symposium (October 2022-May 2023)

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)

Poster Judge for Wayne State University Chemistry Graduate Research Symposium (2022)

MARC Mentor (WSU), 2021-2025

Volunteer for career planning assistance (2021-present)

Poster Judge for undergraduate posters at ANACHEM Symposium (2021)

WSU ACS Pride Month Event Panelist (June 26, 2023)

MARC LGBTQIA+ Panelist (December 1, 2023)

Professional Organizations & Development

American Society for Photobiology (August 2024-present)

Association for Women in Science (November 2018-present)

AGEP Seminar Series (January 2015-September 2016)

STEM Pedagogy Seminar Series (September 2014-September 2016)

BEST Professional Development Program (September 2014-September 2016)

Software Summer School at Virginia Tech (June 2015)

NVIDIA CUDA qwiklabs (April 2015)

American Chemical Society, COMP Member Number: 30858881 (January 2015-present)