

Revolutionizing Materials Innovation through the Materials Genome Project.

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Novel materials design has become a critical capability to address several urgent societal problems. The Materials Genome Project, originally started at MIT (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. Such information can then be datamined to obtain structure-chemistry-property relations, and to develop knowledge based predictive methods.

I will show successful examples of high-throughput calculations in the field of lithium batteries, and show several new materials that have been discovered. I will discuss the public release version of the Materials Genome project, which is making large quantities of computed data freely available to the materials community.