dbkchu@mit.edu

Daniel B. K. Chu

Curriculum Vitae

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

Selected Honors and Awards

2025 – 2026	**Zuckerman Postdoctoral Scholar**, Zuckerman STEM Leadership Program
2025 – 2027	**Postdoctoral Fellowship at The Sackler Center for Computational Molecular and Materials Science**, Tel Aviv University
2019 – 2024	**NSF Graduate Research Fellowship**
2019 – 2020	**Tau Beta Pi Fellowship**
2018 – 2019	**Tau Beta Pi Scholarship**
2018 – 2019	**ESTEEM Scholarship**, UC Santa Barbara
2017 – 2019	**UC LEADS Scholarship**, UC Santa Barbara
2015 – 2019	**Regents Scholarship**, UC Santa Barbara

Research Experience

Dec 2019 – Present **Graduate Research Fellow** Massachusetts Institute of Technology, Cambridge, MA
Project: *Addressing uncertainty in density functional theory* Advisor: *Heather J. Kulik*
- Elucidated method sensitivity trends with metal period, spin state, and Hartree-Fock exchange fraction[2]
- Evaluated agreement within density functionals and with wave function methods[4]

Project: *Accelerate chemical discovery of transition metal complexes*
- Automate quantum chemical computation workflows and calculation recovery
- Develop and apply ligand additivity models to spin-crossover complexes[5] and catalysts[b]

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 CO_2 reduction*[3] Advisor: *Martin Head-Gordon*
- Elucidated reaction mechanisms for a cobalt-based CO_2 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 size[1]

Peer-Reviewed 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
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
3. Matthias Loipersberger, Delmar G. A. Cabral, **Daniel B. K. Chu**, Martin Head-Gordon; "Mechanistic Insights into Co and Fe Quaterpyridine-Based CO_2 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
2. 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
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

Other Publications

b. **Daniel B. K. Chu**, David A. González-Narváez, Ralf Meyer, Aditya Nandy, Heather J. Kulik; "Ligand Many-Body Expansion as a General Approach for Accelerating Transition Metal Complex Discovery." *Submitted*. DOI: 10.26434/chemrxiv-2024-m39d9

a. **Daniel B. K. Chu**; "LaMer Burst Nucleation – A Graphical Interpretation of Microscopic Parameters from Macroscopic Measurements." **2024**. DOI: 10.26434/chemrxiv-2024-vrtp9

Presentations

Oral

II. ACS Fall 2024 Meeting, "Ligand additivity models for accelerated precision molecular catalyst screening." Denver, CO, USA. August 2024, *contributed talk*. Received CATL Division Graduate Student Travel Award.

I. AIChE Annual Meeting, "LaMer Burst Nucleation and Growth: Assumptions, Models, and Data." Minneapolis, MN, USA. November 2017, *substituted for Professor Baron Peters*. (link)

Poster

iii. Cal NERDS Research Showcase, "Computational Study on CO_2 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.

Research Mentorship Experience

Jan 2024 – Present	Davut Muhammetgulyyev via MIT UROP *MIT Class of 2027, Course 6-3*
Jun 2022 – Dec 2022	David A. González-Narváez via MIT MSRP-Bio *`23 B.S. in Chemistry, University of Puerto Rico-Cayey* (now: Columbia Ph.D.)

Teaching Experience

Sep 2023 – Dec 2023 Department of Chemical Engineering, Massachusetts Institute of Technology

Teaching Assistant for 10.637 (Quantum Chemical Simulation)

- Revise and test course materials & prepare rubrics and answer keys
- 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

DEI and Pedagogical Training

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

Community Involvement

2020 – 2024	Chemical engineering Application Mentorship Program (ChAMP) *Assisted nine URM applicants in preparing graduate school applications*	*mentor*
2020 – 2023	GSAB ChemE First-Year Mentorship Program	*peer mentor*
2020 – 2021	Graduate Student Council, Course X (GSC-X)	*budget/event planning*
2018 – 2019	Tau Beta Pi, CA Sigma Chapter	*vice president*