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Electronic correlations determine the phase stability of iron up to the melting temperature I. LEONOV, TPIII, Center for Electr. Correl. & Magnetism, Univ. Augsburg, Germany, A.I. POTERYAEV, Inst.of Metal Physics, Yekaterinburg, Russia, Y.N. GORNOSTYREV, Inst.of Quantum Materials Science, Yekaterinburg, Russia, A.I. LICHTENSTEIN, Inst.of Theor. Phys., Univ. Hamburg, Germany, M.I. KATSNELSON, Inst.for Molecules & Materials, Univ. Nijmegen, Netherlands, V.I. ANISIMOV, Inst.of Metal Physics, Yekaterinburg, Russia, D. VOLLHARDT, TPIII, Center for Electr. Correl. & Magnetism, Univ. Augsburg, Germany — We present results of a theoretical investigation of the phase stability and phonon spectra of paramagnetic iron at high temperatures obtained within the LDA+DMFT scheme. This approach combines *ab initio* band-structure methods with dynamical mean-field theory for correlated electrons and allows one to calculate correlation-induced structural transformations and their temperature evolution [1]. We find that electronic correlations determine the structural phase stability of iron up to the melting temperature. Several peculiarities, including a pronounced softening of the [110] transverse T_1 mode and a dynamical instability of the *bcc* lattice in harmonic approximation, are identified. We relate these features to the α-to-γ and γ-to-δ phase transformations in iron. The high temperature *bcc* phase of iron is found to be highly *anharmonic* and appears to be stabilized by the lattice entropy. This indicates the importance of both electronic correlations and lattice anharmonic effects for a correct description of the high-temperature δ phase of iron. [1] I.Leonov, A.I.Poteryaev, V.I.Anisimov, D.Vollhardt, PRL **106**, 106405 (2011); PRB **85**, 020401 (2012).

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