EXPERIMENTAL DATABASE DEVELOPMENT FOR DATA-DRIVEN MATERIALS DESIGN

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We will describe the program at IIT to develop experimental thermodynamic data on the enthalpies of formation of intermetallic compounds, including B2 and $L2_1$ structures. The data are incorporated into a database that can be accessed by computer for data mining and machine learning based materials design. These data are compared and benchmarked with first-principles results in multiple Materials Genome databases. As an example we will discuss the application of machine learning to elucidate a relationship between the properties of B2 binary compounds and $L2_1$ ternary compounds with the aim of developing rules that can be used to predict the stability of $L2_1$ ternary compounds.