Gerardo Andrés Cisneros
Professor, Department of Physics; and Chemistry & Biochemistry, University of Texas at Dallas

Education and Professional Experience

- Department of Chemistry, University of North Texas, Professor, 2019–2021.
- Department of Chemistry, University of North Texas, Associate Professor, 2016–2019.
- Department of Chemistry, Wayne State University, Associate Professor, 2015–2016.
- Department of Chemistry, Wayne State University, Assistant Professor, 2009–2015.
- National Institute of Environmental Health Sciences–NIH, IRTA Postdoctoral Fellow, 2004–2009.
- Duke University, Durham, NC, Ph.D., 2004.
- Universidad Nacional Autónoma de México (UNAM), Mexico City, México, B.Sc., 1999.

Honors and Awards

2020 SACNAS Outstanding Hispanic Student Mentor.

2019 Early Career Award, Office for Research and Innovation, University of North Texas.

2018 Faculty Award for Research, College of Science, University of North Texas.

2018 Distinguished Visiting Professor, the Mexican Academy of Sciences (AMC).(FUMEC).

2017 Research Exemplar, The P.I. Program at Washington University School of Medicine.

2016 National Strategic Computing Initiative, invited participant, The White House, Washington D.C.

2015 Excellence in Teaching Award, College of Liberal Arts and Sciences, Wayne State University.

2014 Dell–Intel Young Investigator Award, 54th Sanibel Symposium, Quantum Theory Project, University of Florida.

2014 ACS Division of Computers in Chemistry OpenEye Outstanding Junior Faculty Award.

2007 Winner; Emerging Technologies in Computational Chemistry Competition Symposium, 234th ACS National Meeting.

2007 IBM–Löwdin Fellowship, Quantum Theory Project, University of Florida.

2006 Carl Storm Fellowship, Gordon Research Conferences.

2004 Best Graduate Student Poster, 44th Sanibel Symposium.

1999–2002 Scholarship from the Consejo Nacional de Ciencia y Tecnología, (CONACyT).

Funding

Current

- NIH/NIGMS R01GM108583–07 (PI: Cisneros) 08/2019–07/2023 "Investigation of DNA Modifying Enzymes by Computational Simulations: Development and Applications"
- NSF–CHEM/CLP 1856162 (PI: Cisneros, co–PI: Ren) 08/2019–07/2022 "Collaborative Research: Computational Investigation of Solvent Effects on Enzyme Catalysis"
- NSF–OAC 2117247 (PI: Cisneros, co-PIs: Cundari, Yan, Andreussi, Du) 09/2021–08/2024: "MRI: Acquisition of a High Performance Hybrid Computer Cluster for Computational Modeling",
- NIH/NIGMS R01GM108583–07S1 (PI: Cisneros) 08/2019–07/2022, diversity admin. sup.
- NIH/NIGMS R01GM108583–08S1 (PI: Cisneros) 09/2020–08/2021, software admin. sup.
- NIH/NIGMS T32GM136501 (lead PI: P. Padilla, PI: Cisneros, Brugren, Hughes) 06/2021–05/2026 "G–RISE at UNT"
- Microsoft AI for Good Initiative (PI: Cisneros) 03/2020–12/2020, Azure credit for "Using MD and QM/MM to improve drug candidates for nCoV-19 targets", in kind,
- XSEDE Allocation (PI: Cisneros) since 2015, renewed yearly.

Completed

- NIH/NIGMS R01GM108583 (PI: Cisneros) 03/2014–02/2019 "Theory and Simulation of DNA Repair Enzymes; Mechanism, Structure and Function"
- NIH/NIGMS R01GM118501 (PI: Kohli, co–PIs: Bartolomei, and Cisneros) 01/2017–12/2021 (subcontract to GAC) "Investigation of multiple oxidation steps by TET family enzymes"
- NVIDIA Foundation, "Compute the Cure" (PI: Cisneros) 01/2017–12/2019
- NIH/NIGMS R01GM108583–06S1 (PI: Cisneros) 09/2018, equipment administrative suplement

Professional Development

- Academic Leadership Training ALT2020, Cotrell Scholar Collaborative and American Chemical Society, Washington D.C., February, 2020.
- Active Learning for College Teaching, National Institutes of Environmental Health Sciences, RTP, NC, September–December, 2008.

Publications *–in reverse chronological order, star denotes corresponding author*

1. Li A.W.H., Zabrady K., Bainbridge L.J., Zabrady M., Naseem-Khan S., Berger M.B., Kolesar P., Cisneros G.A., Doherty, A.J.*, "Molecular basis for the initiation of DNA primer synthesis", *Nature*, accepted, 2022.
2. Naseem-Khan S., Berger M.B., Leddin E.M., Maghsoud Y., **Cisneros G.A.***, "Impact of Remdesivir Incorporation Along the Primer Strand on SARS-CoV-2 RNA-dependent RNA polymerase", *J. Chem. Inf. Model.*, DOI:10.1021/acs.jcim.2c00201, 2022.
3. Naseem-Khan S., Lagardere L., Narth C., Cisneros G.A., Ren P., Gresh N., Piquemal J.-P.*, "Development of the Quantum Inspired SIBFA Many-Body Polarizable Force Field: I. Enabling Condensed Phase Molecular Dynamics Simulations", *J. Chem. Theo. Comp.*, accepted, 2022.
4. Ravishankar K., Jiang X., Leddin E.M., Morcos, F.*, **Cisneros G.A.**, "Computational Compensatory Mutation Discovery Approach: Predicting a PARP1 Variant Rescue Mutation", *Biophys J.*, accepted, 2022.
5. Naseem-Khan S., Piquemal J.-P., **Cisneros G.A.***, "Improvement of the Gaussian Electrostatic Model by Separate Fitting of Coulomb and Exchange-Repulsion Densities and Implementation of a new Dispersion Term", *J. Chem. Phys*, **155**, 194103, 2021.
6. Berger M.B., Walker A.R., Vazquez-Montelongo E.A., **Cisneros G.A.***, "Computational Investigations of Selected Enzymes From Two Iron and α-ketoglutarate-Dependent Families", *Phys. Chem. Chem. Phys.*, **23**, 22227-22240, 2021.
7. Gaba A., Hix M.A., Suhail S., Flath B., Boysan B., Williams D.R., Pelletier T., Emerman M., Morcos F., Cisneros G.A., Chelico L.*, "Divergence in dimerization and activity of primate APOBEC3C", *J. Mol. Bio.*, **433**, 167306, 2021.
8. Nochebuena J., Quintanar L., Vela A., **Cisneros G.A.***, "Structural and Electronic Analysis of the Octarepeat Region of Prion Protein with Four Cu(II) by Polarizable MD and QM/MM Simulations", *PCCP*, **23**, 21569-21578, 2021.
9. Hix M.A., Leddin E.M., **Cisneros G.A.***, "Combining Evolutionary Conservation and Quantum Topological Analyses to Determine QM Subsystems for Biomolecular QM/MM Simulations", *J. Chem. Theo. Comp.*, **17**, 4524-4537, 2021.
10. Nochebuena J., Naseem-Khan S., **Cisneros G.A.***, "Development and Application of QM/MM Methods with Advanced Polarizable Potentials", *WIREs Comp. Mol. Sci.*, 11:e1515, 2021.
11. Lambros E., Lipparini F., **Cisneros G.A.**, Paesani F*. "A Many-Body, Fully Polarizable Approach to QM/MM Simulations", *J. Chem. Theo. Comp.*, **16**, 7462–7472, 2020.

