

# **Creating It from Bit: Designing Materials by Integrating Quantum Mechanics, Informatics and Computer Science**

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Powered by methodological breakthroughs and computing advances, electronic structure methods have today become an indispensable toolkit in the materials designer's arsenal. In this talk, I will discuss two emerging trends that holds the promise to continue to push the envelope in computational design of materials. The first trend is the development of robust software and data frameworks for the automatic generation, storage and analysis of materials data sets. The second is the advent of reliable central materials data repositories, such as the Materials Project, which provides the research community with efficient access to large quantities of property information that can be mined for trends or new materials. I will show how we have leveraged on these new tools to accelerate discovery and design in energy and structural materials as well as our efforts in contributing back to the community through further tool or data development. I will also provide my perspective on future challenges in high-throughput computational materials design.