

Materials Discovery through Machine Learning: Experimental Validation and Interpretable Models

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Machine learning algorithms have been applied successfully in many areas of materials chemistry. An ongoing challenge is make accurate predictions of the crystal structures of inorganic solids, their site preferences, and their physical properties. We have previously developed machine learning models to predict structures within the large family of intermetallic compounds known as Heusler compounds (used as thermoelectric materials, ferromagnets, magnetocaloric materials, and catalysts), followed by experimental validation. Nevertheless, skeptics rightfully criticize many of these models as being too “black box,” with little chemical insight and explainability. We demonstrate our efforts to generate more interpretable machine learning models, using the structures of binary rare-earth intermetallics RX as an example, to illustrate that it is possible to gain insight and practical guidance to prepare new materials.

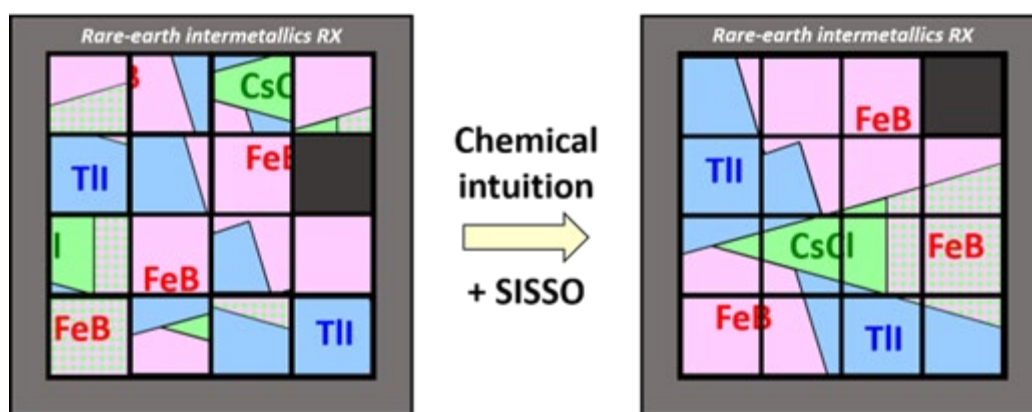


Figure 1