12. Hix M.A., Wong, L, Flath B., Chelico L.*, **Cisneros G.A.***, "Single-nucleotide polymorphism of the DNA cytosine deaminase APOBEC3H haplotype I leads to enzyme destabilization and correlates with lung cancer", *NAR Cancer*, **2**, zcaa023, 2020.
13. Hix M.A., **Cisneros G.A.***, "Computational investigation of APOBEC3H substrate orientation and selectivity", *J. Phys. Chem. B* **124**, 3903–3908, 2020.
14. Vázquez-Montelongo E.A., Vázquez-Cervantes J.E., **Cisneros G.A.**, "Current Status of AMOEBA–IL: A Multipolar/Polarizable Force Field for Ionic Liquids", *Int. J. Mol. Sci.*, **21(3)**, 697, 2020.
15. Vázquez-Montelongo E.A., **Cisneros G.A.**, Flores–Ruiz H.M.*, "Multipolar/Polarizable Molecular Dynamics Simulations of Liquid–Liquid Extraction of Benzene from Hydrocarbons Using Ionic Liquids", submitted to *J. Mol. Liq.*, ChemRxiv preprint, DOI: 10.26434/chemrxiv.8239829.v1, 2019.
16. Duke R.E., **Cisneros G.A.***."Ewald–Based Methods for Gaussian Integral Evaluation: Application to a New Parametrization of GEM*", accepted, *J. Mol. Model.*, **25**:307, 2019.
17. Das R., Vázquez-Montelongo E.A., **Cisneros G.A.**, Wu J.I.*, "Ground State Destabilization in Uracil DNA Deglycosylase (UDG): Let's Not Forget "Tautomeric Strain" in Substrates", *J. Am. Chem. Soc.*, DOI: 10.1021/jacs.9b06447, 2019.
18. Koleva B.N., Gokcan H., Rizzo A.A., Lim R., Dit Fouque K.J., Choy A., Liriano M., Fernandez-Lima F., Korzhnev D., **Cisneros G.A.**, Beuning P.*, "Dynamics of the *E. coli* β clamp dimer interface and its influence on DNA loading", *Biophys J.*, **117**, 587–601, 2019.
19. Leddin E., **Cisneros G.A.***, "Comparison of DNA and RNA Substrate Effects on TET2 Structure", in "Advances in Protein Chemistry and Structural Biology", T. Karabencheva-Christova and C. Christov Eds., Elsevier, DOI:10.1016/bs.apcsb.2019.05.002, 2019.
20. Loco D., Lagardere L, **Cisneros G.A.**, Scalmani G., Frisch M., Lipparini F., Mennucci B., Piquemal J.P.*, "Towards Large Scale Hybrid QM/MM Dynamics of Complex Systems with Advanced Point Dipole Polarizable Embeddings", *Chem. Sci.*, **10**, 7200–7211, 2019.
21. Walker A.R, Baddam N., **Cisneros G.A.***, "Unfolding Pathways of Hen Egg White Lysozyme in Ethanol", *J. Phys. Chem. B*, **123**, 3267-3271, 2019.
22. Gokcan H., Vazquez-Montelongo E.A., **Cisneros G.A.***, "LICHEM 1.1: Recent Improvements and New Capabilities", *J. Chem. Theo. Comput.*, **15**, 3056-3065, 2019.
23. DeNizio J., Liu M., Leddin E., **Cisneros G.A.**, Kohli R.*, "Selectivity and Promiscuity in TET–mediated oxidation of 5–methylcytosine in DNA and RNA", *Biochemistry*, **58**, 411–421, 2018.
24. Vazquez–Montelongo E.A., Vazquez–Cervantes J.A., **Cisneros G.A.***, "Polarizable ab initio QM/MM study of the reaction mechanism of N–tert–butyloxycarbonylation of aniline in [EMIm][BF4]", *Molecules*, **23** (11), 2830, 2018.
25. Torabifard H., **Cisneros G.A.***, "Insight into wild–type and T1372E TET2–mediated 5hmC oxidation using ab initio QM/MM calculations", *Chem. Sci*, **9**, 8433–8445, 2018.
26. Gahlon H.L., Walker A.R., **Cisneros G.A.**, Lamers M.H., and Rueda D.*, "Reduced structural flexibility for an exonuclease deficient DNA polymerase III mutant". *Phys. Chem. Chem. Phys.*, **20**, 26892-26902, 2018.
27. Silvestrov P., Maier S.J., Fang M., **Cisneros G.A.***, "DNArCdb: A Database of Cancer Biomarkers in DNA Repair Genes that Includes Variants Related to Multiple Cancer Phenotypes", *DNA Rep.*, **70**, 10–17, 2018.
28. Antczak N.M., Walker A.R., Leddin E.M., Palad C., Swett R.J., **Cisneros G.A.**, Beuning P.J.*, "Characterization of nine cancer–associated variants in human DNA polymerase κ", *Chem. Res. Tox.*, **31**,

697–711, 2018.

29. Lohrman J., Vázquez-Montelongo E.A., Pramanik S., Day V.W., Hix M.A., Bowman-James K.*, **Cisneros G.A.***, "Characterizing Hydrogen–Bond Interactions in Pyrazinetetracarboxamide Complexes: Insights from Experimental and Quantum Topological Analyses", *Inorg. Chem.*, **57**, 9775-9778, 2018.
30. Gokcan H., Kratz E.G., Darden T., Piquemal J.-P., **Cisneros G.A.***, "QM/MM Simulations with the Gaussian Electrostatic Model, A Density-Based Polarizable Potential", *J. Phys. Chem. Lett.*, **9**, 3062–2067, 2018.
31. Silvestrov P., **Cisneros G.A.***, "Insights on conformational changes in AlkD bound to DNA with a yatakemycin adduct from computational simulations", *Theo. Chem. Acc.*, **137**, 78, 2018.
32. Blanco–Díaz E.G., Vázquez–Mongelongo E.A., **Cisneros G.A.***, Castrejón–González E.O.*, "Computational Investigation of Non–Covalent Interactions in 1–Butyl–3–Methylimidazolium/ bis(Trifluoromethylsufonyl)imide in EMD and NEMD", *J. Chem. Phys.*, **148**, 054303, 2018.
33. Tu Y.–J., Lin Z., Allen M.J., **Cisneros G.A.***, "Molecular Dynamics Investigation of Solvent-Exchange Reactions on Lanthanide Ions in Water/1–Ethyl–3–Methylimidazolium Trifluoromethylsufate ([EMIm][OTf])", *J. Chem. Phys.*, **148**, 024503, 2018.
34. Liyanage P.S., Walker A.R., Brenlla A., **Cisneros G.A.**, Romano L.J.*, Rueda D.*, "Bulky Lesion Bypass Requires Dpo4 Binding in Distinct Conformations", *Sci. Reps.*, **7**, 17383, 2017.
35. Lagardère L., Jolly H.–L., Lipparini F., Aviat F., Stamm B., Jing Z.F., Harger M., Torabifard H., **Cisneros G.A.**, Schnieders M.J., Gresh N., Maday Y., Ren P.Y., Ponder J.W., Piquemal J.–P.*, "Tinker–HP: a Massively Parallel Molecular Dynamics Package for Multiscale Simulations of Large Complex Systems with Advanced Polarizable Force Fields", *Chem. Sci.*, **9**, 956, 2017.
36. Torabifard H., Reed L., Berry M.T., Hein J.E., Menke E., **Cisneros G.A.***, "Computational and Experimental Characterization of a Pyrrolidinum–Based Ionic Liquid for Electrolyte Applications", *J. Chem. Phys.*, **147**, 161731, 2017.
37. Walker A.R., **Cisneros G.A.***, "Computational Simulations of DNA Polymerases: Detailed Insights on Structure/Function/Mechanism from Native Proteins to Cancer Variants", *Chem. Res. Tox.*, **30**, 1922, 2017.
38. Torabifard H., **Cisneros G.A.***, "Computational Investigation of O_2 Diffusion Through an Intra–Molecular Tunnel in AlkB; Influence of Polarization on O_2 Transport", *Chem. Sci.*, **8**, 6230–6238, 2017.
39. O'Brien J.S., Allen M.J., **Cisneros G.A.***, "Computational Study of pH–Responsive Di–Lanthanide Complexes", *Int. J. Quantum Chem.*, in press, **117**, e25406, 2017.
40. Walker A.R., Silvestrov P., Muller T.A., Podolski R.H., Dyson G., Hausinger R.P., **Cisneros G.A.***, "AlkBH7 Variant Related to Prostate Cancer Exhibits Altered Substrate Binding", *PLoS Comp. Bio.*, **13 (2)**, e1005345, 2017.
41. Walker A.R., Bonomi R., Popov V., Gelovani J.G., **Cisneros G.A.***, "Investigating carbohydrate based ligands for galectin–3 with docking and MD studies", *J. Mol. Graph. Model.*, **71**, 211–217, 2017.
42. Liu M.Y., Torabifard H., Crawford D.J., DeNizio J.E., Cao X.–J., Garcia B.A., **Cisneros G.A.***, Kohli R.M.*, "Mutations along a TET2 active Scaffold Stall Oxidation at 5–hydroxymethylcytosine", *Nat. Chem. Bio.*, **13**, 181–187, 2017.
43. Gamage N–D.H., Stasny B., Kratz E.G., Stierstorfer J., Martin P.D., **Cisneros G.A.**, Klapötke T.M.*, Winter C.H.*, "Energetic Materials Trends in 5– and 6–Membered Cyclic Peroxides Containing Hyroperoxy and Hydroxy Subsitutents" *Eur. J. Inorg. Chem.*, **31**, 5036–5043, 2016.
44. Tu Y.–J., Allen M.A., **Cisneros G.A.***, "Simulations of Water Exchange Dynamics on Lanthanide Ions

in 1–Ethyl–3–Methylimidazoium Ethyl Sulfate ([EMim][$EtSO_4$]) and Water" *Phys. Chem. Chem. Phys.*, **18**, 30323–30333, 2016.

