An ab initio based determination of phase stabilities at finite temperatures requires the explicit description of various kinds of excitation mechanisms. For iron-based materials the magnetic entropy contribution is typically the most challenging part. If described independently, the Heisenberg model and its extensions can be used as an elegant way for coupling ground-state ab initio calculations with concepts of many-body theory to fully simulate the temperature dependence. In many materials, however, also the coupling of magnetism to lattice vibrations has a noticeable impact on phase stabilities. We have developed various techniques to meet this challenge, including fixed spin-moment approaches [1], spin-space averaging techniques [2] and the itinerant coherent-potential approximation. The capability of these methods and consequences for thermodynamic properties will be discussed for iron as well as modern magnetocaloric materials.
