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Machine Learning for Materials Hard and Soft

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Materials informatics for predicting materials properties

Abstract:

Over the last decade, we've seen the Materials Genome Initiative encourage 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 made some progress but we are still far from the goals of radically accelerated materials development. Materials Informatics offers a paradigm shift for materials property prediction by leveraging machine learning and data science approaches where patterns in data are exploited rather than mechanistic structure-property relationships. In this talk and tutorial, I'll describe the promise, challenges, and opportunities that this new approach affords materials scientists. Specifically, I will describe some of the ways materials informatics differs from traditional machine learning and what this means in terms of featurization, algorithm selection, data curation and partitioning, and extrapolation. I'll demonstrate the utility of machine learning for materials property prediction with specific examples in thermoelectrics, superhard materials, composite properties of formulations, and more.

Speaker Comment:

Dr. Sparks is an Associate Professor of Materials Science and Engineering at the University of Utah. He holds a BS in MSE from the UofU, MS in Materials from UCSB, and PhD in Applied Physics from Harvard University. He was a recipient of the NSF CAREER Award, the John G. Francis Prize for undergraduate mentoring, and was a speaker for TEDxSaltLakeCity. When he's not in the lab you can find him running his podcast “Materialism” or canyoneering with his 4 kids in southern Utah.