45. Zhao L., Udimbara M., Dewage S.W., Wood W.N., Veltri A.J., **Cisneros G.A.***, Hendrickson T.L.*, "Characterization of tunnel mutants reveals a catalytic step in ammonia delivery by an aminoacyl–tRNA amidotransferase", *FEBS Lett.*, **590**, 3122–3132, 2016.
46. Kratz E.G., Duke R.E., **Cisneros G.A.***, "Long–Range Electrostatic Corrections on Multipolar/Polarizable QM/MM Simulations", *Theo. Chem. Acc.*, **135**, 166, 2016.
47. **Cisneros G.A.**, Wikfeldt K.T., Ojamäe L., Lu J., Xu Y., Bartók A.P., Csányi G., Molinero V., Paesani F*., "Modeling Molecular Interactions in Water: From Pairwise to Many–Body Potential Energy Functions", *Chem. Rev.*, **116**, 7501–7528, 2016.
48. Kratz E.G., Walker A.R., Lagardère F., Lipparini F., Piquemal J.–P., **Cisneros G.A.***, "LICHEM: A QM/MM program for simulations with multipolar–polarizable force fields", *J. Comp. Chem.*, **37**, 1019–1029, 2016.
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51. Torabifard H., Starovoytov O.N., Ren. P., **Cisneros G.A.***, "Development of an AMOEBA water model using GEM distributed multipoles", *Theo. Chem. Acc.*, **134**, 101:1–10, 2015.
52. Fang D., Duke R.E., **Cisneros G.A.***, "A new smoothing function to introduce long–range electrostatic effects in QM/MM calculations", *J. Chem. Phys.*, **143**, 044103, 2015.
53. Bellow J., Yousif M., Fang D., Kratz E., **Cisneros, G.A.***, Groysman S., "Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand [OtBu2Ph]", *Inorg. Chem.*, **54**, 5624–5633, 2015.
54. Dewage S.W., **Cisneros G.A.***, "Computational analysis of ammonia transfer along two intra-molecular tunnels in Staphylococcus Aureus Glutamine–dependent Amidotransferase (GatCAB)", *J. Phys. Chem. B*, **119**, 3669–3677, 2015.
55. Silvestrov P., Müller T.A., Clark K.N., Hausinger R.P., **Cisneros G.A.***, "Homology modeling, molecular dynamics, and site–directed mutagenesis study of AlkB human homolog 1 (ALKBH1)", *J. Mol. Graph. Model*, **54**, 123–130, 2014.
56. Fang D., **Cisneros G.A.***, "Alternative pathway for the reaction catalyzed by DNA dealkylase AlkB from ab initio QM/MM simulations", *J. Chem. Theo. Comp*, **10**, 5136–5148, 2014.
57. Starovoytov O.N.*, Torabifard H., **Cisneros G.A.***, "Development of AMOEBA Force Field for Imidazolium Based Ionic Liquids", *J. Phys. Chem. B*, **118**, 7156–7166, 2014.
58. Chaudret R., Gresh N., Narth C., Lagardère L., Darden T., **Cisneros G.A.***, Piquemal J.P.*, "S/G-1: An Ab Initio Force–field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations", *J. Phys. Chem. A*, **118**, 7156–7166, 2014.
59. Piquemal J.–P.*, **Cisneros G.A.***, "Status of the Gaussian Electrostatic Model, a Density Based Polarizable Force Field", in "Many-body effects and electrostatics in multi-scale computations of biomolecules", Cui Q., Ren P., and Meuwly M., Editors., Pan Stanford Publishing, USA, 2014.
60. Elias A., **Cisneros G.A.***, "Computational Study of Putative Residues Involved in DNA Synthesis Fidelity

Checking in Thermus aquaticus DNA Polymerase I", in "Advances in Protein Chemistry and Structural Biology: Biomolecular Modelling and Simulations Volume 96", Karabencheva-Christova T., Editor, pp. 35–79, Elsevier, Netherlands, 2014.

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64. Burger S.K., **Cisneros G.A.***, "Efficient optimization of van der Waals parameters based on bulk properties", *J. Comp. Chem.*, **34**, 2313–2319, 2013.
65. Bellow J.A., Fang D. Kovacevic N., Martin P.D., Shearer J., **Cisneros G.A.***, Groysman S.*, "Novel Alkoxide Cluster Topologies Featuring Rare Seesaw Geometry at Transition Metals Centers", *Chem. Eur. J.*, **19**, 12225–12228, 2013.
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68. Fang D., Lord R.L., **Cisneros G.A.***, "QM/MM Calculations Show There is an Intersystem Crossing in the Hydrogen Abstraction Step in the Dealkylation Catalyzed by AlkB", *J. Phys. Chem. B*, **117**, 6410–6420, 2013.
69. Chaudret R., Gresh N., **Cisneros G.A.*** Piquemal J.–P.*, "Further refinements of next–generation force fields: non empirical localization of off–centered–points in molecules", *Can. J. Chem.*, **99** 1–7, 2013.
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75. Swett R., **Cisneros G.A.**, Feig A., "Conformational Analysis of Clostridium difficile Toxin B and its Implications for Substrate Recognition", *PLoS ONE*, **7 (7)**, e41518, 2012.
76. Pan W., **Cisneros G.A.**, Hu H., Chaudret R., Hu X., Yang W.*, "Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Protein-Protein Interactions on Proton Transfer Pathways", *J. Phys. Chem. B*, **116**, 6889–6897, 2012.

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87. **Cisneros G.A.***, Perera L.*, García–Díaz M., Bebenek K., Kunkel T.A., Pedersen L.G., "Catalytic mechanism of human DNA polymerase λ with Mg^{2+} and Mn^{2+} from *ab initio* QM/MM studies", *DNA Rep.*, **7**, 1824–1834, 2008.
88. **Cisneros G.A.**, Tholander S.N–I, Parisel O., Darden T.A., Elking D., Perera L., Piquemal J.–P.*, "Simple formulas for improved point–charge electrostatics in classical force fields and hybrid Quantum Mechanical/Molecular Mechanical embedding", *Int. J. Quant. Chem.*, **108**, 1905–1912, 2008.
89. **Cisneros G.A.***, Elking D., Piquemal J.–P., Darden T.A., "Numerical fitting of molecular properties to Hermite Gaussians", *J. Phys. Chem. A*, **111**, 12049–12056, 2007.
90. Gresh N., **Cisneros G.A.**, Darden T.A., Piquemal J.–P.*, "Anisotropic, polarizable molecular mechanics studies of inter–, intra–molecular interactions, and ligand–macromolecule complexes. A bottom–up strategy", *J. Chem. Theo. Comp*, **3**, 1960–1986, 2007.
91. **Cisneros G.A.***, Piquemal J.–P., Darden T.A., "Generalization of the Gaussian Electrostatic Model: extension to arbitrary angular momentum, distributed multipoles and speedup with reciprocal space methods", *J. Chem. Phys.*, **125**, 184101, 2006.
92. Piquemal J.–P.*, Perera L., **Cisneros G.A.**, Ren P, Pedersen L.G., Darden T.A., "Towards accurate

solvation dynamics of divalent cations in water using the polarizable AMOEBA force field: from energetics to structure", *J. Chem. Phys.*, **125**, 054511, 2006.

93. **Cisneros G.A.***, Piquemal J.–P., Darden T.A., "Quantum mechanics/molecular mechanics electrostatic embedding with continuous and discrete functions", *J. Phys. Chem. B*, **110**, 13682–13684, 2006.
94. Piquemal J.–P.*, **Cisneros G.A.**, Reinhardt P., Gresh N., Darden T.A., "Towards a force field based on density fitting", *J. Chem. Phys.*, **124**, 104101, 2006.
95. **Cisneros G.A.**, Wang M., Silinski P., Fitzgerald M.C., Yang W.*, "Theoretical and experimental determination on two substrates turned over by 4–oxalocrotonate tautomerase", *J. Phys. Chem. A*, **110** (2), 700–708, 2006.
96. **Cisneros G.A.***, Piquemal J.–P., Darden T.A., "Intermolecular electrostatics using density fitting", *J. Chem. Phys.*, **123**, 44109, 2005.
97. **Cisneros G.A.**, Liu H., Lu Z., Yang W.*, "Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order "chain–of–replicas" methods", *J. Chem. Phys.*, **122**, 114502, 2005.
98. Liu H., Lu Z., **Cisneros G.A.**, Yang W.*, "Parallel iterative reaction path optimization in *ab initio* quantum mechanical/molecular mechanical modeling of enzyme reactions", *J. Chem. Phys.*, **121** (2), 697–706, 2004.
99. **Cisneros G.A.**, Wang M., Silinski P., Fitzgerald M.C., Yang W.*, "The Protein Backbone Makes Important Contributions to 4–Oxalocrotonate Tautomerase Enzyme Catalysis: Understanding from Theory and Experiment", *Biochem.*, **43** (22), 6885–6892, 2004.
100. Goj L.A., **Cisneros G.A.**, Yang W.*, Widenhoefer R.*, "Dramatic effect of homoallylic substitution on the rate of palladium–catalyzed diene cycloisomerization", *J. Organomet. Chem.*, **687** (2), 498–507, 2003.
101. **Cisneros G.A.**, Liu H., Zhang Y. Yang W.*, "*Ab–initio* QM/MM study shows there is no general acid in the reaction catalyzed by 4–Oxalocrotonate Tautomerase", *J. Am. Chem. Soc.*, **125** (34), 10348–10393, 2003.
102. Pérez–Marín L.*, Castro M., Otazo–Sanchez E., **Cisneros G.A.**, "Density Functional Study of Molecular Recognition and Reactivity in Thiourea Derivatives Used in Sensors for Heavy Metal Polluting Cations", *Int. J. of Quantum Chem.*, **80** (4–5), 609–622, 2000.
103. Ascencio–Gutierrez J.A.*, Pérez–Marín L., Otazo–Sanchez E., Castro M., Contreras–Pulido D., **Cisneros G.A.**, "Molecular and Quantum Mechanics Calculations for the 1–Furoyl–3–Phenylthiourea as a Pb^{2+} sensor", *Afinidad*, **57** (487), 180–184 May–Jun, 2000.
104. **Cisneros G.A.**, Castro M., Salahub D.R.*, "DFT Study of the Structural and Electronic Properties of Small Ni_n (n=2–4) Clusters", *Int. J. of Quantum Chem.*, **75** (4–5), 847–861, 1999.

