

KRISTOPHER S. BROWN

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<https://krisb.org>

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

Postdoctoral researcher, University of Florida <i>Advisor: James Fairbanks</i>	2021
<ul style="list-style-type: none">Model-aware scientific computing, the double category of rewrite rules, regular logic automated theorem provingDPO rewriting + automorphism groups for C-Sets, generalized algebraic theories, sketches, polynomial functors	
Deep Learning / Logical Methods Research Intern, Google	2019-2020
<ul style="list-style-type: none">Higher order logic, proof search, model pruning, feature learning, custom hardwareLean 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
<ul style="list-style-type: none">Explainable AI, algebraic models of the explainability relationSatisfiability modulo theories, inductive datatypes, term rewriting, generalized algebraic theories	
Founder/CTO/Lead researcher, Modelyst LLC	2018-2021
<ul style="list-style-type: none">Declarative programming, API design, knowledge representation, software development	
Graduate Research Assistant, Stanford University <i>Advisor: Jens Norskov</i>	2016 - 2021
<ul style="list-style-type: none">Density functional theory, statistical learning under physics-informed constraints, surface chemistry	
Scientific Modeling Visiting Scholar, École Polytechnique Fédérale de Lausanne <i>Advisor: Jeremy Lutembacher</i>	2015 - 2016
<ul style="list-style-type: none">Catalysis synthesis, molecular dynamics, multi-scale modeling	

EDUCATION

PhD in Chemical Engineering Stanford University	2021
Bachelor of Engineering in Chemical Engineering	2015
Bachelor of Science in Chemistry Dartmouth College, <i>Magna cum laude</i>	2014

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