



INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

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DFT in relation to Calphad assessments

DFT results for zero Kelvin energies and, with assumptions, for finite temperature Gibbs energies for ordered compounds, have become an important supplement to experimental results in Calphad-based phase diagram calculations.

Some limitations, from a Calphad viewpoint, in a wholly physics-based approach for making the best use of the DFT results in carrying out calculations of multicomponent phase diagrams will be discussed.

Finally, some possible alternative ways in which DFT results might be better used by Calphaders in calculating finite temperature Gibbs energies of partially ordered and disordered phases will be suggested.