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NCCR MARVEL Distinguished Lecture

The Materials Genome and the Transformation of Materials Science and Engineering

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Abstract: Novel materials design is a critical capability to address several urgent societal problems. But materials development is difficult and time consuming due to the lack of quantitative information on the properties, synthesis and behavior of novel materials. The confluence of high-throughput computing, big data, and data analytics is likely to transform the way materials development is done in the next decade. I will show several examples of the impact of the Materials Genome in developing new materials and nucleating new ideas in materials science. As one example, the Materials Project (www.materialsproject.com), has as its objective to use high-throughput first principles computations on an unparalleled scale to provide basic materials property data on all known and many potential new inorganic compounds, thereby accelerating the search for new materials.
I believe it is possible to within ten years determine most of the intrinsic properties of all known compounds, thereby generating the Materials Genome. Finally, I will also describe how this will displace the bottleneck of materials development towards materials synthesis, and show some initial work we have started to develop a quantitative theory of materials synthesis, so that materials development can be accelerated all the way from design to device integration.