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High-throughput computational methods for the design of industrial materials

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High-throughput computational materials science methods are being used to aid the prediction, synthesis and characterization of promising candidate materials for many industrial requirements. These methods are producing enormous amounts of derived data that require storage and analysis. Data mining methods provide exploration of this multidimensional property space, at a previously unavailable level of detail, and can rapidly estimate physical properties that are difficult to measure using experimental methods. Given these vast resources of structure and property data it is possible to extract trends on the structure of materials and their properties and use these results at the materials selection and design stages. These informatics approaches, coupled with ab initio quantum mechanics methodologies, provide many of the tools needed to guide materials selection via computational experiments. Examples for the application of these methods coupled with the use of experiments for the design of materials for industrial applications will be presented.