## **Materials Discovery from First Principles Modeling**

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## **Summary**

Large-scale screening of novel materials is at the heart of the Materials Genome Project launched by the Obama administration in the US. Europe is the world leader in the underlying methods and computer software, and is gearing towards mobilization of the relevant research communities. The topics include systematic search for materials with desired functionalities, for example in engineering alloys, in catalysis, and electrochemical applications.