

Thomas Summers

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Education

The University of Memphis, Memphis, TN

Ph.D. in Computational Chemistry

2017–2021

Advisor: Dr. Nathan J. DeYonker

M.S. in Chemistry

2016–2017

Christian Brothers University, Memphis, TN

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

2012–2016

Research Experience

Chemical and Materials Engineering, The University of Nevada, Reno

Nov. 2021–Present

Postdoctoral Researcher

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

Supervisor: Dr. David C. Cantu

Publications

S. J. McElhany, **T. J. Summers**, R. C. Shiery, and D. C. Cantu, “AFICS: a Toolkit to Analyze the Coordination Sphere of Ions” **accepted for publication by J. Chem. Inf. Model.*

B. T. Caswell, **T. J. Summers**, G. L. Licup, and D. C. Cantu, “Mutation Space of Spatially Conserved Amino Acid Sites in Proteins” **under review by ACS Omega*

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).

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

- [Presentation, 2023] “Characterizing Solution Structures of Lanthanide Terpyridyl Complexes with Different Counterions in Non-aqueous Solvent”, 2023 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.

Computer Skills

- **Programming Languages:** Bash, Python, R, C++
- **Computational Chemistry Software:** Gaussian, PSI4, ORCA, AMBER, GROMACS, MOE, Q-Chem, CP2K
- **Visualization Software:** VMD, PyMol, Molden, MacMolplt
- **Typesetting Software:** Microsoft Office, LaTeX
- **Operating systems:** Windows, Linux, MacOS
- **GitHub Repository Contributions:** *Mutation Space* (Cantu), *RINRUS* (DeYonker)
- **Other:** Athena and FEFF XAS data processing softwares; Cytoscape; Experienced with Machine Learning and Bioinformatics techniques; Comfortable with HPC environments

Teaching

- 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*
 - Member of the American Chemical Society (ACS), the Biophysical Society (BPS), and the American Association for the Advancement of Science (AAAS)
 - Reviewer for Nevada Undergraduate Research funding and scholarships 2022-2023
 - Judge for UNR GSA Poster Symposium October 2022
 - 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–Present
 - 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), 2012–2016
Beta Beta Beta Biological Honor Society (Member/Secretary/President)