Challenges in Automated High-Throughput Ab Initio Thermodynamics of Magnetic High-Entropy Alloys

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We investigate the potential and difficulties associated with high-throughput ab initio computation of magnetic high-entropy alloys. Given the often highly automated nature of high-throughput projects [1,2,3], the presence of magnetism can cause workflow-disrupting problems, such as convergence of a calculation into a wrong magnetic state and the presence of multiple magnetic phases in the energy versus volume data used in equation of state fitting [4]. We develop and evaluate different strategies that can be used to overcome these problems, in order to make the results of an automated high-throughput project involving magnetic high-entropy alloys as reliable as possible. A group of 21 magnetic alloys based on the well-known CoCrFeMnNi high-entropy alloy in six different phases is used as a model project to test our strategies.

References