Submitted Manuscripts

1. Nochebuena J., **Cisneros G.A.***, "Polarizable MD and QM/MM Investigation of Acrylamide-based Leads to Target the Main Protease of SARS-CoV-2", https://doi.org/10.26434/chemrxiv-2022-gzk0r, 2022.

Publically Distributed Software

- **LICHEM**: A program to perform QM/MM calculations using advanced FF including AMOEBA (and soon GEM) interfacing several QM codes (PSI4, G09, NWChem) with TINKER(-HP), LAMPSS and AMBER; https://github.com/kratman/LICHEM_QMMM
- **pmemd.gem**: A program to perform classical MD calculations using GEM and AMOEBA. pmemd.gem

is distributed with the Amber 18 suite; http://ambermd.org

- **HyDn–SNP–S** (pronounced hidden–SNPs): (Hypothesis Driven–SNP–Search) A program to search for SNPs on genes for a target protein or protein family for a particular disease given a set of genome wide association studies (GWAS)
- **TINKER–HP**: The Cisneros group is part of the team developing TINKER-HP, a massively parallel software for new generation polarizable molecular dynamics; http://www.ip2ct.upmc.fr/tinkerHP/
- **GEM_Fit**: A program to calculate fitted densities and distributed multipoles from Gaussian Electrostatic Model (GEM) Hermite functions
- **VDW_Opt**: A program to calculate optimized Van der Waals parameters from QM intermolecular interactions and experimental data

Teaching and Mentoring

Students and Postdocs

Current

Postdoctoral Researchers:
Dr. Sehr Naseem–Khan
Dr. Jorge A. Nochebuena–Hernández

Graduate Students:
Mark Allen Hix
Emmett Leddin
José Enrique Vázquez Cervantes
Madison Berger
Yazdan Maghsoud
Arkanil Roy
Upeksha Walimuni Dewage
Shubham Chatterjee

Undergraduate Students:
Cole Stevens

High School Students:
Neel Shanmugam (TAMS, UNT)
Sanjana Bolnedi (TAMS, UNT)

Former

Dr. Rebecca Swett (Ph.D. 07/2013, now Senior Scientist at Relay Pharmaceuticals)
Dr. Dong Fang (Ph.D., 07/2014, now Scientist at Xtalpi, Shenzhen, China)
Dr. Sajeewa W. Dewage (Ph.D., 05/2015, now Senior Lecturer at Wayamba University, Sri Lanka.)
Dr. Hedieh Torabifard (Ph.D., 04/2017, now Asst. Prof. at University of Texas at Dallas)
Dr. Alice Walker (Ph.D., 03/2018, now Asst. Prof. at Wayne State U.)
Dr. Pavel Silvestrov (Ph.D., 03/2018)
Dr. Tu Yi–Jung (Ph.D., 05/2018, H.B. Schlegel co–adv., Asst. Prof. at Natl. Chi Nan Univ., Taiwan)
Dr. Erik A. Vázquez–Montelongo, (Ph.D., 03/2020, now postdoc at U Maryland College of Pharmacy)
Dr. Stanley M. Smith (postdoc, 2010–2011, Scientist at Waters Inc.)
Dr. Steven Burger (postdoc, 2012–2012, now seasonal lecturer at McMaster University)
Dr. Oleg Starovoytov, (postdoc, 2013–2014, now Asst. Prof. at Southern Univ. LA, Comp. Sci.)
Dr. Eric Kratz, (postdoc, 2014–2016, now algorithms specialist at Continental)
Dr. Hatice Gökcan, (postdoc, 2016–2018, now postdoc at Carnegie Mellon U.)
Dr. Robert E. Duke, Senior Scientific Software Developer, retired

Syeda Fatima Sultana (MA 2010, now Lead Health Data Analyst at BCBS RI)
Sarah E. Rowe (B.Sc. 2011, now Staff Scientist at University of Michigan Chemistry)
Michael Bell (B.Sc. 2011, now PhD student at University of Michigan Chemistry)
Chava Goldberg (B.Sc. 2014, honors)
Angela Elias (B.Sc. 2014, now PhD student at Wayne State University BME)
Elena Hunsanger (B.Sc. 2018, honors, now medical student at Wayne State University Med. School)
Joseph Senan O'Brien (B.Sc. 2018, honors, now PhD student at GATech)
Ally Smith (B.Sc. 2020, now PhD student at U Maryland School of Pharmacy)
Jordan Frank–Darío García
Sarah Maier (NSF–REU Summer 2017, now PhD student at Indiana University Chemistry)
Peter Camacho (NSF–REU Summer 2018)
Bernadette Broderick (Summer 2010, now staff scientist at University of Missouri)
Gregorio Alanís–Lobato (Summer 2010, now PhD student at KAUST)
Farjana Alam (project SEED summer 2012, now at University of Michigan)
Mumta Kadir (project SEED summer 2013, now at University of Michigan)
Fahmida Ahmed (project SEED summer 2014, and summer 2015, now at University of Michigan)
Nikhil Baddam (volunteer high school student, 2015–2016, now at Johns Hopkins University)
Michelle Fang (volunteer high school student, 2017, now at Yale University)
Katherine Shei (TAMS, 2017–2018, UNT)
Corey Shen (TAMS, 2017–2019, UNT)
Krithika Ravishankar (TAMS, 2017–2019, UNT)

Visiting Researchers

Prof. Jean Philip–Piquemal, University Paris VI, Pierre et Marie Curie/Sorbonne, France (multiple visits).
Prof. Maria Clelia Milletti, Eastern Michigan University, USA (2014).
Prof. Marco Tulio Gallo Estrada, Universidad Autónoma de San Luis Potosí, México (2015).
Prof. Hugo Marcelo Flores Ruiz, Universidad Autónoma del Estado de Hidalgo, México (2017).
Prof. Richard D. Lord, Grand Valley State University (2018).
Robin Chaudret, visiting graduate student, University Paris VI, Pierre et Marie Curie/Sorbonne (2011).
Dulce María Vázquez–Zavala, visiting graduate student, LANGEBIO/CINVESTAV, México (2015).
Christophe Narth, visiting graduate student, University Paris VI, Pierre et Marie Curie/Sorbonne (2015).
Edgar Guadalupe Blanco Díaz, visiting graduate student, Instituto Tecnológico de Celaya, México (2017).
Sehr Naseem–Kahn, visiting graduate student, University Paris VI, Pierre et Marie Curie/Sorbonne (2018).

Courses and Workshops

CHM3520, Physical Chemistry II, University of North Texas, Spring 2020.

CHM4660/5660, Computational Chemistry, University of North Texas, Fall 2016, Fall 2017, Fall 2018, Fall 2019, Fall 2021.

CHM5210, Quantum Chemistry, University of North Texas, Spring 2017, Spring 2018, Spring 2019.

CHM1030, Survey of Organic Chemistry and Biochemistry, Wayne State University, Fall 2012.

CHM5400 (co–instructor), Biological Physical Chemistry, Wayne State University, Winter 2012, Winter 2013, Winter 2014, Winter 2016.

CHM7440/6440 (co–instructor), Computational Chemistry, Wayne State University, Winter 2011, Winter 2012, Winter 2013, Winter 2014, Winter 2015, Winter 2016.

