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Mapping the Materials Genome through Combinatorial Informatics

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The recently announced White House Materials Genome Initiative provides an exciting challenge to the materials science community. To meet that challenge one needs to address a critical question, namely *what* is the materials genome? Some guide on how to the answer this question can be gained by recognizing that a "gene" is a carrier of information. In the biological sciences, discovering how to manipulate these genes has generated exciting discoveries in fundamental molecular biology as well as significant advances in biotechnology. Scaling that up to molecular, cellular length scales and beyond, has spawned from genomics, fields such as proteomics, metabolomics and essentially systems biology. The "omics" approach requires that one needs to discover and track these "carriers of information" and then correlate that information to predict behavior. A similar challenge lies in materials science, where there is a diverse array of modalities of materials "discovery" ranging from new materials chemistries and molecular arrangements with novel properties, to the development and design of new micro- and mesoscale structures. Hence to meaningfully adapt the spirit of "genomics" style research in materials science, we need to first identify and map the "genes" across different materials science applications On the experimental side, combinatorial experiments have opened a new approach to generate data in a high throughput manner, but without a clear way to link that to models, the full value of that data is not realized. Hence along with experimental and computational materials science, we need to add a "third leg" to our toolkit to make the "Materials Genome" a reality, the science of Materials Informatics. In this presentation we provide an overview of how information science coupled to materials science can in fact achieve the goal of mapping the "Materials Genome".