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Mo in steels – An ab initio perspective

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The role of Mo in steels as an alloying element is manifold and often key to obtain excellent mechanical properties in the final product. In many cases, ab initio calculations on the atomic level can give valuable insights into the mechanisms at work, which then provides direct guidelines for alloy design and optimization. Molybdenum is present in steels in solid solution and in various precipitated phases, leading to a diverse set of influences in the process-microstructure-property relationships. In dissolved state, Mo acts as a ferrite stabilizer and as solid solution strengthener, which can be quantified with ab initio methods in dependence on the specific composition and temperature. Furthermore, dissolved Mo binds to grain boundaries and by that affects the strength of grain boundaries and their mobility, which in turn slows down kinetics of grain growth, recrystallization, and phase transformation. For predictive modelling of these effects, accurate interaction energies are needed, which can only be obtained from ab initio calculations. In the form of precipitates, Mo-containing phases may contribute to precipitation strengthening or Hydrogen trapping. Ab initio calculation of precipitates and their interfaces with the Fe matrix helps to understand the effect of Mo in the relevant mechanism and allows to derive material design guidelines.
In this talk, a short overview on the available ab initio approaches to study Mo effects in steels, how they link to higher scales, and some examples are provided.

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