CHM5440 (co–instructor), Physical Chemistry 2, Wayne State University, Winter 2011, Winter 2015.

CHM7470, Quantum Chemistry, Wayne State University, Fall 2010, Fall 2011, Fall 2013.

CHM7430, Chemical Kinetics and Dynamics, Wayne State University, Fall 2009, Fall 2014, Fall 2015.

CHM7740 (co–instructor), Responsible Conduct of Research, Wayne State University, Fall 2010, Fall

2011, Fall 2013.

Invited Lecturer, Chemistry 22 "Gen. Chem.", Department of Chemistry, Duke University, Summer 2007.

Graduate Student Mentor for independent study undergraduate research student, Department of Chemistry, Duke University, Fall 2003.

Teaching Assistant, Gaussian98 lab for graduate course Chem 203.1 "Introduction to Quantum Mechanics I", Department of Chemistry, Duke University, Fall 1999.

Lead Instructor, Workshop: Introduction to UniChem, in "First Autumn School in Computational Chemistry", Mexico City, November 12 and 13, 1998.

Invited Talks at Institutions

1. Programa de Ingeniería Química, "Simulaciones híbridas QM/MM con potenciales polarizables avanzados", Universidad Autónoma de Zacatecas, Zacatecas, México, November, 2021.
2. Department of Chemistry and Biochemistry, "QM/MM Simulations with Advanced Polarizable Potentials", University of Lethbridge, Lethbridge, Alberta, November, 2021.
3. Departmento de Química, "Simulaciones híbridas QM/MM con potenciales polarizables avanzados", Universidad Nacional Autónoma de México, Mexico City, México, November, 2021.
4. Boston Area Group for Informatics and Modeling, "QM/MM Simulations with Advanced Polarizable Potentials", Boston, MA, June, 2021.
5. Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, "QM/MM Simulations with Advanced Polarizable Potentials", Xiamen University, Xiamen, China, April, 2021.
6. Grupo de Fisicoquímica Teórica, "QM/MM Simulations with Advanced Polarizable Potentials", Universidad Autónoma del Estado de Morelos, Cuernavaca, Morelos, México, March, 2021.
7. Department of Chemistry, "QM/MM Simulations with Advanced Polarizable Potentials", University of Colorado–Denver, Denver, CO, January, 2021.
8. 2020 Theory Seminar, "QM/MM Simulations with Advanced Polarizable Potentials", Kansas State University, Manhattan, KS, November, 2020.
9. Department of Chemistry and Biochemistry, "Leveraging Computational Approaches to Uncover and Characterize Cancer–Associated Missense Mutations", Texas Technological University, Lubbock, TX, November, 2020.
10. Bio-Discovery Institute, "Leveraging Computational Approaches to Uncover and Characterize Cancer–Associated Missense Mutations", University of North Texas, Denton, TX, October, 2020.
11. Biological Soft Matter Seminar Series, "Computational Approach to Discover and Characterize Cancer–Associated Mutations in DNA Modification Enzymes", Virtual Presentation, University of Newcastle, Newcastle, UK, May, 2020.
12. Department of Biochemistry, Molecular Biology and Immunology, "Computational Discovery and Characterization of Cancer Mutants", University of Saskatchewan, Saskatoon, Saskatchewan, Canada, January, 2020.
13. Department of Chemistry & Biochemistry, "Computational Prediction of Structural and Functional Characteristics of Fe/α–KG Enzymes", University of Texas at Dallas, Dallas, TX, March, 2019.
14. Department of Chemistry, "Insights on DNA modifying enzymes from computational simulations", University of Texas at Arlington, Arlington, TX, March, 2019.
15. Department of Biological Sciences, "Insights on DNA modifying enzymes from computational simulations", University of Texas at Dallas, Dallas, TX, August, 2018.

16. Department of Physics, "Development and Application of Classical and QM/MM Methods for Ionic Liquids and Biomolecular Simulations", University of North Texas, August, 2018.
17. AMC–FUMEC Distinguished visiting professor, Department of Chemistry, Centro de Investigación y de Estudios Avanzados (CINVESTAV), Workshop: "QM/MM Simulations with LICHEM and Advanced Potentials" Mexico City, Mexico, January, 2018.
18. AMC–FUMEC Distinguished visiting professor, Department of Chemistry, Centro de Investigación y de Estudios Avanzados (CINVESTAV), Seminar: "Insights on AlkB family enzymes, from native proteins to cancer variants", Mexico City, Mexico, January, 2018.
19. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", Grand Valley State University, Allendale, MI, April, 2016.
20. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", University of Florida, Gainesville, FL, February, 2016.
21. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", University of North Texas, Denton, TX, November, 2015.
22. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", University of Tennessee, Knoxville, TN, October, 2015.
23. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", Texas A&M University, College Station, TX, October, 2015.
24. "Workshop: Fitting of GEM densities and distributed multipoles", University Paris VI, Pierre et Marie Curie/Sorbonne, Paris, France, May–June, 2015.
25. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", University of Western Ontario, London, Ontario, Canada, April, 2015.
26. Department of Chemistry, "Development and application of advanced force fields for classical simulations", University of North Carolina, Chapel Hill, NC, February, 2015.
27. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", Duke University, Durham, NC, February, 2015.
28. LANGEBIO, "Investigación de Enzimas de Reparación de ADN Mediante Métodos Computationales", CINVESTAV, Irapuato, Guanajuato, México, January, 2015.
29. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", Vanderbilt University, Nashville, TN, October, 2014.
30. Center for Structural Biology, "Development of accurate polarizable potentials for water and ionic liquid simulations", National Heart Lung and Blood Institute/NIH, Rockville, MD, May, 2014.
31. Center for Functional Nanomaterials, "Insights on liquid systems and DNA repair enzymes from computational simulations", Brookhaven National Laboratory, Brookhaven, NY, March, 2014.
32. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", State University of New York–Stony Brook, Stony Brook, NY, March, 2014.
33. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", Georgia Institute of Technology, Atlanta, GA, March, 2014.
34. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", Wayne State University, Frontiers Seminar Series, Detroit, MI, February, 2014.
35. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", University of Chicago, Chicago, IL, January, 2014.

36. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", University of Southern California, Los Angeles, CA, November, 2013.
37. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", University of California–San Diego, San Diego, CA, November, 2013.
38. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", University of California–Santa Barbara, Santa Barbara, CA, November, 2013.
39. Department of Chemistry, "Insights on liquid systems and DNA repair enzymes from computational simulations", University of Wisconsin–Madison, Madison, WI, November, 2013.
40. Department of Chemistry, "Toward an electronic density based force field for classical simulations", University of Pittsburgh, Pittsburgh, PA, November, 2013.
41. Department of Biomedical Engineering and Department of Chemistry, "Toward an electronic density based force field for classical simulations", University of Texas at Austin, Austin, TX, October, 2013.
42. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", University of Michigan, Ann Arbor, MI, October, 2013.
43. Department of Chemistry, Highlands in Chemistry Seminar Series, "Toward an electronic density based force field for classical simulations", Virginia Institute of Technology, Blacksburg, VA, September, 2013.
44. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", New York University, New York, NY, September, 2013.
45. Department of Chemistry, "Insights on DNA repair enzymes from computational simulations", Rutgers University, New Brunswick, NJ, September, 2013.
46. Department of Chemistry, "Insights on fidelity of DNA synthesis from computational simulations", McMaster University, Hamilton, Ontario, Canada, May, 2013.
47. School of Natural Sciences, "Insights on fidelity of DNA synthesis from computational simulations", University of California–Merced, Merced, CA, April, 2013.
48. Department of Chemistry, "Insights on fidelity of DNA synthesis from computational simulations", University of California–Davis, Davis, CA, April, 2013.
49. Department of Chemistry, "Insights on fidelity of DNA synthesis from computational simulations", Michigan State University, East Lansing, MI, October, 2012.
50. Department of Chemistry, "Insights on fidelity of DNA synthesis from computational simulations", Oakland University, Rochester, MI, March, 2012.
51. Department of Medicinal Chemistry, "Insights on fidelity of DNA synthesis from computational simulations", University of Michigan, Ann Arbor, MI, March, 2012.
52. Theoretical Biophysics Section, "Computational investigation of metal ion mutagenicity in DNA synthesis from QM/MM calculations", NIDDK/NIH, Bethesda, MD, May 2011.
53. Department of Biochemistry, "Computational prediction of residues involved in post–insertion fidelity checking in DNA polymerase I", Wayne State University, Detroit, MI, March, 2011.
54. Department of Chemistry, "Computational prediction of residues involved in post–insertion fidelity checking in DNA polymerase I", Western Michigan University, Kalamazoo, MI, March, 2011.
55. Department of Chemistry, "Insights on metal mutagenicity in DNA polymerases from quantum chemistry", Eastern Michigan University, Ypsilanti, MI, October, 2010.
56. Aging, Senescence and Cellular Immortalization committee, "Computational studies of DNA repair: The

reaction mechanism of DNA polymerase λ", Karmanos Cancer Institute, Detroit, MI, October 2009.

