KRISTOPHER S. BROWN

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https://krisb.org/root

HONORS

Topos Institute seminar speaker: *Combinatorial representation of scientific knowledge*	2022
JuliaCon speaker: *Declarative data transformation via graph transformation*	2022
SIAM Discrete Mathematics Speaker: *Extending McKay's Canonical Isomorph Algorithm to C-Sets*	2022
AMS Applied Category Theory Mathematics Research Community conference (selected participant)	2022
Catalysis and Modeling Symposium, Rungstedagaard DK: *Combinatorial scientific knowledge* (poster)	2022
ACT 2021 short talk: *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: 1st 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
- 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 2020
Advisors: Thomas Icard and Clark Barrett

- 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

Graduate Research Assistant, Stanford University 2016 - 2021
Advisor: Jens Norskøv

- 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 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. (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