Thomas Summers

Email: thomassummers@unr.edu
Phone: (901)-338-0934
GitHub: github.com/tsmmers1

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. 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", *under review by J. Chem. Phys.*

T. J. Summers and N. J. DeYonker. "QM-cluster Model Study of CO_2 Hydration Mechanisms in Metal-substituted Human Carbonic Anhydrase II", *under review by Elect. Struct; 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

- 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, 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.
- [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 Repositories**: *Mutation Space* (Cantu), *RINRUS* (DeYonker)
- **Other**: Cytoscape; Athena and FEFF XAS data processing softwares; Experienced with Machine Learning and Bioinformatics techniques; Comfortable with HPC environments

Teaching

- 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*
  - Member of the American Chemical Society (ACS), the Biophysical Society (BPS), and the American Association for the Advancement of Science (AAAS)
  - Member of United Campus Workers (UCW)
  - Reviewer for Nevada Undergraduate Research Award funding May 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, Memphis, TN 2015−2020
  - Judge, Memphis and Shelby County Science Fairs, Memphis, TN 2015−2020
  - Judge, Pleasant View School Science Fair, Memphis, TN 2019

References

- **Dr. David Cantu**
  Assistant Professor
  Chemical and Materials Engineering, MSC 0388, University of Nevada, Reno
  1664 N. Virginia Street, Reno, NV 89557, USA
  dcantu@unr.edu
- **Dr. Nathan DeYonker**
  Assistant Professor
  Department of Chemistry, University of Memphis
  3744 Walker Avenue, Memphis, TN 38152, USA
  ndyonker@memphis.edu
- **Dr. Qianyi Cheng**
  Research Scientist
  Department of Chemistry, University of Memphis
  3744 Walker Avenue, Memphis, TN 38152, USA
  qcheng1@memphis.edu
- **Dr. Abby Parrill-Baker**
  Dean / Professor
  Department of Chemistry, University of Memphis
  450 University, Memphis, TN 38111, USA
  aparrill@memphis.edu