

KRISTOPHER S. BROWN

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<https://krisb.org/docs/research.html>

HONORS

ICGT Best Paper Award <i>Computational Category Theoretic Rewriting</i>	2022
Topos Institute seminar speaker: <i>Combinatorial representation of scientific knowledge</i>	2022
JuliaCon speaker: <i>Declarative data transformation via graph transformation</i>	2022
SIAM Discrete Mathematics Speaker: <i>Extending McKay's Canonical Isomorph Algorithm to C-Sets</i>	2022
Catalysis and Modeling Symposium, Rungstedagaard DK: <i>Combinatorial scientific knowledge</i> (poster)	2022
ACT 2021 short talk: <i>Implementing polynomial functors and mode-dependent dynamical systems in Matlab</i>	2021
The Applied Category Theory Adjoint School (selected participant)	2021
<i>Comput. Mat. Sci.</i> 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

Research software engineer, Topos Institute <i>with Evan Patterson and Owen Lynch</i>	2022
· Graphical linear algebra, scientific computing, categorical databases, combinatorial algorithms	
Postdoctoral researcher, University of Florida <i>Advisor: James Fairbanks</i>	2021
· Model-aware scientific computing, the double category of rewrite rules, regular logic automated theorem proving	
· DPO rewriting + automorphism groups for C-Sets, generalized algebraic theories, sketches, polynomial functors	
Deep Learning / Logical Methods Research Intern, Google	2019-2020
· Higher order logic, proof search, model pruning, feature learning, custom hardware	
· Lean Theorem Prover, separation logic, dependent type theory, formal software verification	
Independent Studies in Philosophical Logic and Formal Methods, Stanford University <i>Advisors: Thomas Icard and Clark Barrett</i>	2020
· Explainable AI, algebraic models of the explainability relation	
· Satisfiability modulo theories, inductive datatypes, term rewriting, generalized algebraic theories	
Founder/CTO/Lead researcher, Modelyst LLC	2018-2021
· Declarative programming, API design, knowledge representation, software development	

RESEARCH EXPERIENCE - NATURAL SCIENTIFIC

Graduate Research Assistant, Stanford University 2016 - 2021

Advisor: Jens Norskov

- Density functional theory, statistical learning under physics-informed constraints, surface chemistry

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

Advisor: Jeremy Luterbacher

- Catalysis synthesis, molecular dynamics, multi-scale modeling

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**, *T Hanks, J Fairbanks*. Compositional Exploration of Combinatorial Scientific Models. *Applied Category Theory 2022* (2022).
- *S Wu*, **K S Brown**, *S Libkind*. Individual.jl: a Julia package for specifying and simulating individual-based models based on graph rewriting. *Applied Category Theory 2022* (2022).
- **K S Brown**, *T Hanks, E Patterson, J Fairbanks*. Computational category-theoretic graph rewriting. *International Conference on Graph Transformation* (2022).
- *M Mann, A Wilson, Y Zohar, L Stuntz, A Irfan*, **K S Brown**, *C Donovan, 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. (2022 - in preparation).
- **K S Brown**, *Y Maimaiti, J Voss, T Bligaard.* MCML: Combining physical constraints with experimental data for a multipurpose metageneralized gradient approximation. *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

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

TEACHING ASSISTANTSHIPS

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