# KRISTOPHER S. BROWN

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## OBJECTIVE

I'm interested in formal methods, applied category theory, and database engineering such that human expert knowledge can be applied to concrete problems *at scale* through safe AI. My research address systemic challenges with data sharing, transparency of methodologies, and the automatic generation of code to allow computational scientists to work at the level of abstraction in which they naturally reason about their domains.

## HONORS

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| ACT 2021 speaker: *Implementing polynomial functors and mode-dependent dynamical systems in Catlab* | 2021 |
| The Applied Category Theory Adjoint School (selected participant) | 2021 |
| *Comput. Mat. Sci.* Editor's Choice: Categorical data integration for computational science | 2019 |
| Applied Category Theory: Bridging Theory & Practice, at NIST (invited guest) | 2018 |
| CS230 Deep Learning: $1^{st}$ Prize Poster Award (Stanford University) | 2018 |
| National Defense Science and Engineering Graduate (NDSEG) Fellowship | 2017 - 2021 |
| James B. Reynolds Scholarship for Foreign Study | 2015 |
| Phi Beta Kappa and Tau Beta Pi (Vice President of NH-B Chapter) | 2014 |
| American Chemical Society National Scholar | 2012 - 2014 |

## RESEARCH EXPERIENCE

**Postdoctoral researcher, University of Florida** — 2021
*Advisor: James Fairbanks*

· Model-aware scientific computing, the double category of rewrite rules, regular logic automated theorem proving

**AlgebraicJulia Development Research, ACT Adjoint School** — 2021
*Advisors: James Fairbanks and Evan Patterson*

· DPO rewriting + automorphism groups for C-Sets, generalized algebraic theories, sketches, polynomial functors

**Logical Methods Research Intern, Google** — 2020

· Lean Theorem Prover, separation logic, dependent type theory, formal software verification

**Philosophical Logic Independent Study, Stanford University** — 2020
*Advisor: Thomas Icard*

· Explainable AI, algebraic models of the explainability relation

**Formal Methods Independent Study, Stanford University** — 2020
*Advisor: Clark Barrett*

· Satisfiability modulo theories, inductive datatypes, term rewriting, generalized algebraic theories

**Deep Learning Research Intern, Google** — 2019

· Higher order logic, proof search, model pruning, feature learning, custom hardware

**Founder/CTO/Lead researcher, Modelyst LLC** — 2018-2021

· Declarative programming, API design, knowledge representation, software development

### Graduate Research Assistant, Stanford University
2016 - 2021

*Advisor: Jens Norskøv*

· Density functional theory, constrained statistical learning, surface chemistry

### Scientific Modeling Visiting Scholar, École Polytechnique Fédérale de Lausanne
2015 - 2016

*Advisor: Jeremy Luterbacher*

· Catalysis synthesis, molecular dynamics, multi-scale modeling

### Automation Engineering Visiting Scholar, Helmut Schmidt Universität
2015

*Advisor: Alexander Fay*

· Fuzzy digraphs, control theory, chemical process design, safety engineering

### R&D Intern, Bayer CropScience
2014

· Bioreactor design, agricultural science, mechanical engineering, fluid mechanics

## EDUCATION

### PhD in Chemical Engineering
2021

Stanford University

### Bachelor of Engineering in Chemical Engineering
2015
### Bachelor of Science in Chemistry
2014

Dartmouth College, *Magna cum laude*

## PUBLICATIONS - COMPUTER SCIENTIFIC

· **K S Brown**, *E Patterson, J Fairbanks.* Double pushout rewriting for C-Sets. (2021 - in preparation).

· *M Mann, A Wilson, Y Zohar, L Stuntz, A Irfan,* **K S Brown**, *C Donovick, A Guman, C Tinelli, C Barrett.* Smt-Switch: A Solver-agnostic C++ API for SMT Solving. *24th International Conference on Theory and Applications of Satisfiability Testing: SAT* (2021).

· *M Mann, A Irfan, F Lonsing, Yahan Yang, H Zhang,* **K S Brown**, *A Gupta, C Barrett.* pono: a Flexible and Extensible SMT-based Model Checker. *33rd International Conference on Computer-Aided Verification: CAV* (2021).

