

Thomas Summers

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Research Experience

Los Alamos National Laboratory, Theoretical Division

Jan. 2024 – Present

Postdoctoral Research Associate

Supervisors: Dr. Ping Yang and Dr. Enrique Batista

The University of Nevada, Reno, Chemical and Materials Engineering

Nov. 2021–Jan. 2024

Postdoctoral Researcher

Project: "Quantum Dynamics of Spin-based Molecular Systems" funded by the DOE

Supervisor: Dr. David C. Cantu

Education

The University of Memphis, Memphis, TN

2017–2021

Ph.D. in Computational Chemistry

Advisor: Dr. Nathan J. DeYonker

M.S. in Chemistry

2016–2017

Christian Brothers University, Memphis, TN

2012–2016

B.Sc. in Biochemistry, *summa cum laude*

Publications

† Equal contribution

12 published articles; 9 first-author

T. J. Summers, J. Diaz-Sanchez, and D. C. Cantu, "Molecular Dynamics Modeling of Gd-HDEHP Complexes Across Aqueous-Organic Interfaces", **under review in J. Mol. Liq.*

D. A. Agbaglo, **T. J. Summers**, Q. Cheng, N. J. DeYonker, "The Influence of Model Building Schemes and Molecular Dynamics Sampling on QM-cluster Models: the Chorismate Mutase Case Study", **under review in Phys. Chem. Chem. Phys.*

G. L. Licup, **T. J. Summers**, J. A. Sobrinho, A. de Bettencourt-Dias, and D. C. Cantu, "Elucidating the Structure of the Eu-EDTA Complex in Solution at Various Protonation States", *Eur. J. Inorg. Chem.* (2024)
**accepted for publication*

T. J. Summers,† R. D. O'Brien,† J. A. Sobrinho, A. de Bettencourt-Dias, and D. C. Cantu, "Structural Changes to the Gd-DTPA Complex at Varying Ligand Protonation State", *Eur. J. Inorg. Chem.*, e202300507 (2023).
**invited special issue *featured cover article of 01/21/2024 issue*

T. J. Summers, J. A. Sobrinho, A. de Bettencourt-Dias, S. D. Kelly, J. L. Fulton, and D. C. Cantu, "Solution Structures of Europium Terpyridyl Complexes with Nitrate and Triflate Counterions in Acetonitrile", *Inorg. Chem.*, **62**, 13 (2023).

B. T. Caswell,† **T. J. Summers**,† G. L. Licup, and D. C. Cantu, "Mutation Space of Spatially Conserved Amino Acid Sites in Proteins", *ACS Omega*, **8**, 27 (2023).

S. J. McElhany, **T. J. Summers**, R. C. Shiery, and D. C. Cantu, "AFICS: a Toolkit to Analyze the Coordination Sphere of Ions", *J. Chem. Inf. Model.*, **63**, 9 (2023).

- T. J. Summers**, R. Hemmati, J. E. Miller, D. A. Agbaglo, Q. Cheng, and N. J. DeYonker. "Evaluating the Active Site-Substrate Interplay Between X-ray Crystal Structure and Molecular Dynamics in Chorismate Mutase", *J. Chem. Phys.*, **158**, 065101 (2023).
- T. J. Summers** and N. J. DeYonker. "QM-cluster Model Study of CO₂ Hydration Mechanisms in Metal-substituted Human Carbonic Anhydrase II", *Electron. Struct.*, **5**, 1 (2023). **invited special issue*
- R. D. O'Brien, **T. J. Summers**, D. S. Kaliakin, and D. C. Cantu. "The Solution Structures and Relative Stability Constants of Lanthanide-EDTA Complexes Predicted from Computation", *Phys. Chem. Chem. Phys.*, **24**, 17 (2022).
- T. J. Summers**, Q. Cheng, M. A. Palma, D.-T. Pham, D. K. Kelso III, C. E. Webster, and N. J. DeYonker. "Cheminformatic Quantum Mechanical Enzyme Model Design: a Catechol-O-methyltransferase Case Study", *Biophys. J.*, **120**, 17 (2021).
- T. J. Summers**, H. Tupkar, T. M. Ozvat, Z. Tregillus, K. A. Miller, and N. J. DeYonker. "Computational Insight into the Rope-skipping Isomerization of Diarylether Cyclophanes", *Symmetry*, **13**, 11 (2021).
- T. J. Summers**, B. P. Daniel, Q. Cheng, and N. J. DeYonker. "Quantifying Inter-Residue Contacts through Interaction Energies", *J. Chem. Inf. Model.*, **59**, 12 (2019).
- T. J. Summers**, Q. Cheng, and N. J. DeYonker. "A Transition State 'Trapped'? Modeling Biphenyl Torsional Rotation with a QM-cluster Model of Engineered Threonyl-tRNA Synthetase", *Org. Biomol. Chem.*, **16**, 22 (2018). **featured cover article of 06/14/2018 issue*

