

Education

2025 (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 Research Assistant** Massachusetts Institute of Technology, Cambridge, MA

Project: *Addressing uncertainty in density functional theory* Advisor: *Heather J. Kulik*

- Discovered method sensitivity trends with metal period, spin state, and Hartree-Fock exchange fraction²
- Established agreement within density functionals and with wave function methods

Project: *Accelerate chemical discovery of transition metal complexes*

- Automate quantum chemical calculation workflows and job recovery
- Develop and apply ligand additivity models to spin-crossover complexes⁵ and catalysts

Jul 2019 – Aug 2019 **Research Assistant** 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 Research Assistant** University of California, 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, CA

Project: *Density functional theory investigation of CO₂ reduction*³ Advisor: *Martin Head-Gordon*

- Elucidated reaction mechanisms for a cobalt-based CO₂ reduction catalyst using density functional theory
- Discovered that a distorted ligand framework provides favorable reaction conditions in the cobalt catalyst

Apr 2017 – Dec 2018 **Undergraduate Research Assistant** University of California, Santa Barbara, CA

Project: *Macroscopic modeling of LaMer burst nucleation* Advisor: *Baron Peters*

- Developed a macroscopic model of LaMer burst nucleation which improves upon a prior model by incorporating critical nucleus size¹

Publications (Equal contributors indicated by #)

5. Naveen Arunachalam[#], Stefan Gugler[#], Michael G. Taylor[#], Chenru Duan, Aditya Nandy, Jon Paul Janet, Ralf Meyer, Jonas Oldenstaedt, **Daniel B. K. Chu**, and Heather J. Kulik; “Ligand additivity relationships enable efficient exploration of transition metal chemical space.” *Journal of Chemical Physics*, **2022**, (in press). DOI:[10.1063/5.0125700](https://doi.org/10.1063/5.0125700)
4. 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)
3. 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)
2. Aditya Nandy[#], **Daniel B. K. Chu**[#], Daniel R. Harper, Chenru Duan, Naveen Arunachalam, Yael Cyttter, 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)
1. **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

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

Posters

- iii. Cal NERDS Research Showcase, “Computational Study on CO₂ Reduction by a Co(II) Quaterpyridine Electrocatalyst.” Berkeley, CA. August 2018.
- ii. Koret UC LEADS Research & Leadership Symposium, “LaMer Burst Nucleation.” Santa Barbara, CA. March 2018. *Honorable mention*.
- i. 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 2023 – Dec 2023 Department of Chemical Engineering, Massachusetts Institute of Technology
Teaching Assistant for 10.637 (Computational Chemistry)

- Update and test course materials
- Hold weekly office hours to assist students with concepts and scripting

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](#)

Research Mentorship Experience

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| 2024 | Davut Muhammetgulyyev via MIT UROP (Jan – Present)
<i>First-year undergraduate researcher at MIT</i> |
| 2022 | David A. González-Narváez via MIT MSRP-Bio (Jun – Dec)
<i>Visiting undergraduate researcher from University of Puerto Rico-Cayey</i> |

DEI and Pedagogical Training

2024	I Am a LEADer DEI Training	<i>conference</i>
2023	Kaufman Teaching Certificate Program	<i>interactive workshop series</i>
2023	TA Days Training (evidence-based teaching practices for TAs)	<i>workshop series</i>
2021	Fundamentals of Facilitation for Racial Justice Work	<i>workshop series</i>
2020	Jewish Learning Fellowship: Pursuing Justice	<i>experiential seminar</i>

Community Involvement

2020 – 2023	Chemical engineering Application Mentorship Program (ChAMP) <i>Assisted eight URM applicants in preparing applications to MIT ChemE</i>	<i>mentor</i>
2020 – 2023	GSAB ChemE First-Year Mentorship Program	<i>peer mentor</i>
2020	Graduate Student Council, Course X (GSC-X)	<i>budget/event planning</i>
2018	Tau Beta Pi, CA Sigma Chapter	<i>vice president</i>