MM 43: HV Hickel

Time: Wednesday 18:30–19:00 Location: H 0107

Invited Talk MM 43.1 Wed 18:30 H 0107

Advancing ab initio methods to finite temperatures for applications in materials design — •Tilmann Hickel, Alexey Dick, Fritz Körmann, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The performance of materials such as steels, their strength and formability, are based on an impressive variety of competing mechanisms on the atomic/microscopic scale, ranging from point defects up to mechanical twinning or structural phase transformations. Whereas many of these mechanisms are currently described with empirical concepts and experimental data, it becomes more and more apparent that further improvement of materials needs to be based on fundamental theories. Recent progress in the field of ab initio methods now makes the exploration of chemical trends, the determination of parameters for phenomenological models and the identification of new routes for the optimization of material properties feasible. A major challenge in applying these methods to a true materials design is, however, the inclusion of temperature-driven effects on the desired properties. This talk will, therefore, address the large range of computational tools we have developed in order to improve the capability and accuracy of first-principles methods in determining free energies. These combine electronic, vibrational, and in particular magnetic excitations, but also structural defects in an integrated approach. Based on these simulation tools, we are able to successfully predict with a hitherto not achievable accuracy mechanical and thermodynamic properties of metals, such as high-strength steels and magnetic shape-memory alloys.