Text and Data Mining for Material Synthesis.

Predictive materials modeling can provide properties of real and virtual compounds and will be available on demand, thereby enabling rapid iteration time in materials design. However, the allure (and necessity) of accelerated discovery that motivates computational materials design is diminished by the prevalent heuristic approaches to materials synthesis and optimization. This delay in moving from promising materials concept to validation, optimization, and scale-up is a significant burden to commercialization. I will describe our work to extract information from peer reviewed academic literature across a range of inorganic solid state materials synthesis approaches. We have demonstrated not only the potential of the natural language processing (NLP) approach to assemble materials data from the literature, but we have also shown that one can develop hypotheses for what synthesis conditions drive a particular target material outcome using learning approaches.

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Tuesday, February 12 • 4 pm | Tech L211