Abstract Submitted
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Ab initio **study of Fe-rich Fe-Cu alloys**[1] DAVID REITH, RAIMUND PODLOUCKY, Department of Physical Chemistry, University of Vienna — Cu precipitates are important for strengthening steel. Our *ab initio* study aims to model the thermodynamical stability of Cu precipitations in α-Fe. As a first step, a density functional theory (DFT) supercell approach is applied to study $Fe_{1-x}Cu_x$ alloys at small concentrations x. From the DFT total energies a strongly nonbonding substitutional energy $E_{subs} \approx 0.7eV$ is derived, which is significantly larger than results of a previous DFT study [1]. Based on force constants derived by the same DFT approach the temperature dependent vibrational free energy is determined [2]. In particular at higher temperatures the vibrational entropy significantly reduces the formation energy. Finally, by using the entropy of mixing the dilute Fe-Cu alloy becomes stabilized. The derived phase diagram is in good agreement with experimental data [3]. According to our analysis, the vibrational free energy is very important for a correct modelling of the phase stability of Fe-rich Fe-Cu alloys. [1] C. Domain et al., PRB, 65, 024103 (2001) [2] D. Alfè et al, PRB, 65, 045123 (2001) [3] B. Predel, Landolt-Börnstein - IV, Springer, Volume 5d (1994)

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