57. Molecular Biology & Genetics Program, "Computational studies of DNA repair: The reaction mechanism of DNA polymerase λ", Karmanos Cancer Institute, Detroit, MI, September 2009.
58. Biotechnology High Performance Computing Software Applications Institute, Fort Detrick: "Penta–coordinated metal in the ϵ subunit of E. coli DNA polymerase III promotes catalysis", Frederick, MD, February 2009.
59. Department of Chemistry, Wayne State University: "Penta–coordinated metal in the ϵ subunit of E. coli DNA polymerase III promotes catalysis", Detroit, MI, January 2009.
60. Department of Molecular Structure, Amgen: "Penta–coordinated metal in the ϵ subunit of E. coli DNA polymerase III promotes catalysis ", Cambridge, MA, December 2008.
61. Center for Structural Biology, Wake Forest University: "Penta–coordinated metal in the ϵ subunit of *E. coli* DNA polymerase III promotes catalysis", Winston–Salem, NC, November 2008.
62. Department of Chemistry, Mount Olive College: "How metal ions aid in the replication of DNA", Mount Olive, NC, October 2008.
63. Laboratory of Computational Biology, NHLBI–NIH: "Catalytic mechanism of human DNA polymerase λ with Mg^{2+} and Mn^{2+} from *ab initio* QM/MM studies", Bethesda, MD, April 2008.
64. Department of Chemistry, Centro de Investigación y Estudios Avanzados–IPN; Physical Chemistry seminar series: "QM/MM theoretical study of enzymatic reaction mechanisms", Mexico City, August 2007.
65. Department of Chemistry, Universidad Nacional Autónoma de México (UNAM); Theoretical Chemistry seminar series: "QM/MM computational studies and theoretical development: The reaction mechanism of 4–oxalocrotonate tautomerase", Mexico City, March 2005.
66. Department of Chemistry, Universidad Autónoma Metropolitana (UAM); Physical Chemistry seminar: "QM/MM computational studies and theoretical development: The reaction mechanism of 4–oxalocrotonate tautomerase", Mexico City, March 2005.

Congresses and Symposia

Invited Talks

1. "*Ab initio* QM/MM Simulations with Advanced Polarizable Potentials", ACS Spring 2022 National Meeting, San Diego, CA, March, 2022.
2. "Discovery and Characterization of Cancer Mutations on DNA Transaction Enzymes", BIPOC make COMP Symposium, ACS Spring 2022 National Meeting, San Diego, CA, March, 2022.
3. "Computational investigation of SARS-CoV-2 main protease and RNA directed RNA polymerase inhibitors", ACS Fall 2021 National Meeting, Atlanta, GA, August, 2021 (Virtual).
4. "Computational mutational analysis of two APOBEC3 family enzymes", ACS Fall 2021 National Meeting, Atlanta, GA, August, 2021 (Virtual).
5. "Development and implementation of GEM and AMOEBA-IL for classical and QM/MM methods", ACS Fall 2021 National Meeting, Atlanta, GA, August, 2021 (Virtual).
6. "Discovery and Characterization of Cancer Mutations on DNA Transaction Enzymes", IUPAC CCCE 2021-48th World Chemistry Congress & 104th Canadian Chemistry Conference and Exhibition, Ottawa, CA, August, 2021 (Virtual).
7. "Discovery and Characterization of Cancer Mutations on DNA Transaction Enzymes", MolSSI Tapia Center Workshop, Houston, TX, July, 2021 (Virtual).

8. Boston Area Group for Informatics and Modeling, "QM/MM Simulations with Advanced Polarizable Potentials", Boston, MA, May, 2021.
9. "Discovery and Characterization of Cancer Mutations on DNA Transaction Enzymes", ACS National Meeting, San Diego, CA, April, 2021 (Virtual).
10. "Computational Investigation of SARS–CoV–2 RNA–dependent RNA Polymerase and Main Protease", ACS National Meeting, San Diego, CA, April, 2021 (Virtual).
11. "Leveraging Computational Approaches to Uncover and Characterize Cancer-Associated Missense Mutations", "Next Generation Biophysics Symposium 2020" A Virtual Meeting Hosted by MRC Laboratory of Molecular Biology, Cambridge, Cambridge, UK, October, 2020.
12. "MD and QM/MM Simulations of SARS-CoV-2 Main Protease and RNA Dependent RNA Polymerase", "COVID-19 HPC Consortium", Virtual Presentation, University of Pittsburg, Pittsburg, PA, June, 2020.
13. "Development and Implementation of GEM and AMOEBA–IL for Classical and QM/MM Methods", "Beyond point charges: novel electrostatic developments in force fields" CECAM workshop, Lausanne, Switzerland, December, 2019.
14. "Development and Applications of AMOEBA–IL", 11th Symposium on Molecular Simulations, Mexico City, México, November, 2019.
15. "Desarrollo y Aplicación de Métodos Computacionales Para Descubrir y Caracterizar Mutantes de Cáncer", Red Latinoamericana de Fisicoquímica Teórica, Webinar (multiple sites in México, Argentina, Colombia, and Venezuela), October 2019.
16. "Development and Implementation of GEM and AMOEBA–IL for Classical and QM/MM Simulations", Joint CHARMM–Tinker developer's meeting, Paris, France, July 2019.
17. "Adventures in Free Energy Simulations of ALKB Family DNA Oxidases", Free Energy Calculations Symposium, Santa Fe, NM, June, 2019.
18. "Development and Implementation of Classical and QM/MM Methods with Advanced Polarizable Potentials: LICHEM and pmemd.gem", ACS National Meeting, Orlando, FL, April, 2019.
19. "Development of Advanced Simulation Methods with Polarizable Potentials: LICHEM and pmemd.gem", XVIII Mexican Physicochemical Theory Reunion, Monterrey, MX, November, 2018.
20. "Computational Chemistry in Cancer Research", 2018 SACNAS National Conference, San Antonio, TX, October, 2018.
21. "Insights on AlkB family native and cancer variant enzymes", 255th ACS National Meeting, New Orleans, LA, March, 2018.
22. "Introduction to quantum chemistry and QM simulations", 255th ACS National Meeting, New Orleans, LA, March, 2018.
23. "Insights on the Role of an Active Site Scaffold in TET2 Required for the Step–Wise Oxidation of 5mC", 254th ACS National Meeting, Washington DC., August, 2017.
24. "Development of the Gaussian Electrostatic Model, GEM", 2017 Tinker Software Developers Meeting, St Louis, MO, March, 2017.
25. "Development of pmemd.gem: current capabilities and perspective", 2017 AMBER Developers Meeting, Athens, GA, February, 2017.
26. "Development and Application of Advanced Potentials and QM/MM Methods", 8th Meeting on Molecular Simulations, Mexico City, Mexico, December, 2016.
27. "Discovery and Characterization of Cancer Biomarkers in DNA Repair Enzymes" Frontiers in Computa-

tional Chemistry 2016, UNAM, Mexico City, MX August, 2016.

