

Education

2024 (expected)	Ph.D. in Chemical Engineering Doctoral advisor: Heather J. Kulik	Massachusetts Institute of Technology Cambridge, MA
2019	B.S. in Chemical Engineering with Highest Honors and a minor in Physics	University of California, Santa Barbara Santa Barbara, CA

Honors and Awards

2019	NSF Graduate Research Fellowship	\$138,000 over 5 years
2019	Tau Beta Pi Fellowship	\$10,000 over 1 year
2018	Tau Beta Pi Scholarship	\$2,000 over 1 year
2018	ESTEEM Scholarship, UC Santa Barbara	\$4,400 over 1 year
2017	UC LEADS Scholarship, UC Santa Barbara	\$7,000 over 2 years
2015	Regents Scholarship, UC Santa Barbara	\$24,000 over 4 years

Research Experience

- Dec 2019 – Present **Graduate Student Researcher**, Massachusetts Institute of Technology, Cambridge, MA
 Project: *Addressing uncertainty in density functional theory* Advisor: *Heather J. Kulik*
- Uncover trends in method sensitivity relating the following:
 - o Agreement within density functionals and deviations from more accurate methods
 - o Metal period, spin state, and Hartree-Fock exchange fraction (publication #2 below)
- Jul 2019 – Aug 2019 **Postgraduate Researcher**, University of Illinois, Urbana-Champaign, Champaign, IL
 Project: *Deterministic modeling of LaMer burst nucleation* Advisor: *Baron Peters*
- Derived system of unbounded Volterra delay integro-differential equations for LaMer burst nucleation
 - Implemented numerical solutions for the derived equations via method of lines with collocation methods
- Jan 2019 – Jun 2019 **Undergraduate Researcher**, University of California, Santa Barbara, Santa Barbara, CA
 Project: *Phase diagrams of thermoresponsive nanoemulsions* Advisors: *M. Scott Shell & Glenn Fredrickson*
- Calculated phase diagrams for model systems with histogram reweighting and grand-canonical Monte Carlo
 - Produced effective force fields for colloidal systems from field theoretical simulations on bridging polymers
- Jun 2018 – Aug 2018 **Summer Research Intern**, University of California, Berkeley, Berkeley, CA
 Project: *Density functional theory investigation of CO₂ reduction* Advisor: *Martin Head-Gordon*
- Elucidated reaction mechanisms for a cobalt-based CO₂ reduction catalyst using density functional theory (publication #3 below)
 - Discovered that a distorted ligand framework provides favorable reaction conditions in the cobalt catalyst
- Apr 2017 – Dec 2018 **Undergraduate Researcher**, University of California, Santa Barbara, Santa Barbara, CA
 Project: *Macroscopic modeling of LaMer burst nucleation* Advisor: *Baron Peters*
- Developed a macroscopic model of LaMer burst nucleation which improves upon the prior model by incorporating critical nucleus size (publication #1 below)

Publications (Equal contributors indicated by #)

- Chenru Duan, **Daniel B. K. Chu**, Aditya Nandy, and Heather J. Kulik; “Detection of multi-reference character imbalances enables a transfer learning approach for virtual high throughput screening with coupled cluster accuracy at DFT cost.” *Chemical Science*, **2022**, 13 (17), 4962-4971. DOI:[10.1039/D2SC00393G](https://doi.org/10.1039/D2SC00393G)
- Matthias Loipersberger, Delmar G.A. Cabral, **Daniel B. K. Chu**, Martin Head-Gordon; “Mechanistic Insights into Co and Fe Quaterpyridine-Based CO₂ Reduction Catalysts: Metal–Ligand Orbital Interaction as the Key Driving Force for Distinct Pathways.” *Journal of the American Chemical Society*, **2021**, 143 (2), 744-763. DOI:[10.1021/jacs.0c09380](https://doi.org/10.1021/jacs.0c09380)
- Aditya Nandy[#], **Daniel B. K. Chu**[#], Daniel R. Harper, Chenru Duan, Naveen Arunachalam, Yael Cytter, and Heather J. Kulik; “Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics.” *Physical Chemistry Chemical Physics*, **2020**, 22 (34), 19326-19341. DOI:[10.1039/D0CP02977G](https://doi.org/10.1039/D0CP02977G)
- Daniel B. K. Chu**, Jonathan S. Owen, and Baron Peters; “Nucleation and growth kinetics from LaMer burst data.” *The Journal of Physical Chemistry A*, **2017**, 121 (40), 7511-7517. DOI:[10.1021/acs.jpca.7b08368](https://doi.org/10.1021/acs.jpca.7b08368)

Presentations

Talks

- AICChE Annual Meeting, “LaMer Burst Nucleation and Growth: Assumptions, Models, and Data.” Minneapolis, MN. November 2017, *substituted for Professor Baron Peters*. ([link](#))

Posters

- Cal NERDS Research Showcase, “Computational Study on CO₂ Reduction by a Co(II) Quaterpyridine Electrocatalyst.” Berkeley, CA. August 2018.
- Koret UC LEADS Research & Leadership Symposium, “LaMer Burst Nucleation.” Santa Barbara, CA. March 2018. [Honorable mention](#).
- UCSB Summer Undergraduate and Graduate Research Colloquium, “Understanding the Influence of Nucleation Kinetics in LaMer Burst Nucleation.” Santa Barbara, CA. August 2017.

Teaching Experience

Sep 2016 – Jun 2019

Campus Learning Assistance Services ([link](#)), UC Santa Barbara

Math-Science Tutor and Group Instructor

- Reinforce course material in a classroom setting (of ~20 students) & hold office hours for additional questions
- Design practice tests/worksheets for lower division [linear algebra](#), [differential equations](#), and [vector calculus](#)

Mentorship Experience

2022 | David González Narváez via [MIT MSRP-Bio](#)
Visiting undergraduate researcher from University of Puerto Rico

Community Involvement and Diversity, Equity, & Inclusion

2021	Fundamentals of Facilitation for Racial Justice Work (workshop)	<i>participant</i>
2020	Jewish Learning Fellowship: Pursuing Justice (experiential seminar)	<i>participant</i>
2020	Chemical engineering Application Mentorship Program (ChAMP)	<i>mentor</i>
2020	Graduate Student Council, Course X (GSC-X)	<i>budget/event planning</i>
2020	Graduate Student Affairs Board (GSAB) ChemE Mentorship Program	<i>peer mentor</i>
2018	Tau Beta Pi, CA Sigma Chapter	<i>vice president</i>