Daniel S. Graham, Ph.D.

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EDUCATIONAL HISTORY

Education

2016 - 2022	Ph.D., Chemistry, University of Minnesota Main Research Project: Developing Projection based Quantum Embedding Methods Research Advisor: Professor Jason Goodpaster
2012 - 2016	B.S., Chemistry, <i>magna cum-laude,</i> Centre College Research Project: Identifying MurA Inhibitors using DOCK6 Undergraduate Advisor: Professor Jennifer Muzyka

Positions

Fall 2023 - Present	Assistant Chemistry Professor, Millsaps College
Fall 2022 - Fall 2023	Assistant Chemistry Professor, Birmingham-Southern College
Fall 2021	Adjunct Chemistry Professor, Concordia University
2019 - 2022	System Administrator of Bohr HPC cluster, University of Minnesota
2018 - Present	Lead Developer for QSoME quantum embedding software, University of Minnesota
2016 - 2018	Teaching Assistant, University of Minnesota

2014 - 2016	Undergraduate Research Assistant, Centre College
Summer 2015	Summer Undergraduate Research Fellow, NIST Gaithersburg
Summer 2014	Summer Computational Chemistry Research Fellow, Centre College
2014 - 2015	Chemistry Department Undergraduate Tutor
2013 - 2015	Undergraduate General Chemistry Lab Teaching Assistant, Centre College

SCHOLARSHIP AND TEACHING

Teaching Experience

Fall 2023 - Present	Assistant Chemistry Professor teaching Physical Chemistry and Senior Seminar, Millsaps College
Fall 2022 - Fall 2023	Assistant Chemistry Professor teaching Physical Chemistry and Gen. Chemistry labs, Birmingham-Southern College
Fall 2021	Adjunct Chemistry Faculty teaching Gen. Chemistry, Concordia University
Fall 2019	Mentorship Program for Aspiring Chemistry Teachers (MPACT), University of Minnesota
Volunteer Work	
2018 - 2020	Teen Mentor and Tutor at People Serving People Shelter
2018 - 2020	Youth Mentor with Mentors For Success Youth on Probation Program
Summer 2018, Summer 2019, Summer 2021	Youth Track and Field Coach for Minneapolis Parks and Rec.

Awards and Honors

Nov. 2014	2 nd Place Kentucky Academy of Sciences Presentation
Nov. 2015	2 nd Place NIST Reference Data Challenge
Mar. 2020	APS DCOMP March Meeting Travel Award

Professional Organizations

2016 - present	Phi Beta Kappa National Honor Society
2017 - 2022	Nanoporous Materials Genome Center
2017 - 2022	Chemical Theory Center, University of Minnesota

Conference Talks

- 8) <u>Graham, D. S.</u>; Wen, X.; Chulhai, D.; Goodpaster, J. D. "Huzinaga Projection Operator QM/QM Embedding for Complex Systems" ACS Spring Meeting, March 22nd, 2022.
- 7) <u>Graham, D. S.</u>; Wen, X.; Chulhai, D.; Goodpaster, J. D. "Absolutely Localized Open-shell WF-in-DFT Huzinaga Embedding" APS March Meeting, March 16th, 2021.
- 6) <u>Graham, D. S.</u>; Goodpaster, J. D. "Absolutely Localized Multi-reference DFT Embedding" University of Minnesota Mini March Meeting, March 12th, 2020.
- 5) <u>Graham, D. S.</u>; Goodpaster, J. D. "Absolutely Localized Huzinaga WF-in-DFT Embedding: Robustness and Applications" University of Minnesota Chemistry Graduate Student Research Symposium, Minneapolis, Minnesota, June 4th, 2019.
- 4) <u>Graham, D. S.</u>; Goodpaster, J. D. "Absolutely Localized Huzinaga WF-in-DFT Embedding: Robustness and Applications" ACS Great Lakes Regional Meeting , Lisle, Illinois, May 1-4, 2019.
- 3) Graham, D. S.; Chulhai, D. V.; Goodpaster, J. D. "Huzinaga Operator WF-in-DFT

Embedding" Nanoporous Materials Genome Center All Hands Meeting, Minneapolis, Minnesota, September 16, 2018.

- 2) <u>Graham, D. S.</u>; Muzyka, J. L. "LabPal: Chemical Information for Android" 251st ACS National Meeting, San Diego, California, March 13 17, 2016
- 1) <u>Graham, D. S.</u>; Muzyka, J. L. "Identifying MurA Inhibitors Using DOCK6 Screening" 100th Annual Kentucky Academy of Sciences Meeting, Lexington, Kentucky, November 14-16, 2014

Poster Presentations

- 4) <u>Graham, D. S.</u>; Wen, X..; Goodpaster, J. D. "Huzinaga WF-in-DFT Embedding for Complex Open-shell Systems" Nanoporous Materials Genome Center Annual Meeting, Minneapolis, Minnesota, October 8-9, 2020.
- **3)** <u>Graham, D. S.</u>; Chulhai, D. V.; Goodpaster, J. D. "Huzinaga Level-Shift Projection-based Embedding Method Analysis" Midwest Theoretical Chemistry Conference, Chicago, Illinois, June 21 - 23, 2018.
- 2) <u>Graham, D. S.</u>; Chulhai, D. V.; Goodpaster, J. D. "Rigorous Projection-based DFT Embedding Methodology" Nanoporous Materials Genome Center Phase II Kick-off Meeting, Minneapolis, Minnesota, October 8 - 9, 2017.
- <u>Graham, D. S.</u>; Chulhai, D. V.; Goodpaster, J. D. "Analysis of Projection-based Embedding: Determining Error Origin by Individual Subsystem Energies" Minnesota Workshop on ab initio Modeling in Solid State Chemistry, Minneapolis, Minnesota, July 12th, 2017

Publications

- 5) <u>Graham, D. S.</u> Absolutely Localized Huzinaga Projection Based Embedding for Efficient and Accurate Molecular Modeling. PhD Dissertation. University of Minnesota: Minneapolis, MN, 2022
- Graham, D. S.; Wen, X.; Goodpaster, J. D. "Huzinaga Projection Embedding for Efficient, Accurate Energies of Systems with Complex, Localized Spin-densities" J. Chem. Phys. 2022, 156, 054112
- **3)** <u>Graham, D. S.</u>; Wen, X.; Chulhai, D. V.; Goodpaster, J. D. "Robust, Accurate, and Efficient: Quantum Embedding Using the Huzinaga Level-Shift Projection Operator for Complex Systems" *J. Chem. Theory Comput.* **2020**, *16*, 4, 2284-2295

- Wen, X.; <u>Graham, D. S.</u>; Chulhai, D. V.; Goodpaster, J. D. "Absolutely Localized Projection-Based Embedding for Excited States" *J. Chem. Theory Comput.* 2020, 16, 1, 385-398
- **1)** <u>Graham, D. S.</u>; Petras, H.R.; Ramadugu, S. K.; Goodpaster, J.D.; Shepherd, J. J. "Fully quantum embedding with density functional theory for full configuration interaction quantum Monte Carlo" *J. Chem Theory Comput.* **2019**, 15, 10, 5332-5342