28. "Polarizable/Multipolar and Long–Range Corrected Methods for QM/MM simulations", 252nd ACS National Meeting, Philadelphia, PA August, 2016.
29. "Development of AMOEBA for water and ionic liquids", Many Body Interactions: From QM to force fields, Telluride Science Research Center, Telluride, CO, July, 2016.
30. "Development and Application of Advanced Methods for QM/MM Simulations of Enzyme Catalysis", 251st ACS National Meeting, San Diego, CA, March, 2016.
31. "Development of AMOEBA for Ionic Liquids and Applications for Li^+ Transport", 251st ACS National National Meeting, San Diego, CA, March, 2016.
32. "Development and Application of Advanced Force Fields for Classical Simulations", 2015 Midwest Theoretical Chemistry Conference, Ann Arbor, MI, June, 2015.
33. "Extension and Implementation of Ewald–Based Methods for Classical Simulations of a Density–Based Force Field", Platform for Advanced Scientific Computing Conference (PASC), Zürich, Switzerland, June, 2015.
34. "Development and Application of Advanced Force Fields for Classical Simulations", 248th ACS national meeting, Denver, CO, March, 2015.
35. "*Ab initio* QM/MM Simulations Point to an Alternative Mechanism for the AlkB Catalyzed Repair of 1mA5", 248th ACS national meeting, Denver, CO, March, 2015.
36. "Development of advanced potentials for water based on molecular electronic density", Water: The Most Anomalous Liquid, Stockholm, Sweden, October, 2014.
37. "Development of advanced polarizable force fields for water and ionic liquids", Current Trends in Computational Chemistry, Nha Trang, Vietnam, August, 2014.
38. "Development of advanced polarizable force fields for water and ionic liquids", Many Body Interactions: From QM to force fields, Telluride Science Research Center, Telluride, CO, June, 2014.
39. "Development of advanced force fields for water and ionic liquids", 54th Sanibel Simposium, St. Simons Island, GA, February, 2014.
40. "GEM$\star$: Toward an electronic density based force field", 20 years of PME: A tribute to Tom Darden, Lee Pedersen and Darrin York, 246th ACS national meeting, Indianapolis, IN, September, 2013.
41. "Insights on DNA repair enzymes from computational simulation", DNA replication repair and recombination, Telluride Science Research Center, Telluride, CO, June, 2013.
42. "Hypothesis Driven–SNP–Search: A new method to find disease related SNPs", Molecular Therapeutics Program Annual Research Retreat, Karmanos Cancer Institute, Detroit, MI, June, 2013.
43. "QM/MM study of the rate limiting step in the dealkylation reaction catalyzed by AlkB", Exploring Potential Energy Surfaces in Quantum Chemistry: A Tribute to H. Bernhard Schlegel, Philadelphia, PA, August, 2012.
44. "Using GEM distributed multipoles in the AMOEBA force field", Many Body Interactions: From QM to force fields, Telluride Science Research Center, Telluride, CO, July, 2012.
45. "Insights on metal ion mutagenicity in DNA polymerase λ from ab initio QM/MM calculations", ACS Award for Computers in Chemical and Pharmaceutical Research, San Diego, CA, March, 2012.
46. "Correlation between electronic localization and mutagenicity of metallic ions in DNA synthesis from QM/MM calculations", 37th Congress of Theoretical Chemists of Latin Expression, Riviera Maya, Mexico, December, 2011.

47. "Estudios computacionales revelan diferencias entre cationes mutagénicos e inhibidores en la ADN polimerasa", Química Teórica para el siglo XXI Donde esta?, Donde estara?, Mexico City, Mexico, September, 2011.
48. "Insights on metal ion mutagenicity in DNA polymerases from QM/MM calculations", 43rd IUPAC World Chemistry Congress, San Juan, Puerto Rico, August, 2011.
49. "ELF analysis of the active site of human DNA polymerase λ provides insight on metal ion mutagenicity in DNA synthesis", 51st Sanibel Symposium, St. Simons Island, GA, February, 2011.
50. "Topological analysis of the active site of human DNA polymerase λ provides insight on metal ion mutagenicity in DNA synthesis", ELF 20 years, Paris, France, July, 2010.

Talks

1. "Computational prediction of residues involved in putative post–insertion fidelity checking in DNA polymerase", TSRC, DNA replication repair and recombination workshop, Telluride, CO, June 2011.
2. "Toward the computational determination of residues for nucleotide misincorporation discrimination in *E. coli* DNA polymerase I", ACS Spring National Meeting, San Francisco, CA, March 2010.
3. "Quantum mechanical/molecular mechanical studies of the reaction mechanism of human DNA polymerase λ with Mg^{2+} and Mn^{2+}", ACS Spring National Meeting, Salt Lake City, UT, March 2009.
4. "The Gaussian electrostatic model: Towards a molecular density based force field"; Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, East Lansing, MI, July 2008.
5. "Generalization of the Gaussian Electrostatic Model: A molecular density based force field"; Emerging Technologies in Computational Chemistry Competition, 234th ACS National Meeting, Boston, MA, August 2007.
6. "Extensions of the Gaussian Electrostatic Model", 121st NC–ACS Sectional Conference, Durham, NC, April 2007.
7. "Towards a force field based on density fitting"; Thomas Kuhn Paradigm Shift Award Competition, 231st ACS National Meeting, Atlanta, GA, March 2006.
8. "Protein Backbone Contributions to 4–Oxalocrotonate Tautomerase Catalysis: Understanding from Experiment and Theory", 118th NC–ACS Sectional Conference, Durham, NC, April 2004.

Posters

1. "Characterizing the Impact of Cancer Mutations in DNA Base Editing Enzymes", 65th Biophysical Society Annual Meeting, Virtual, February, 2021.
2. "Role of a conserved scaffold in TET2 is crucial for sequential oxidation of 5mC", 6th EU–US Conference on Endogenous DNA Repair, Udine, Italy, September, 2017.
3. "Using GEM distributed multipoles in the AMOEBA force field", 243rd ACS National Meeting, Philadelphia, PA, August, 2012.
4. "Topological analysis of the active site of human DNA polymerase λ provides insight on metal ion mutagenicity in DNA synthesis"; 240th ACS National Meeting, Boston, MA, August 2010.
5. "Catalytic mechanism of human DNA polymerase λ with Mg^{2+} and Mn^{2+} from *ab initio* QM/MM studies"; 32nd Reaction Mechanisms Conference, Chapel Hill, NC, June 2008.
6. "Generalization of the Gaussian Electrostatic Model: A force field based on density fitting"; 47th Sanibel Symposium, St. Simons Island, GA, February 2007.
7. "Generalization of the density fitting based Gaussian Electrostatic Model: Extension to arbitrary angular moment, distributed multipoles and computational speedup", Computational Chemistry GRC, Les

Diablerets, Switzerland, October 2006.

8. "Molecular Properties from Density Fitting: Part I"; 45th Sanibel Symposium, St. Simons Island, GA, March 2005.
9. "Protein Backbone Contributions to 4–Oxalocrotonate Tautomerase Catalysis: Understanding from Experiment and Theory"; 44th Sanibel Symposium, St. Augustine, FL, March 2004.
10. "QM/MM Study of the Reaction Mechanism of 4–Oxalocrotonate Tautomerase"; 223rd ACS National Meeting, Orlando, FL, April 2002.
11. "DFT Study of the Structural and Electronic Properties of Small Ni_n (n=2–4) Clusters"; XXXIX Sanibel Symposium, St. Augustine, FL, March 1999.

Service

Departmental

Awards Committee, Department of Chemistry, University of North Texas, 2019–.

Chair, Diversity, Equity, Inclusion & Justice Committee, Department of Chemistry, University of North Texas, 2020–2021.

UNT Chemistry Department Research Roadmap, Department of Chemistry, University of North Texas, 2020–2021.

Comp. Chem. Faculty Search Committee co–Chair, Department of Chemistry, University of North Texas, 2020–2021.

Graduate Admissions Committee, Department of Chemistry, University of North Texas, 2016–2020.

Chair, Promotion & Tenure Sub–Committee, Department of Chemistry, University of North Texas, 2019–.

Chair, Mentoring Committee for Tenure Track Professor Hao Yan, Department of Chemistry, University of North Texas, 2019–.

Org. Chem. Faculty Search Committee, Department of Chemistry, University of North Texas, 2019.

Phys. Chem. Faculty Search Committee, Department of Chemistry, University of North Texas, 2017, 2018.

Welch Chair Search Committee, Department of Chemistry, University of North Texas, 2017, 2018.

Committee on Retention, Department of Chemistry, University of North Texas, 2018.

ad–hoc Committee on Workload Assignment Rules, Department of Chemistry, University of North Texas, 2019.

Host for Departmental Speakers, Department of Chemistry, University of North Texas, 2016–.

Chair, computer security committee, Department of Chemistry, Wayne State University, 2012–2015.

Graduate admissions committee member, Department of Chemistry, Wayne State University, 2011–2013, 2014–2015.

Awards committee member, Department of Chemistry, Wayne State University, 2010–2011, 2013–2014.

Diversity Equity committee member, Department of Chemistry, Wayne State University, 2015.

Organizer, Physical Chemistry Seminar Series, Fall 2012, Winter 2014.

College

Member of the College By-laws update committee, 2022.

Chair, ad–hoc faculty committee, College of Science, University of North Texas, 2019.

University

SACNAS/UNT Chapter co–advisor (with Prof. P. Padilla), University of North Texas 2016–.

Intellectual Property Committee, University of North Texas, 2017–.

A2RU Committee, University of North Texas, 2017–.

NIH Grants Workshop, Office of the Vice President for Research, University of North Texas, September, 2019.

Parking and Transportation Advisory Committee, University of North Texas, 2017–2018.

Ally, UNT Initiative Supporting Women Faculty, University of North Texas, 2017–.

Research Computing Infrastructure Task Force committee member, Wayne State University, 2015.

Conference Organization–in reverse chronological order

Organizing Committee, @LatinXChem twitter conference, Computational Chemistry Division, September 2021

Organizing Committee, Life Sciences: "PASC21 (Platform for Advanced Scientific Computing)", Geneva, Switzerland (Digital Event), July 2021.

Organizer: "1st North Texas/Oklahoma Theory Meeting", Denton, TX, January 2019.

Organizer: "Leading Edge Research in Computational Chemistry", 2018 SACNAS National Meeting, San Antonio, TX, October 2018.

