Accelerating the Discovery of Solid State Materials: From Traditional to Machine-Learning Approaches

Abstract: Traditional approaches to search for new solid state materials can involve systematic investigations (e.g., phase diagrams), serendipitous discoveries, or, for limited classes of compounds, rational strategies for manipulating building blocks. Answering the call of the Materials Genome Initiative, launched in 2011, to “discover, develop, and deploy new materials twice as fast,” we are applying high-throughput machine-learning methods to predict the structures of new compounds and optimize properties of materials. An ambitious goal is to classify structures of intermetallics, including unknown ones, solely on the basis of their compositions; these encompass binary AB compounds, ternary ABC compounds, Heusler and half-Heusler phases. In collaboration with Citrine Informatics, machine-learning approaches have also been used to search for unconventional candidates for thermoelectric materials.

Wednesday, February 21, 2018
Cram Conference Room, 3440 Mol Sci
4:30 p.m.

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