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

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", *submitted to Eur. J. Inorg. Chem.*

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, 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 CO_2 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.*

†equal contribution

Honors and Awards

- 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
- **Visualization Software**: VMD, PyMol, Molden, MacMolplt
- **XAS Data Processing Software**: FEFF, Demeter
- **Typesetting Software**: Microsoft Office, LaTeX
- **Operating systems**: Windows, Linux, MacOS
- **GitHub Repository Contributions**: *AFICS* (Cantu), *Mutation Space* (Cantu), *RINRUS* (DeYonker)
- **Languages**: English (native), American Sign Language (intermediate)
- **Other**: Cytoscape; Experienced with Machine Learning and Bioinformatics techniques; HPC environments

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, 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), Beta Beta Beta Biological Honor Society (Member/Secretary/President) — 2012−2016