[L13] Material Informatics: Statistical Modeling in Material Sciences

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Materials informatics is engaged with the application of informatics principles to materials science in order to assist in the discovery and development of new materials. Central to the field is the application of data mining techniques and in particular machine learning approaches, often referred to as QSAR modeling, to derive predictive models for a variety of materials-related "activities". Such models can accelerate the development of new materials with favorable properties and provide insight into the factors governing these properties. Here we provide a comparison between medicinal chemistry / drug design and materials-related QSAR modeling and highlight the importance of developing new, materials-specific descriptors. We survey some of the most recent QSAR models developed in materials science with focus on energetic materials and on solar cells. Finally we present new examples of chemoinformatic analyses of solar cells libraries produced from metal oxides using combinatorial material synthesis. Different analyses lead to interesting physical insights as well as to the design of new cells with potentially improved photovoltaic parameters.