

POSTDOCTORAL SCHOLAR

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Education _____

University of California, Berkeley

Berkeley, California

PHD IN CHEMISTRY

2014

• Dissertation: "Short-range Correlation Models in Electronic Structure Theory"

Butler University Indianapolis, Indiana

BS IN CHEMISTRY CUM LAUDE 2008

· American Chemical Society certified degree

Research _____

Institute for Molecular Engineering, University of Chicago

Research group of Professor Giulia

Galli

Postdoctoral Scholar 2014-present

- Developed and implemented methodology for modeling charge transport in electronic materials.
- Characterized structure-property relationships for organic polymers and quantum dots.
- Coordinated regular meetings with collaborators in the Center for Hierarchical Materials Design.
- Prepared reports for funding agencies.

College of Chemistry, University of California, Berkeley

Research group of Professor Martin

Head-Gordon

GRADUATE STUDENT RESEARCHER

2008-2014

- Developed series of new methods for efficient treatment of bonded and non-bonded interactions using perturbation theory approaches.
- Designed efficient new parallel algorithm for the evaluation of total energies.
- Improved active space methods for molecular systems where static correlation is important.
- Mentored a masters student on a shared project, resulting in published work.

Research group of Professor Todd

Hopkins

Undergraduate Researcher

2006-2008

• Synthesized ionic liquids and lanthanide complexes.

Department of Chemistry, Butler University

- Characterized the environment dependence of lanthanide luminescence.
- Designed experimental setup for chiral luminescence measurements.

Teaching _

Quantum Chemistry for graduate students

University of California, Berkeley

2010

GRADUATE STUDENT INSTRUCTOR

- Taught occasional lectures.
- Tutored students during regular office hours.
- Prepared and graded exams and homework assignments.

General Chemistry for chemistry majors

University of California, Berkeley

2009

GRADUATE STUDENT INSTRUCTOR

- Supervised four hours of laboratory practice per week.
- Tutored students during twice-weekly office hours.
- Graded exams and homework assignments.

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General Chemistry for nonmajors

University of California, Berkeley

GRADUATE STUDENT INSTRUCTOR

• Supervised four hours of laboratory practice per week.

- Hosted class-wide exam review sessions.
- Lectured one hour per week.
- Tutored students during twice-weekly office hours.
- Graded exams and homework assignments.

Service Activities _____

Meeting coordinator

Center for Hierarchical Materials

Design

ORGANIC PHOTOVOLTAICS USE CASE GROUP

• Coordinated agenda and schedules across three institutions before monthly meetings

Mentor University of California, Berkeley

• Supervised research project with masters student, resulting in a joint publication

ReviewerJournal of Chemical Theory and

Computation

Reviewer Molecular Physics

MemberAmerican Chemical Society

2007-2008,2016-

MemberAmerican Physical Society

2014-

Honors & Awards

Production Allocation Award, 4 million hours , National Energy Research Scientific Computing	2016
Center	2010
NSF Graduate Research Fellowship Honorable Mention, National Science Foundation	2008
Freud Fellowship (Declined), University of Chicago	2008
Undergraduate Research Fellowship , Butler Summer Institute, Butler University	2007
ACS Undergraduate Fellowship in Nuclear Chemistry and Radiochemistry, San Jose State	2006
University	2006

Publications _

- 15. Brawand, N., Goldey, M. B., Vörös, M., and Galli, G. Defect states and charge transport in quantum dot solids. Under review
- 14. Goldey, M. B., Reid, D., de Pablo, J., and Galli, G. Planarity and multiple components promote organic photovoltaic efficiency by improving electronic transport. *Phys. Chem. Chem. Phys.* 18 (2016), 31388–31399. Chosen for front cover
- 13. Goldey, M. B., Belzunces, B., and Head-Gordon, M. Attenuated MP2 with a

