Jason D. Goodpaster, Ph.D.

CONTACT INFORMATION

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CURRENT

University of Minnesota, Twin Cities, Minneapolis, Minnesota USA

Assistant Professor (Tenure Track), Department of Chemistry

- Research Focus: Multiscale modeling of complex chemical systems

EDUCATION AND RESEARCH

University of California, Berkeley, Berkeley, California USA

Postdoctoral Researcher - Joint Center for Artificial Photosynthesis (JCAP)

- Research Focus: The fundamental quantum chemical modeling of CO_2 reduction
- Advisors: Martin Head-Gordon and Alexis Bell

California Institute of Technology, Pasadena, California USA

Ph.D., Chemical Engineering, June 2014

- Dissertation Title: "Density functional theory embedding for correlated wavefunctions"
- Advisor: Thomas F. Miller, III

M.S., Chemical Engineering, June 2011

University of Illinois, Urbana-Champaign, Urbana, Illinois USA

B.S., Chemical Engineering, May 2008
Thesis Title: "Role of Platinum Surface Structure in Anode Catalysts for Fuel Cells"

ACADEMIC EXPERIENCE

University of Minnesota, Twin Cities, Minneapolis, Minnesota USA

Assistant Professor **Starting June 2016**

My research group focuses on the development of new multiscale models for the study of large, complex chemical systems. These projects aim to develop new chemical theories with increased accuracy and improved computational efficiency. Specific target applications include metalloenzymes, heterogenous catalysts, and metal-organic frameworks.

University of California Berkeley, Berkeley, California USA

Postdoctoral Researcher **September 2014 - Present**

This project aims to contribute mechanistic insight from electronic structure computations on experimentally relevant systems, as well as attempting to give insights that can impact the design principles for future catalysts. In support of this main objective, the project includes the development of new computational methods used for the modeling.

California Institute of Technology, Pasadena, California USA

Graduate Student **September 2008 - June 2014**

Includes current Ph.D. research, Ph.D. and Masters level coursework, and research projects centered on the development and application of embedded density functional theory and embedded wave function theory methods.

Teaching Assistant **September 2009 - June 2010**

Teaching assistant for senior undergraduate level lab and process controls class. Responsible for

examination preparation, homework grading, and weekly office hours.

- ChE 105-Dynamics and Control of Chemical Systems, Spring 2010
- ChE 126-Chemical Engineering Laboratory, Fall 2009

University of Illinois Urbana-Champaign, Urbana, Illinois USA

Undergraduate Research **October 2004 - August 2008**

Included experimental research focused on the fundamental understanding of surface structure's effect on catalytic activity for fuel cell anodes.

Teaching Assistant **September 2006 - May 2008**

Teaching assistant for a general chemistry class for incoming chemistry majors. Responsible for examination writing and preparation, homework grading, and weekly discussion sections.

- CHEM 202-Accelerated Chemistry I, Fall 2006-07
- CHEM 204-Accelerated Chemistry II, Spring 2007-08

Professional Experience

Argonne National Laboratory, Argonne, Illinois USA

Summer researcher **May 2005 - August 2005**

Carried out several research projects, including the synthesis and characterization of transition metal catalysts for fuel cell cathodes.

Honors and Awards

Chemical Computing Group Excellence Award for Graduate Students, 2014

American Physical Society Division of Chemical Physics Graduate Student Travel Awards, 2014

National Science Foundation Graduate Research Fellowship Honorable Mention, 2009

University of Illinois: graduated with high honor, thesis with distinction, 2008

Merck Travel Award, 2007

Publications

J. D. Goodpaster, T. A. Barnes, F. R. Manby, and T. F. Miller III, *Accurate and systematically improvable density functional theory embedding for correlated wavefunctions*, J. Chem. Phys., **140**, 18A507 (2014).

T. A. Barnes, J. D. Goodpaster, F. R. Manby, and T. F. Miller III, *Accurate basis set truncation for wavefunction embedding*, J. Chem. Phys., **139**, 024103 (2013).

