



Inorganic Chemistry Seminar Series

Tuesday, October 9, 2018, 12:30 pm

Seaver Science Library, Room 150

SSC Auditorium next to the library

Professor Taylor Sparks

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The Promises Challenges, and Opportunities in Materials Informatics

More than seven years ago the White House announced the Materials Genome Initiative (MGI), asking computational materials scientists and experimentalists to find ways to “discover, develop, manufacture, and deploy materials twice as fast at a fraction of the cost.” High throughput computation and experiments have helped make progress but we are still far from the MGI goal. However, the emerging field of Materials Informatics offers a completely new and underutilized approach via machine learning and big data approaches to materials problems. In this talk, I’ll describe the promise, challenges, and opportunities that this new approach affords materials scientists. Specifically, I describe some of the new data-driven tools we are developing in our group as well as tools developed in conjunction with Citrine Informatics such as the “Materials Recommendation Engine.” These tools allow us to reduce the risk associated with exploring chemical whitespace for new, interesting materials and enable rapid material discovery. I’ll demonstrate the utility of machine learning with specific examples in thermoelectrics, superhard materials, crystal structure classification, and thermochemical data prediction.

Hosted by Professor Brent Melot

The scientific community is invited

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