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Materials Design based on Predictive Ab Initio Thermodynamics

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A key requirement in developing predictive multi-scale modeling is the availability of accurate computational tools determining energies not only at T = 0 K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities such as heat capacity, thermal expansion coefficients, and elastic constants with an accuracy that matches and often even rivals available experimental data. In the talk a brief overview of the fundamentals and recent developments of combining modern fully parameter-free ab initio methods with thermodynamic concepts will be given with special emphasize on structural materials. The flexibility and the predictive power of these approaches and the impact they can have in developing new strategies in materials design will be discussed e.g. for modern high strength TWIP/TRIP steels, for understanding failure mechanisms such as hydrogen embrittlement, or for identifying chemical trends in the performance of light weight metallic alloys. Work has been done in collaboration with Fritz Kormann, Blazej Grabowski, and Tilmann Hickel.