

Thermodynamic and physical databases and their combinatorial applications

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A database for retrieval of thermodynamic and physical properties of solids and fluids has been constructed at CeSMEC through the International Materials Institute project. The database is a result of data collection from multiple sources and new experiments; the new experiments were particularly carried out for MAX carbide/nitride phases and light-element hydrides. Additionally several phases have been modeled using ab-initio/MD method. The database can help search for regularity of physical property trends among over 3000 solids and help recognize the possible novel properties. Using this approach several interesting correlation of properties within classes of solids have been recognized.