· *M J Statt,* **K S Brown**, *S Suram, L Hung, J Gregoire, B Rohr.* DBgen: A Python Library for Defining Scalable, Maintainable, Accessible, Reconfigure, Transparent (SMART) Data Pipelines. *SoftwareX* (2021 - in preparation).

· *M J Statt, B A Rohr,* **K S Brown**, *D Guevarra, J Hummelshoej, L Hung, A Anapolsky, J M Gregoire, S K Suram.* ESAMP: Event-Sourced Architecture for Materials Provenance management and application to accelerated materials discovery. (2021 - in preparation).

· **K S Brown**, *D I Spivak, R Wisnesky.* Categorical data integration for computational science. *Computational Materials Science* (2019).

· *L Hung, B Rohr,* **K S Brown**, *M Statt, P Herring, A Bhargava, H Kwon, S Suram, M Aykol, J Hummelshoej.* Deep neural networks to accelerate and reproduce DFT. *APS Abstracts* (2019).

## PUBLICATIONS - NATURAL SCIENTIFIC

· *A Krishnapriyan,* **K S Brown**. Sensitivity Analysis of Tight-Binding Theory Parameters. (2021 - in preparation).

· **K S Brown**, *J Voss.* Linear constraints for improving transferability of empirical DFT functionals. (2021 - in preparation).

· **K S Brown**, *Y Maimaiti, J Voss, T Bligaard.* MCML: Constraints and machine learning applied to surface chemistry. *Journal of Computational Chemistry* (2021).

· *T Ludwig, J A Gauthier, C F Dickens,* **K S Brown**, *S Ringe, K Chan, J K Norskov.* Atomistic Insight into Cation Effects on Binding Energies in Cu-Catalyzed Carbon Dioxide Reduction . *Nature Communications* (2019).

· *X Liu, P Schlexer, J Xiao, Y. Ji, L. Wang, R B Sandberg, M. Tang,* **K S Brown**, *H. Peng, S Ringe, C Hahn, T F Jaramillo, J K Norskov, K Chan.* pH effects on the electrochemical reduction of CO2 towards C2 products on stepped copper. *Nature Communications* (2019).

· *T Ludwig, J A Gauthier,* **K S Brown**, *S Ringe, J K Nrskov, K Chan .* Solvent adsorbate interactions and adsorbate specific solvent structure in carbon dioxide reduction on a stepped Cu surface. *Journal of Physical Chemistry C* (2019).

· **K S Brown**, *C Saggese, B P Le Monnier, F Heroguel, J S Luterbacher.* Simulation of Gas-and Liquid-Phase Layer-By-Layer Deposition of Metal Oxides by Coarse-Grained Modeling. *Journal of Physical Chemistry C* (2018).

· *F Heroguel, B P Le Monnier,* **K S Brown**, *J C Siu, J S Luterbacher.* Catalyst stabilization by stoichiometrically limited layer-by-layer overcoating in liquid media. *Applied Catalysis B: Environmental* (2017).

· *D Chen, K Chen,* **K S Brown**, *A Hang, J X J Zhang.* Liquid-phase tuning of porous PVDF-TrFE film on flexible substrate for energy harvesting. *Applied Physics Letters* (2017).

## SKILLS

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| **Programming Languages** | Julia, Python, SQL, Haskell, Lean, Coq, Prolog, C++ |
| **Spoken Languages** | Spanish, German, French (beginner level) |
| **Scientific Software** | VASP, Quantum Espresso, Gaussian 09, COMSOL, SolidWorks, Aspen Plus |

## TEACHING ASSISTANTSHIPS

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| Stanford University (Energy and mass transport) | Spring 2020 |
| Stanford University (Energy: Chemical Transformations for Production, Storage, and Use) | Winter 2018 |
| Thayer School of Engineering at Dartmouth College (Chemical Engineering Fundamentals) | Fall 2015 |
| Dartmouth College (Organic Chemistry) | Fall 2012 |