Curriculum Vitae

Jacqueline A. R. Shea

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Affiliation

Postdoctoral Scholar	Stanford University, Stanford, CA Advisor: Todd Martínez	2021-present

Education

Ph. D. in Chemistry	University of California Berkeley, Berkeley, CA Thesis Advisor: Eric Neuscamman	2016-2021

Thesis Title: *On the Construction of a Novel Mean Field Platform and Broadly Applicable Variational Principle Methods for Electronically Excited States*

B. S. in Chemistry	Texas A&M University, College Station, TX Thesis Advisor: Steven E. Wheeler	2013-2016

Thesis Title: *Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*

Academic Honors and Awards

National Science Foundation GRFP Fellow	NSF	2018
ACS Undergraduate Award in Analytical Chemistry	American Chemical Society	2016
ACS Undergraduate Award in Organic Chemistry	American Chemical Society	2016
Graduated Summa Cum Laude	Texas A&M University	2016
Undergraduate Research Scholar	Texas A&M University	2016
Summer Research Fellowship	Texas A&M University	2015
College of Science Dean's List	Texas A&M University	2013-2016
Phi Eta Sigma Honor Society Membership	Texas A&M University	2013-2016
President's Endowed Scholarship	Texas A&M University	2013-2016
Houston Endowment Scholarship	Jones Scholar Program	2013-2015
Top 10 Percent State Scholarship	State of Texas	2013-2014
The Pete Hunter Dunham Jr. '74 Scholarship	Texas A&M University	2013-2014
National Merit Finalist	National Merit Scholars	2013

Teaching Experience

Graduate Quantum Chemistry II (Chem 221B)	University of California Berkeley	2019
Physical Chemistry (Chem 120A)	University of California Berkeley	2017
Bay Area Scientists in Schools Volunteer	Community Resources for Science	2017
Organic Chemistry Lab (Chem 3B)	University of California Berkeley	2016
Organic Chemistry II (Chem 228)	Texas A&M University	2015
Organic Chemistry I (Chem 227)	Texas A&M University	2014

Research Experience

- Developing algorithms for excited state optimizations to transform between variational principles to achieve size consistency, state selectivity, and compatibility with quantum Monte Carlo methods.
- Integrating neural network technology into theoretical chemistry algorithms to improve optimization methods for excited state modeling
- Constructing, implementing, and benchmarking novel mean field excited state methods
- Utilizing density functional theory (DFT) to understand the performance of commonly used dual-hydrogen bonding organocatalysts for Diels-Alder cycloadditions and Friedel-Crafts alkylations.
- Applying DFT to novel silanediol catalysts to identify the mode of catalysis and stereoinduction, with an aim of developing more selective catalysts.

Posters and Presentations

1. "*Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*." Texas A&M REU, College Station, Texas (August 5, 2015). (Poster)
2. "*Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*." Texas A&M REU, College Station, Texas (August 6, 2015). (Presentation)
3. "*Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*." Gulf Coast Undergraduate Research Symposium, Houston, Texas (October 17, 2015). (Presentation) **Awarded the Outstanding Presentation in Computational Chemistry.**
4. "*Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*." 251st National Meeting of the American Chemical Society, San Diego, California (March 17-22, 2016). (Poster)
5. "*Quantifying the Strengths of Dual Hydrogen Bonding Organocatalysts*." Texas A&M Student Research Week, College Station, Texas (March 30, 2016). (Presentation) **Awarded 2nd place oral presentation in the Astronomy, Chemistry, Physics, and Material Sciences Division.**
6. "*Enforcing Size Consistency in an Excited State Variational Principle*." 254th National Meeting of the American Chemical Society, Washington DC (August 21-23, 2017). (Poster)
7. *"Size Consistent Excited States via Algorithmic Transformations between Variational Principles."* UC Berkeley Graduate Research Conference, Berkeley, CA (March 22, 2018). (Presentation)
8. *"Size Consistent Excited States via Variational Principle Transformations."* West Coast Theoretical Chemistry Symposium, Stanford, CA (March 28, 2018). (Poster)
9. *"Excited State Mean Field Theory."* Penn Conference in Theoretical Chemistry, University of Pennsylvania, PN (June 12, 2018). (Poster)
10. *"Excited State Mean Field Theory: Building upon a mean field platform for excited state quantum chemistry."* Northern California Theoretical Chemistry Meeting, UC Berkeley, CA (May 19, 2019). (Poster)
11. *"Building upon a mean field platform for excited state quantum chemistry."* ACS National Meeting & Expo, San Diego, CA (August 28, 2019). (Poster)

Invited Talks

1. *"Excited State Mean Field Theory & A Generalized Variational Principle."* Pitzer Center Theoretical Chemistry Seminar, UC Berkeley, CA (February 26, 2020).

2. *"A Generalized Variational Principle and its Application to Excited State Mean Field Theory."* Quantum Chemistry by the Lake Seminar Series, The University of Chicago, IL (May 5, 2021).

Publications

1. "*Size consistent excited states via algorithmic transformations between variational principles."* Jacqueline A. R. Shea and Eric Neuscamman, *Journal of Chemical Theory and Computation*. **2017**, *13* (12), 6078-6088. http://pubs.acs.org/doi/abs/10.1021/acs.jctc.7b00923

2. *"QMCPACK: An open source ab initio Quantum Monte Carlo package for the electronic structure of atoms, molecules, and solids."* Jeong Kim *et al. Journal of Physics: Condensed Matter*, **2018**, *30*, 195901. https://iopscience.iop.org/article/10.1088/1361-648X/aab9c3

3. *"Communication: A mean field platform for excited state quantum chemistry."* Jacqueline A. R. Shea and Eric Neuscamman. *Journal of Chemical Physics*. **2018**, *149*, 081101. **(Editor's Pick)** https://aip.scitation.org/doi/10.1063/1.5045056

4. *"Tracking excited states in wave function optimization using density matrices and variational principles."* Lan Nguyen Tran, Jacqueline A. R. Shea, and Eric Neuscamman. *Journal of Chemical Theory and Computation*. **2019**, *15* (9), 4790-4803. https://pubs.acs.org/doi/abs/10.1021/acs.jctc.9b00351

5. *"A Generalized Variational Principle with Applications to Excited State Mean Field Theory."* Jacqueline A. R. Shea, Elise Gwin, and Eric Neuscamman. *Journal of Chemical Theory and Computation*. **2020**, *16* (3), 1526-1540. **(ACS Editor's Choice)** https://pubs.acs.org/doi/10.1021/acs.jctc.9b01105

6. *"N^5-Scaling Excited-State-Specific Perturbation theory."* Rachel Clune, Jacqueline A. R. Shea, and Eric Neuscamman. *Journal of Chemical Theory and Computation*. **2020**, *16* (10), 6132-6141. https://pubs.acs.org/doi/10.1021/acs.jctc.0c00308