Thermodynamic database development based on ab initio calculations: challenges and opportunities

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All the databases available at GTT-Technologies currently rely solely on experimental input. In the framework of the Materials Genome Initiative several open *ab initio* databases have been made available. These contain results of several tens to hundreds of thousands quantum mechanical calculations at 0K. It will be discussed how these can be used by database developers as well as by normal FactSage users. Challenges relating to accuracy and interoperability are discussed as well as opportunities for the design of new materials and processes.