Honors and Awards

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| ▪ FOMMS 2022 Early Career Researcher Award | July 2022 |
| ▪ National Science Foundation Graduate Research Fellowship Program awardee | 2018–2021 |
| ▪ Second Place Presentation Award – 33rd Annual Student Research Forum at the University of Memphis | April 2021 |
| ▪ First Place Presentation Award – 32nd Annual Student Research Forum at the University of Memphis | April 2020 |
| ▪ Best Poster Award – 2019 Southeast Theoretical Chemistry Association Meeting at the University of Tennessee, Knoxville | May 2019 |
| ▪ Outstanding Graduate Researcher Award by The University of Memphis | April 2019 |
| ▪ First Place Poster Award at the 31st Annual Student Research Forum at the University of Memphis | March 2019 |

Conferences, Presentations, and Workshops

- [Poster, 2023] "Applying Molecular Dynamics, Deep Learning, and Global Optimization to Resolve Lanthanide Solution Structures", 2023 Fall American Chemical Society National Meeting and Exposition, San Francisco, CA
- [Poster, 2023] "AFICS: An Open-source Tool to Analyze the Coordination Sphere of Ions", 2023 Fall American Chemical Society National Meeting and Exposition, San Francisco, CA
- [Presentation, 2023] "Characterizing Solution Structures of Lanthanide Terpyridyl Complexes with Different Counterions in Non-aqueous Solvent", 2023 Spring American Chemical Society National Meeting and Exposition, Indianapolis, IN

- [Workshop, 2023] "Computationally Modeling Solution Structures of Eu(terpyridyl) Complexes in Acetonitrile", Virtual Winter School on Computational Chemistry, Virtual
- [Poster, 2022] "Characterizing Lanthanide-ligand Complexes in Organic Solvents with Ab Initio and Classical Molecular Dynamics Simulations", Foundations of Molecular Modeling and Simulation 2022 Conference, Delavan, WI.
- [Poster, 2022] "Quantifying Dynamic Enzyme Active Site Chemical Interaction Networks throughout MD Simulations", Virtual Winter School on Computational Chemistry, Virtual.
- [Workshop, 2022] "Quantifying Dynamic Enzyme Active Site Chemical Interaction Networks Throughout MD Simulations", Virtual Winter School on Computational Chemistry, Virtual
- [Poster, 2021] "Incorporating Cheminformatics into the Design of Quantum Mechanical Cluster Models", 2021 American Chemical Society National Meeting and Exposition, Virtual.
- [Presentation, 2021] "Designing Cheminformatics-based Enzyme Quantum Mechanical Models: a Catechol-O-methyltransferase Case Study", 33rd Annual Student Research Forum, Memphis, TN. Virtual.
- [Presentation, 2021] "Automating, Analyzing, and Databasing Enzyme Simulations", The Memphis DATA Conference, Memphis, TN. Virtual.
- [Workshop, 2021] Virtual Winter School on Computational Chemistry, Virtual.
- [Workshop, 2021] Machine Learning for Everybody, FedEx Institute of Technology, Virtual.
- [Presentation, 2020] "Incorporating Cheminformatics into Rational Enzyme Modeling", Seminar, The University of Memphis, Memphis, TN. Virtual.
- [Presentation, 2020] "Atomic Insights into Metal-substituted Human Carbonic Anhydrase II through QM-cluster Modeling", 32nd Annual Student Research Forum, Memphis, TN. Virtual.
- [Presentation, 2020] "Towards Automation of the Design and Construction of Protein QM-models", Seminar, National Institutes of Health, Bethesda, MD.
- [Poster, 2019] "Quantifying Protein Contact Networks Through Residue-Residue Pair Interaction Energies", 2019 Annual Meeting of the Southeast Theoretical Chemistry Association, University of Tennessee, Knoxville, TN.
- [Poster, 2019] "Correlating Protein Topological and Chemical Descriptors to Inter-Residue Interaction Strength", 31st Annual Student Research Forum, Memphis, TN.
- [Poster, 2019] "Improving Protein Modeling Through Residue Interaction Network Analyses", The Memphis DATA Conference, Memphis, TN.
- [Presentation, 2019] "Investigating Structural and Mechanistic Changes in Metal-substituted Human Carbonic Anhydrase II QM-cluster Models", American Chemical Society National Meeting and Exposition, Orlando, FL.
- [Poster, 2018] "A Transition State 'Trapped'? QM-cluster Models of Engineered Threonyl-tRNA Synthetase", 2018 Annual Meeting of the Southeast Theoretical Chemistry Association, Louisiana State University, LA.
- [Presentation, 2018] "A Transition State 'Trapped'? QM-cluster Models of Engineered Threonyl-tRNA Synthetase", Lester Andrews Graduate Research Symposium, Mississippi State University, MS.
- [Poster, 2018] "QM-cluster Model Examination of a Biphenyl Transition State 'Trapped' within an Engineered Thr-tRNA Synthetase", 255th American Chemical Society National Meeting, New Orleans, LA.
- [Workshop, 2017] MolSSI Software Summer School, Virginia Tech, Blacksburg, VA.

