**Biographical Sketch -- C. DAVID SHERRILL**

##### A. Professional Preparation

Massachusetts Institute of Technology, Cambridge, MA, Chemistry, B.S. 1992

University of Georgia, Athens, GA, NSF Graduate Fellow, Chemistry, Ph.D. 1996

University of California, Berkeley, CA, NSF Postdoctoral Fellow, Chemistry, 1996-1999

##### B. Appointments

Georgia Institute of Technology, School of Chemistry and Biochemistry

Professor, 2008-present

Associate Director, Institute for Data Science and Engineering, 2017-present

Associate Professor, 2005-2008

Assistant Professor, 1999-2004

###### C. Products

*Five most closely related to the proposed project*

1. “Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development,'' D. G. A. Smith, L. A. Burns, D. A. Sirianni, D. R. Nascimento, A. Kumar, A. M. James, J. B. Schriber, T. Zhang, B. Zhang, A. S. Abbott, E. J. Berquist, M. H. Lechner, L. A. Cunha, A. G. Heide, J. M. Waldrop, T. Y. Takeshita, A. Alenaizan, D. Neuhauser, R. A. King, A. C. Simmonett, J. M. Turney, H. F. Schaefer, F. A. Evangelista, A. E. DePrince, T. D. Crawford, K. Patkowski, and C. D. Sherrill, *J. Chem. Theory Comput.* **14**, 3504-3511 (2018).
2. “Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability,” R. M. Parrish, L. A. Burns, D. G. A. Smith, et al., and C. D. Sherrill, *J. Chem. Theory Comput*. **13**, 3185-3197 (2017).
3. “The BioFragment Database (BFDb): An Open-Data Platform for Computational Chemistry Analysis of Noncovalent Interactions,” L. A. Burns, J. C. Faver, Z. Zheng, M. S. Marshall, D. G. A. Smith, K. Vanommeslaeghe, A. D. MacKerell, K. M. Merz, and C. D. Sherrill, *J. Chem. Phys.* **147**, 161727 (2017).
4. “Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory,” D. G. A. Smith, L. A. Burns, K. Patkowski, and C. D. Sherrill, *J. Phys. Chem. Lett.* **7**, 2197-2203 (2016).
5. “Density-Fitted Open-Shell Symmetry-Adapted Perturbation Theory and Application to π-Stacking in Benzene Dimer Cation and Ionized DNA Base Pair Steps,” J. F. Gonthier and C. D. Sherrill, *J. Chem. Phys*. **145**, 134106 (2016).

*Five other significant products*

1. “Tipping the Balance Between S-π and O-π Interactions,” J. Hwang, P. Li, M. D. Smith, C. E. Warden, D. A. Sirianni, E. C. Vik, J. M. Maier, C. J. Yehl, C. D. Sherrill, and K. D. Shimizu, *J. Am. Chem. Soc*. **140**, 13301-13307 (2018).
2. “Assessment of Density Functional Methods for Geometry Optimization of Biomolecular van der Waals Complexes,” D. A. Sirianni, A. Alenaizan, D. L. Cheney, and C. D. Sherrill, *J. Chem. Theory Comput.* **14**, 3004-3013 (2018).
3. “Analysis of Transition State Stabilization by Non-Covalent Interactions in Organocatalysis: Application of Atomic and Functional-Group Partitioned Symmetry-Adapted Perturbation Theory to the Addition of Organoboron Reagents to Fluoroketones,” B. W. Bakr and C. D. Sherrill, *Phys. Chem. Chem. Phys.* **20**, 18241-18251 (2018).
4. “Comparison of Explicitly Correlated Methods for Computing High-Accuracy Benchmark Energies for Noncovalent Interactions,” D. A. Sirianni, L. A. Burns, and C. D. Sherrill, *J. Chem. Theory Comput.* **13**, 86-99 (2017).
5. “Analytic Energy Gradients for the Coupled-Cluster Singles and Doubles Method with the Density-Fitting Approximation,” U. Bozkaya and C. D. Sherrill, *J. Chem. Phys*. **144**, 174103 (2016).

D. Synergistic Activities

Co-organizer, Conference on Machine Learning in Science and Engineering, Carnegie Mellon University, June 6-8, 2018; Georgia Tech, June 10-12, 2019

Organizer, Data Science Bootcamp, August 5-9, 2019 (80 undergraduate and graduate participants from Georgia Tech, Morehouse, Spelman, Agnes Scott, and Kennesaw State)

Associate Editor, Journal of Chemical Physics, 2009-present

Vice-Chair, Division of Physical Chemistry, American Chemical Society, present

Created online lecture notes in quantum chemistry (http://vergil.chemistry.gatech.edu/notes/) used by many chemistry educators as supplementary material