

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

Project : *Charge transport models for nanostructured materials*

Tools:

- ◆ Algorithm design and implementation of constrained DFT inside the Quantum ESPRESSO software package
- ◆ Fortran90, MPI, OpenMP, Python, Unsupervised machine learning (python/sklearn)

Results:

- ◇ Employed machine learning (affinity propagation) to cluster and discover unexpected structural features in twisted organic polymers.
- ◇ Identified structure-property relationships for organic polymers, finding a 50-fold decrease in charge transport rates inside of polymers with increasing twisting.
- ◇ Demonstrated that double-bonded oxygen defects were up to 10^6 -fold faster at trapping charge carriers than dangling bond defects in silicon quantum dots and found that other commonly used methods fail to describe the physics of these systems qualitatively correctly.
- ◇ Coordinated regular meetings with collaborators across 3 institutions and prepared written reports within the Center for Hierarchical Materials Design.
- ◇ Published 3 papers, delivered 5 oral presentations and 7 poster presentations, and embedded developed methodology in Quantum ESPRESSO, providing training for 2 other researcher teams for projects on novel materials.

College of Chemistry, University of California, Berkeley

Research group of Professor Martin Head-Gordon

GRADUATE STUDENT RESEARCHER

2008-2014

Project : *Improved models for noncovalent interactions*

Tools:

- ◆ Nonlinear parameter optimization within new theoretical models (based on second order Møller-Plesset perturbation theory), multiprecision arithmetic, and symbolic algebra
- ◆ C++, Fortran90, Python

Results:

- ◇ Reduced errors by 80% in predicted energies of noncovalent complexes while reducing the cost of calculations by 1-2 orders of magnitude through the development of new mathematical models.
- ◇ Generated new methods for predicting the geometries noncovalent complexes which fix qualitative errors of finite basis perturbation theory for intramolecular noncovalent interactions.
- ◇ Mentored masters student who successfully entered PhD program after joint project.
- ◇ Published 8 papers (6 first author) and made code available within the Q-Chem commercial software.

Project : Parallel integral transformation using the resolution of the identity approximation**Tools:**

- ◆ Algorithm design and parallelization of integral transformations inside of the Q-Chem quantum chemistry package
- ◆ C++, OpenMP

Results:

- ◇ Demonstrated strong scaling of 9x increase in speed on 12 cores for new implementation of resolution of the identity second order Møller-Plesset perturbation theory.
- ◇ Created new methodologies for modeling strong correlation using new active space methods.
- ◇ Published 3 papers in collaboration with 6 other authors and embedded framework in Q-Chem commercial software.

Department of Chemistry, Butler University*Research group of Professor Todd Hopkins*

UNDERGRADUATE RESEARCHER

2006-2008

Project : Ionic liquids as media for novel lanthanide fluorescence probes**Tools:**

- ◆ Syntheses of ionic liquids butyl methyl imidazolium bromide and butyl methyl imidazolium bis(trifluoromethylsulfonyl)imide and Europium and Terbium complexes.
- ◆ Experimental design of fluorescent and optical spectroscopy table.

Results:

- ◇ Measured the effect of ionic liquid solvent on Europium complexes, finding that halide and aqueous complexes were strongly affected by presence of ionic liquids, while complexes with 2,6-pyridine dicarboxylate were effectively isolated from ionic liquid environment.
- ◇ Published 1 paper, delivered 1 conference presentation and 1 poster presentation, and developed methodology later used for 3 more papers by 4 other researchers for chiral luminescence studies.

Teaching

Quantum Chemistry for graduate students*University of California, Berkeley*

GRADUATE STUDENT INSTRUCTOR

2010

- Taught occasional lecture and led discussion sections.
- Tutored students during 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-

Member

American Physical Society

2014-

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. *Chem. Mater.* 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 Chemical Society

APR. 2017

Design principles for organic photovoltaic materials from ab initio simulations

Spring Meeting

San Francisco, CA

American Chemical Society	<i>Spring Meeting</i>
APR. 2017	San Francisco, CA
Ab initio modeling of charge transport defects in quantum dot arrays	
American Physical Society	<i>March Meeting</i>
MAR. 2016	Baltimore, MD
Electronic structure properties as signatures of morphological motifs in organic photovoltaics	
Advances and Challenges in Soft Matter Photovoltaic Research	<i>Center for Hierarchical Materials Design</i>
Nov. 2015	Chicago, IL
invited speaker	
American Physical Society	<i>March Meeting</i>
MAR. 2015	Austin, TX
Attenuated second order Møller-Plesset perturbation theory: correcting finite basis set errors and infinite basis set inaccuracies	
Aspuru-Guzik Group Meeting	<i>Harvard University</i>
MAR. 2014	Cambridge, MA
invited speaker	
Chemical Sciences Division Seminar	<i>Lawrence Berkeley Laboratory</i>
APR. 2013	Berkeley, CA
invited speaker	
Martin Head-Gordon Group Meetings	<i>University of California, Berkeley</i>
2010-2013	Berkeley, CA
Graduate Research Seminar	<i>University of California, Berkeley</i>
APR. 2010	Berkeley, CA
Undergraduate Research Conference	<i>Butler University</i>
APR. 2008	Indianapolis, IN
Departmental Seminar	<i>Butler University</i>
OCT. 2007	Indianapolis, IN
Butler Summer Institute	<i>Butler University</i>
JUL. 2007	Indianapolis, IN
POSTER PRESENTATIONS	
Center for Hierarchical Materials Annual Meeting	<i>Northwestern University</i>
MAR. 2017	Evanston, IL
Argonne Postdoctoral Research and Career Symposium	<i>Argonne National Laboratory</i>
OCT. 2016	Lemont, IL
Car-Parrinello Molecular Dynamics 2016 conference	<i>University of Chicago</i>
MAY 2016	Chicago, IL
Center for Hierarchical Materials Annual Meeting	<i>Northwestern University</i>
MAR. 2016	Evanston, IL
Mindbytes Research Computing Expo	<i>University of Chicago</i>
OCT. 2015	Chicago, IL

Argonne Postdoctoral Research and Career Symposium

OCT. 2015

*Argonne National Laboratory**Lemont, IL***Center for Hierarchical Materials Annual Meeting**

MAY 2015

*Northwestern University**Evanston, IL***American Conference on Theoretical Chemistry**

JUL. 2014

*Telluride, CO***Molecular Quantum Mechanics**

MAY 2010

*University of California, Berkeley**Berkeley, CA***Local ACS Section**

OCT. 2007

*Indianapolis, IN***ACS General Meeting**

AUG. 2007

Boston, MA