Matthew B. **Goldey**

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"
- GPA 3.98/4.0

Butler University

Indianapolis, Indiana

BS in chemistry cum laude — *2008*

- American Chemical Society certified degree
- GPA 3.92/4.0

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.

Department of Chemistry, Butler University

Research group of Professor Todd Hopkins

Undergraduate Researcher — *2006-2008*

- Synthesized ionic liquids and lanthanide complexes.
- Characterized the environment dependence of lanthanide luminescence.
- Designed experimental setup for chiral luminescence measurements.

Teaching

Quantum Chemistry for graduate students

University of California, Berkeley

Graduate Student Instructor — *2010*

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

General Chemistry for chemistry majors

University of California, Berkeley

Graduate Student Instructor

2009

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

General Chemistry for nonmajors

University of California, Berkeley

Graduate Student Instructor

2008

- 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.

Honors & Awards

Production Allocation Award, 4 million hours, National Energy Research Scientific Computing Center — *2016*

NSF Graduate Research Fellowship Honorable Mention, National Science Foundation — *2008*

Freud Fellowship (Declined), University of Chicago — *2008*

Top 100 student, Butler University — *2008*

Undergraduate Research Fellowship, Butler Summer Institute, Butler University — *2007*

ACS Undergraduate Fellowship in Nuclear Chemistry and Radiochemistry, San Jose State University — *2006*

Highest GPA award within Jordan College of Fine Arts, Butler University — *2004*

Outstanding Student of General Chemistry, Butler University — *2004*

National Merit Scholar, Butler University — *2004*

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

Reviewer

Journal of Chemical Theory and Computation

Reviewer

Chemical Physics Letters

Reviewer

Molecular Physics

Member

American Chemical Society

2007-2008,2016-

Publications

16. **Goldey, M. B.**, Brawand, N. P., Vörös, M., and Galli, G. Charge Transport in Nanostructured Materials: Implementation and Verification of Constrained Density Functional Theory. **Under review**
15. Brawand*, N. P., **Goldey*, M. B.**, Vörös, M., and Galli, G. Defect states and charge transport in quantum dot solids. *Chemistry of Materials 29*, 3 (2017), 1255–1262. ***Co-first authors**
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.** Tb^{+3} and 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*

Advances and Challenges in Soft Matter Photovoltaic Research — *Center for Hierarchical Materials Design*
Nov. 2015 — *Chicago, IL*
invited speaker

American Physical Society — *March Meeting*
Mar. 2015 — *Austin, TX*

Aspuru-Guzik Group Meeting — *Harvard University*
Mar. 2014 — *Cambridge, MA*
invited speaker

Chemical Sciences Division Seminar — *Lawrence Berkeley Laboratory*
Apr. 2013 — *Berkeley, CA*
invited speaker

Martin Head-Gordon Group Meetings — *University of California, Berkeley*
2010-2013 — *Berkeley, CA*

Graduate Research Seminar — *University of California, Berkeley*
Apr. 2010 — *Berkeley, CA*

Undergraduate Research Conference — *Butler University*
Apr. 2008 — *Indianapolis, IN*

Departmental Seminar — *Butler University*
Oct. 2007 — *Indianapolis, IN*

Butler Summer Institute — *Butler University*
Jul. 2007 — *Indianapolis, IN*

Poster Presentations

Argonne Postdoctoral Research and Career Symposium — *Argonne National Laboratory*
Oct. 2016 — *Lemont, IL*

Car-Parrinello Molecular Dynamics 2016 conference — *University of Chicago*
May 2016 — *Chicago, IL*

Center for Hierarchichal Materials Annual Meeting — *Northwestern University*
Mar. 2016 — *Evanston, IL*

Mindbytes Research Computing Expo — *University of Chicago*
Oct. 2015 — *Chicago, IL*

Argonne Postdoctoral Research and Career Symposium — *Argonne National Laboratory*
Oct. 2015 — *Lemont, IL*

Center for Hierarchichal Materials Annual Meeting — *Northwestern University*
May 2015 — *Evanston, IL*

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*