- [Presentation, 2017] "Modeling Biphenyl Torsional Rotation with a QM-cluster Model of Thr-tRNA Synthetase", Seminar, University of Memphis, Memphis, TN.
- [Poster, 2017] "A Transition State Trapped? QM-model Examination of Biphenyl Torsional Rotation within an Engineered Thr-tRNA Synthetase", 2017 Annual Meeting of the Southeast Theoretical Chemistry Association, University of Mississippi, MS.

Skills

- **Programming Languages:** Python, R, Bash, C++
- **Computational Chemistry Software:** Gaussian, PSI4, ORCA, AMBER, GROMACS, MOE, Q-Chem, CP2K, ADF
- **XAS Data Processing Software:** FEFF, Demeter
- **Visualization Software:** VMD, PyMol, Molden, MacMolplt
- **Typesetting Software:** Microsoft Office, LaTeX
- **Operating systems:** Windows, Linux, MacOS
- **GitHub Repository Contributions:** [AFICS](#) (Cantu), [Mutation Space](#) (Cantu), [RINRUS](#) (DeYonker)
- **Other:** Cytoscape; Experience with HPC environments, Machine Learning, Bioinformatics

Teaching

- Assistant Instructor - University of Nevada, Reno Spring 2023
Computer Applications in Chemical Engineering Laboratory (CHE 245)
- Teaching Assistant - University of Memphis Fall 2016 - Fall 2017
General Chemistry I and II Laboratory (CHEM 1111 and CHEM 1121)

Service

Professional

- Peer reviewer for *JACS Au*, *Journal of Applied Physics*, *European Physical Journal Plus*
- Member of the American Chemical Society (ACS), the Biophysical Society (BPS), and the American Association for the Advancement of Science (AAAS)
- Reviewer for Nevada NASA Space Grant Consortium, 2022-2023
Nevada Undergraduate Research funding and scholarships
- Judge for UNR GSA Poster Symposium, ACS COMP undergraduate posters 2022-2023
- Member of United Campus Workers (UCW) 2017-2022
- Presider at the 2021 ACS National Meeting and Exposition April 2021
- Presider at the 31st National Conference on Undergraduate Research April 2017

Community

- Volunteer, Food Bank of Northern Nevada 2022-2023
- Big Brother volunteer, Big Brothers Big Sisters of America 2017-2022
- Volunteer, Science Olympiad Regional Competition 2015-2020

- Judge, Memphis and Shelby County Science Fairs, Pleasant View School Science Fair 2015–2020
- Student Members of the American Chemical Society (Member/President), Beta Beta Beta Biological Honor Society (Member/Secretary/President) 2012–2016