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**Preliminary results in data mining for materials**[1] DA GAO, YOUSEF SAAD, University of Minnesota at Twin Cities, JAMES CHELIKOWSKY, University of Texas at Austin — In recent years, materials scientists have started exploiting data mining techniques, i.e., methods for extracting meaningful information and patterns from data, for the discovery and design of materials. One of the grand challenges in this methodology is to establish correlations and intrinsic features in materials database in order to facilitate the extraction of useful information that can be exploited to discover new hypothetical materials. Using an atomic properties database of 110 elements, obtained from quantum mechanical calculations and several macroscopic properties database of binary compounds, we explored several sample data mining techniques to study the correlations among them with the goal of predicting macroscopic properties from knowledge of the atomic constituents. In this talk, preliminary results of such efforts will be presented to demonstrate how simple data mining can be applied in materials science and what they can achieve. These preliminary results indicate a good potential for data mining applications in materials science.

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