Updated 2 Nov 2022

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Daniel B. K. Chu

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 Research Assistant** Massachusetts Institute of Technology, Cambridge, MA
Project: *Addressing uncertainty in density functional theory* Advisor: *Heather J. Kulik*
- Uncover method sensitivity trends
  - Agreement within density functionals and with wave function methods
  - Metal period, spin state, and Hartree-Fock exchange fraction[2]

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 complexes[5] 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 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]

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

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 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.

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 (June – present)
Visiting undergraduate researcher from University of Puerto Rico

Community Involvement

2020 & 2022 | Chemical engineering Application Mentorship Program (ChAMP) — *mentor*
Gave feedback and advice to 3 historically underrepresented applicants

2020 & 2022 | Graduate Student Affairs Board (GSAB) ChemE Mentorship Program — *peer mentor*

2020	Graduate Student Council, Course X (GSC-X)	*budget/event planning*
2018	Tau Beta Pi, CA Sigma Chapter	*vice president*

Diversity, Equity, & Inclusion Training

2021	Fundamentals of Facilitation for Racial Justice Work	*workshop*
2020	Jewish Learning Fellowship: Pursuing Justice	*experiential seminar*