- Long-Range Dispersion Correction for Treating Nonbonded Interactions. J. Chem. Theory Comput. 11, 9 (2015), 4159–4168
- 12. WITTE, J., GOLDEY, M. B., NEATON, J. B., AND HEAD-GORDON, M. Beyond energies: Geometries of nonbonded molecular complexes as metrics for assessing electronic structure approaches. *J. Chem. Theory Comput.* 11, 4 (2015), 1481–1492
- 11. Yihan Shao, et al. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* 113, 2 (2015), 184–215
- 10. Goldey, M. B., and Head-Gordon, M. Convergence of attenuated second order Møller-Plesset perturbation theory towards the complete basis set limit. *Chem. Phys. Lett.* 608 (2014), 249 254. Editor's choice
- 9. Huang, Y., Goldey, M. B., Head-Gordon, M., and Beran, G. Achieving high-accuracy intermolecular interactions by combining Coulomb-attenuated second-order Møller-Plesset perturbation theory with a long-range dispersion correction. *J. Chem. Theory Comput.* 10 (2014), 2054
- 8. Goldey, M. B., and Head-Gordon, M. Separate Electronic Attenuation Allowing a Spin-Component Scaled Second Order Møller-Plesset Theory to Be Effective for Both Thermochemistry and Non-Covalent Interactions. *J. Phys. Chem. B* 118 (2014), 6519
- 7. MAYHALL, N. J., GOLDEY, M. B., AND HEAD-GORDON, M. A Quasidegenerate Second-Order Perturbation Theory Approximation to RAS-nSF for Excited States and Strong Correlations. J. Chem. Theory Comput. 10, 2 (2014), 589–599
- 6. Goldey, M. B., Distasio, Jr., R. A., Shao, Y., and Head-Gordon, M. Shared memory multiprocessing implementation of resolution-of-the-identity second-order Møller-Plesset perturbation theory with attenuated and unattenuated results for intermolecular interactions between large molecules. *Mol. Phys.* 112, 5-6 (2014), 836–843
- 5. Goldey, M. B., Dutoi, A., and Head-Gordon, M. Attenuated Second-Order Møller-Plesset Perturbation Theory: Performance within the aug-cc-pVTZ Basis. *Phys. Chem. Chem. Phys.* 15 (2013), 15869–15875
- 4. Goldey, M. B., and Head-Gordon, M. Attenuating Away the Errors in Inter- and Intramolecular Interactions from Second Order Møller-Plesset Calculations in the Small Aug-cc-pVDZ Basis Set. J. Phys. Chem. Lett. 3 (2012), 3592–3598
- 3. Bell, F., Zimmerman, P. M., Casanova, D., Goldey, M. B., and Head-Gordon, M. Restricted active space spin-flip (RAS-SF) with arbitrary number of spin-flips. *Phys. Chem. Chem. Phys.* 15 (2013), 358–366
- 2. ZIMMERMAN, P. M., BELL, F., GOLDEY, M. B., BELL, A. T., AND HEAD-GORDON, M. Restricted active space spin-flip configuration interaction: Theory and examples for multiple spin flips with odd numbers of electrons. *J. Chem. Phys.* 137 (2012), 164110
- 1. Hopkins, T., and Goldey, M. B. ${\rm Tb^{+3}}$ and ${\rm Eu^{+3}}$ luminescence in imidazolium ionic liquids. J. Alloy Compd. 488, 2 (2009), 615–618

Presentations

ORAL PRESENTATIONS

American Physical Society

March Meeting

Mar. 2016 Baltimore, MD

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Advances and Challenges in Soft Matter Photovoltaic Research

Center for Hierarchical Materials

Design Chicago, IL

Austin, TX

Nov. 2015

invited speaker

American Physical Society

MAR. 2015

March Meeting

Harvard University

Cambridge, MA

Aspuru-Guzik Group Meeting

MAR. 2014

invited speaker

Chemical Sciences Division Seminar

APR. 2013

invited speaker

Martin Head-Gordon Group Meetings

2010-2013

Lawrence Berkeley Laboratory

Berkeley, CA

University of California, Berkeley

Berkeley, CA

Graduate Research Seminar

APR. 2010

University of California, Berkeley

Berkeley, CA

Undergraduate Research Conference

APR. 2008

Butler University
Indianapolis, IN

Departmental Seminar

OCT. 2007

Butler University

Indianapolis, IN

Butler Summer Institute

JUL. 2007

Butler University
Indianapolis, IN

POSTER PRESENTATIONS

Argonne Postdoctoral Research and Career Symposium

OCT. 2016

Argonne National Laboratory

Lemont, IL

Car-Parrinello Molecular Dynamics 2016 conference

MAY 2016

University of Chicago Chicago, IL

Center for Hierarchichal Materials Annual Meeting

MAR. 2016

Northwestern University

Evanston, IL

Mindbytes Research Computing Expo

OCT. 2015

University of Chicago

Chicago, IL

Argonne Postdoctoral Research and Career Symposium

OCT. 2015

Argonne National Laboratory

Lemont, IL

Center for Hierarchichal Materials Annual Meeting

MAY 2015

Northwestern University

Evanston, IL

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American Conference on Theoretical Chemistry

Jul. 2014 Telluride, CO

Molecular Quantum Mechanics

University of California, Berkeley

MAY 2010 Berkeley, CA

Local ACS Section

Oct. 2007 Indianapolis, IN

ACS General Meeting

Aug. 2007 Boston, MA