J. D. Goodpaster, T. A. Barnes, F. R. Manby, and T. F. Miller III, *Density functional theory embedding for correlated wavefunctions: Improved methods for open-shell systems and transition metal complexes*, J. Chem. Phys., **137**, 224113 (2012).

F. R. Manby, M. Stella, J. D. Goodpaster, and T. F. Miller III, *A simple, exact density-functional-theory embedding scheme*, J. Chem. Theory Comput., **8**, 2564 (2012).

J. D. Goodpaster, T. A. Barnes, and T. F. Miller III, *Embedded density functional theory for covalently bonded and strongly interacting subsystems*, J. Chem. Phys., **134**, 164108 (2011).

J. D. Goodpaster, T. A. Barnes, N. Ananth, and T. F. Miller III, *Exactly embedded density functional theory methods for the first-principles modeling of reactions in complex systems*, Proceedings of the 27th Army Science Conference, Orlando, FL (2010).

J. D. Goodpaster, N. Ananth, F. R. Manby, and T. F. Miller III, *Exact non-additive kinetic potentials for embedded density functional theory* J. Chem. Phys., **133**, 084103 (2010).

X. P. Wang, N. Kariuki, J. T. Vaughey, J. D. Goodpaster, R. Kumar, and D. J. Myers, *Bimetallic Pd-Cu oxygen reduction electrocatalysts*, J. Electro. Soc., **155**, B602-B609 (2008).

J. S. Spendelow, X. Qinqin, J. D. Goodpaster, P. J. A. Kenis, and A. Wieckowski, *The role of surface defects in CO oxidation, methanol oxidation, and oxygen reduction on Pt(111)*, J. Electro. Soc., **154**, F238-F242 (2007).

J. S. Spendelow, J. D. Goodpaster, P. J. A. Kenis, and A. Wieckowski, *Methanol dehydrogenation and oxidation of Pt(111) is alkaline solutions*, J. Electro. Soc., **22**, 10457-10464 (2006).

J. S. Spendelow, J. D. Goodpaster, P. J. A. Kenis, and A. Wieckowski, *Mechanism of CO oxidation of Pt(111) in alkaline media*, J. Phys. Chem. B., **110**, 9545-9555 (2006).

Papers in preparation

J. D. Goodpaster, A. T. Bell, and M. Head-Gordon, *Identification of Possible Pathways for C-C bond Formation during Electrochemical Reduction of CO2: New Theoretical Insights from an Improved Electrochemical Model.*

J. D. Goodpaster, A. T. Bell, and M. Head-Gordon, *Theoretical insights into the role of metal oxides as a promoter for Fischer-Tropsch Synthesis.*

J. D. Goodpaster, M. Singh, A. T. Bell, and M. Head-Gordon, *First principles microkinetic modeling of CO_2 reduction on Silver.*

P. Huo, C. Uyeda, J. D. Goodpaster, T. F. Miller III, and J. C. Peters, *Intra-molecular proton transfer and hydrogen production in pyridine modified cobalt oxime catalyst.*

Conference Lectures

J. D. Goodpaster, T. F. Miller, III, A. T. Bell, and M. Head-Gordon *Accurate and robust embedding methodologies for enzymatic and catalytic systems*, Pacifichem, Honolulu, Hawaii, December, 2015.

J. D. Goodpaster and T. F. Miller, III, *Exactly Embedded Density Functional Theory for Modeling Chemical Reactions*, CECAM, Lausanne, Switzerland, March, 2014.

J. D. Goodpaster, T. A. Barnes, and T. F. Miller, III, *Accurate and systematically improvable quantum embedding methods for complex systems*, American Physical Society, Denver, Colorado, March, 2014.

J. D. Goodpaster, T. A. Barnes, and T. F. Miller, III, *Multi-level partitioning using embedded density functional theory*, American Physical Society, Boston, Massachusetts, March, 2012.

J. D. Goodpaster, T. A. Barnes, and T. F. Miller, III, *Embedded Density Functional Theory for Large Scale Electronic Structure Calculations*, Chemistry and Chemical Engineering Seminar Day, Pasadena, California, October, 2010.