CHEMICAL ENGINEERING

DISTINGUISHED YOUNG SCHOLARS SERIES

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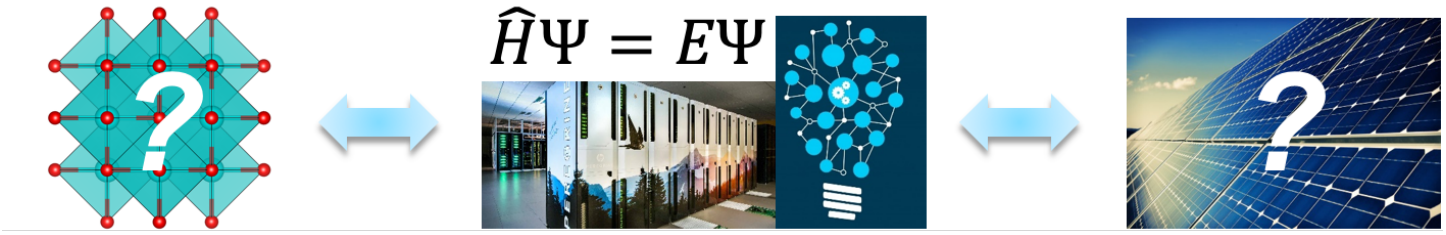
Predictive descriptors for the stability of new solid-state materials

ABSTRACT: Throughout history, emergent technologies have been enabled by the discovery and application of new or improved materials. Materials-driven societal advancement dates back at least to the Stone Age, when early hominins made use of naturally occurring rock in the form of tools to obtain food and build shelter. A transformational change occurred with the dawn of metallurgy and the observation that naturally occurring elements, copper and tin, could be mixed (alloyed) at high temperature, to form bronze, a much harder material than pure copper. Historically, these material discoveries have been predicated on some serendipitous accident where two compounds might have been accidentally mixed, and a new material emerges with some exciting property. Today, we strive to rationally design new materials with state-ofthe-art properties for some application of technological relevance. This challenge is made daunting by the vast diversity of chemistries, compositions, and structures that can be realized in the solid state, motivating the emergence of a field termed materials informatics. Following the lead of bio- and cheminformatics, the immense combinatorial challenge of solid-state materials design is addressed by marrying computational chemistry (predominantly density functional theory, DFT) and machine learning to rapidly identify and design new materials with emergent phenomena.



Fundamental to the viability of a new material for any application is that it is synthesizable and stable under the conditions of implementation. It is therefore paramount to the success of materials informatics approaches that when we identify a new material with promising properties, we can answer the question – are we going to be able to make it? This question was the driving force behind my Ph.D. thesis and will be addressed in my seminar talk through three vignettes – 1) understanding the role of structure in determining perovskite stability,[1] 2) machine-learning the effects of temperature on solid-state thermodynamics,[2] and 3) discovering new nitride semiconductors.[3] In each of these projects, we integrated experimental data, DFT calculations, and statistical learning to establish a framework for rapid predictions of thermodynamic stability. Importantly, the predictive models themselves are not the end-game, and we demonstrate the application of these models to accelerate the prediction of new materials including perovskite optoelectronics[4] and redox materials for ammonia synthesis.[5] Beyond model validation and demonstration, we also invert the learning problem to gain new physicochemical insights into the driving forces for materials stability by interrogation of the statistical models and development of chemical descriptors parsed from the DFT-calculated electronic structure. These projects form the basis for my recognition as the 2019 Max Peters Outstanding Graduate Student in the Department of Chemical & Biological Engineering at the University of Colorado Boulder.

BIOGRAPHY: Chris Bartel is a Chemical Engineer who uses computational materials science and statistical learning to understand the nature of solid-state materials and accelerate the advancement of emergent energy conversion and storage technologies. He obtained his B.S. in Chemical Engineering at Auburn University in 2014 and was awarded an NSF Graduate Research Fellowship that same year. He chose to use this fellowship at the University of Colorado Boulder (CU) where he obtained a Ph.D. in Chemical Engineering in 2018 under the direction of Professors Charles Musgrave and Al Weimer. While at CU, he co-authored 11 papers in journals including Nature Materials, Nature Communications, Science Advances, and JACS, and was named the 2018 Max Peters Outstanding Graduate in Chemical Engineering. Chris is currently a Postdoctoral Scholar in Prof. Gerbrand Ceder's group at UC-Berkeley and Lawrence Berkeley National Lab developing computational approaches for predictive solid-state synthesis.

LECTURE 4:00 – 5:00 (PAA) A118
Happy Hour in Benson Hall Lobby Following

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[1] C. Bartel et al., New tolerance factor to predict the stability of perovskite oxides and halides, Science Advances, 2019, 5, eaav0693

[2] C. Bartel et al., Physical descriptor for the Gibbs energy of inorganic crystalline solids and temperature-dependent materials chemistry, Nature communications, 2018, 9, 4168

[3] W. Sun, C. Bartel et al., A map of the inorganic ternary metal nitrides, Nature Materials, 2019, Accepted

[4] C. Bartel et al., Computational discovery of cesium chloride double perovskite optoelectronics, In Prep

[5] C. Bartel et al., High-throughput equilibrium analysis of active materials for solar thermochemical ammonia synthesis, 2019, ACS Applied Materials & Interfaces, Accepted & online