The Materials Genome: Overview, Success Stories and Outlook

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The Materials Genome Initiative (MGI) aims to develop an infrastructure to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost. The exponential growth of computer-processing power, combined with the laws of physics expressed through quantum mechanics, has made it possible to design new materials from scratch using supercomputers and first-principle physics. Concurrently, high-throughput (HT) synthesis and measurement experimental techniques are being developed which enable rapid validation and benchmarking.

This presentation will give an overview of goals of the Initiative and exemplify the materials genomic approach by describing singular efforts that have used it to optimize and discover novel materials from computations and experimental efforts as well as the data and tools emerging from these efforts. Among these examples are innovative novel materials and electrolytes in energy storage and energy production, the broad searchable dissemination of phase stability, solid-aqueous stability, elastic properties and electronic structure information across structure and chemical space. Finally it will be recognized that the information age has finally reached the materials science field and that the infrastructure tools being prevalently utilized in other fields should be leveraged for accelerating materials research.