Co-organizer: "Insights into Structure, Function and Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation", 255th ACS National Meeting, New Orleans, LA, March 2018.

Co-organizer: "16th annual midwest DNA repair symposium", Wayne State University, Detroit, MI, May 2014.

Co-organizer: Symposium "20 years of PME: A tribute to Thomas Darden, Lee Pedersen and Darrin York", 246th ACS National Meeting, Indianapolis, IN, September 2013.

Co-organizer: Workshop on "DNA replication repair and recombination", Telluride Science Research Center, Telluride, CO, June 2013.

Co-organizer: ACS Award for Computers in Chemical and Pharmaceutical Research in honor of Prof. H. Bernhard Schlegel, New Orleans, LA, April, 2013.

Co-organizer: Workshop on "DNA replication repair and recombination", Telluride Science Research Center, Telluride, CO, June 2011.

Planning committee member: 10^{th} and 11^{th} NIEHS Biomedical Career Fair, RTP, NC, 2007 and 2008.

Organizing Committee Member, "1st Autumn School in Computational Chemistry", Mexico City, November 1998.

Outreach and Other

School of Science and Engineering, Dallas Independent School District, "My Journey to Use Computers to Discover and Understand Cancer Mutations", April, 2022.

Career Panel for Mid-Career to Early Career Academics, OpenEye Early Faculty Award Symposium, ACS Spring 2022 National Meeting, San Diego, CA, March, 2022.

Promotion/Tenure Case Evaluation: Florida International University (2017), University of Texas at Arlington (2020), University of South Florida (2020), Michigan Technological University (2020), National Heart Lung and Blood Institute (2021), University of Texas at El Paso (2021), University of Oklahoma (2021).

SACNAS national conference, poster and talk submission volunteer reviewer, 2016–2021

ACS Computers in Chemistry Division CCG Excellence Award for Graduate Students reviewer, 2017–2020.

Invited Panelist, "Who Will Win the #ChemNobel? Predicting the 2021 Nobel Laureate(s) in Chemistry", ACS Webinar, September, 2021

Invited Lecture: "Force Fields and Molecular Dynamics; An Overview", MolSSI Tapia Center Workshop, Houston, TX, July, 2021 (Virtual).

Invited Panelist, Faculty State Schools, 2021 NIH Career Symposium (Virtual), April, 2021.

Invited Panelist, Academic Careers Conversation, Computers in Chemistry Division (COMP), 2021 ACS National Conference (Virtual), April, 2021.

Invited Judge, Undergraduate Presentations, Computers in Chemistry Division (COMP), 2021 ACS National Conference (Virtual), April, 2021.

Invited Judge, LatinXChem Virtual Scientific Conference, Theoretical Chemistry Division, Twitter Conference, September, 2020.

Invited speaker, "Navigating an Academic Job Search during the COVID-19 Pandemic", (virtual panel) Northeastern University, Boston, MA, August, 2020.

PenPal, Leters for a PreScientist program, 9/2020-5/2021.

Invited Volunteer speaker, "Skype a Scientist", Ms. Heidi Bacon's 5th grade Science class, Levine Academy, Dallas, TX, May 2020.

Invited Volunteer speaker, "Skype a Scientist", Ms. Noreen Hayes' 4th grade class, Whittier Elementary, Blue Island, IL, May 2020.

Invited Participant (virtual), Beyond the Professoriate:"Academic Job Market Conference", "Faculty Career Panel: Research–Intensive Institutions", Online Webinar, September, 2019.

Invited Participant (virtual), NASEM Workshop: "Science of Mentoring in STEM", Knoxville, TN, February 2018.

Volunteer speaker, "Skype a Scientist", Ms. Tracy Anderson's 1st grade class, Esparto Elementary, Esparto, CA, January 2018.

Invited Volunteer Speaker, Earhart Middle School, Detroit MI, April, 2010; Detroit Cristo Rey, Detroit, MI, May 2013.

Organizer and leader of "Advancing Latinos Aptitudes in Science" (ALAS) workshop for highschool students, Department of Chemistry, Wayne State University, August, 2012.

Panelist, College2Career Undergraduate and Graduate Latino/a Studies Research Conference: "Navigating the Sciences: Exploring Careers in Health", Wayne State University, Detroit, MI, 2011.

Poster Judge, Michigan-Luis Stokes Alliance for Minority Participation, Detroit, MI, January 2011

Invited Volunteer Speaker, Earhart Middle School, Detroit MI, April, 2010;

Panelist, PAD Seminar: "How to succeed as a New Faculty Member", Welcome Center, Wayne State University, October, 2010.

Panelist, NIH Career symposium: "Life as a junior faculty member", Bethesda, MD, May 2011.

Workshop Leader, "GO GIRLs Go Nano (G^3N) workshop on smart medicine", Department of Chemistry, Wayne State University, Detroit, MI, November 2009.

Invited Volunteer Speaker, Phillips Middle School, Chapel Hill NC, Oct. 2007 and Brentwood Elementary

School, Raleigh NC, March 2008.

Panelist, Howard Hughes Summer Program–Career Panel, Biology Department, Duke University, July 2007.

Chief Reviewer, Chemistry and Biophysics study section, "Fellows Award for Research Excellence" (FARE) competition, National Institutes of Health 2006.

Graduate Student Assistant, "Chemistry for Executives" Program, Department of Chemistry, Duke University, Summer 2000.

Editorial Service

Advisory Board: "Physical Chemistry Chemical Physics", Royal Society of Chemistry, 2020–

Review Editor: "Frontiers in Structural Biology", 2018–

Review Editor: "Frontiers in Theoretical and Computational Chemistry", 2013–2018

Editorial Board Member: "Computational Chemistry Highlights"

Guest Editor: Physical Chemistry Chemical Physics, themed issue "Insights from advanced methods in molecular dynamics"

Guest Editor: International Journal of Molecular Sciences, special issue "Computational Modeling of Ionic Liquids and Solutions for Modern Applications"

Review Service to Granting Agencies

NIH/CSR; Macromolecular Structure and Function D (MSFD), charter member 2018–2024, *ad hoc* panel member 06/2015, 10/2016.

NIH/CSR; Macromolecular Structure and Function A (MSFA) *ad hoc* panel member 06/2017.

NIH/CSR; Fellowship: Macromolecular Structure and Function (F04B) *ad hoc* panel member 07/2017, 11/2018.

NIH/CSR; Special Emphasis Panel/Scientific Review Group ZRG1 BCMB–X (07)L 10/2017, 11/2018.

National Science Foundation, CLP Computational Theory, and Modeling Virtual Panel, 4/2018

National Science Foundation, *ad hoc* reviewer

Center for Functional Nanomaterials, Brookhaven National Laboratory

Army Research Office–Biochemistry

National Sciences and Engineering Research Council of Canada

Consejo Nacional de Ciencia y Tecnología, CONACyT (National Science and Technology Council of Mexico)

National Science Center, Poland

Swiss National Science Foundation

Swiss National Supercomputing Center

US–Israel Binational Science Foundation

Petroleum Research Fund–American Chemical Society

Research Corporation for Scientific Advancement

FONDECYT (National Research and Development Agency), Chile.

Austrian Science Fund, Vienna, Austria.

Review Service to Professional Journals

Journal of the American Chemical Society
Journal of Chemical Theory and Computation
Journal of Physical Chemistry
Journal of Computational Chemistry
Journal of Chemical Physics
Nature Communications
Angewandte Chimie, Intl. Ed.
Chemical Science
Chemistry, a European Journal
Physical Chemistry Chemical Physics
Journal of Molecular Graphics and Modeling
PLoS One
PLoS Computational Biology
ACS Omega
Scientific Reports
Inorganic Chemistry
ACS Catalysis
ACS Central Science
Nucleic Acids Research
Journal of Biological Chemistry
Journal of Computer–Aided Molecular Design
RSC Medicinal Chemistry
Frontiers in Computational and Theoretical Chemistry
Theoretical Chemistry Accounts
Chemical Communications
Chemical Physics
Chemical Physics Letters
Molecular Physics
Biochemistry
DNA Repair
WIREs Computational Molecular Science
Journal of Molecular Biology
Journal of Molecular Liquids
Coordination Chemistry Reviews
Organic Biomolecular Chemistry
Interdisciplinary Sciences: Computational Life Sciences

Journal of the Mexican Chemical Society

Canadian Journal of Chemistry

Results in Chemistry

Professional Affiliations

Member, Molecular Therapeutics Program, Barbara Ann Karmanos Cancer Institute (since Nov. 2009).

Sigma Xi

American Chemical Society

Biophysical Society

Phi Lambda Upsilon

SACNAS: Society for the Advancement of Chicanos and Native Americans in Science

SHPE: Society of Hispanic Professional Engineers

Languages

Fluent in Spanish and English.