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Strain-induced metal-hydrogen interactions across the first transition series – An *ab initio* study of hydrogen embrittlement JOHANN VON PEZOLD, UGUR AYDIN, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH — The attractive interaction between hydrogen and distorted regions of the host matrix underlies all the currently discussed mechanisms of hydrogen-induced embrittlement of metals, such as hydrogen enhanced local plasticity (HELP), hydrogen enhanced decohesion (HEDE) and stress-induced hydride formation. In this study we investigate these interactions systematically by determining heat of solutions, H-H binding energies within the metal matrix, as well as phase diagrams as a function of the lattice strain and the H chemical potential across the first transition series (3d elements) using Density Functional Theory (DFT) calculations. The results will be interpreted in terms of the likely embrittlement mechanisms of these metals.

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