Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Large effects of subtle electronic correlations on the energetics of vacancies in alpha-Fe PASCAL DELANGE, Centre de Physique Thorique, Ecole Polytechnique, France, THOMAS AYRAL, Institut de Physique Thorique, CEA, France, SERGEI SIMAK, Department of Physics, Chemistry and Biology, Linkping University, Sweden, MICHEL FERRERO, Centre de Physique Thorique, Ecole Polytechnique, France, OLIVIER PARCOLLET, Institut de Physique Thorique, CEA, France, SILKE BIERMANN, LEONID POUROVSKII, Centre de Physique Thorique, Ecole Polytechnique, France — We apply an ab initio theoretical framework combining the density functional and dynamical mean field theories (DFT+DMFT) to study the effect of electronic Coulomb correlations on the vacancy formation energy if paramagnetic alphe-Fe. The calculated value using different implementations of DFT are compared, and we show that the formation energy is substantially lower than in standard density-functional calculations and in excellent agreement with experiment. The reduction is caused by an enhancement of electronic correlations at the nearest neighbors of the vacancy. This effect is explained by subtle changes in the corresponding spectral function of the d-electrons, and is linked to the reduction of coordination on these atoms. The local lattice relaxations around the vacancy are substantially increased by many-body effects, and must be consistently calculated within DFT+DMFT to obtain a consistent vacancy formation energy.

Pascal Delange
Centre de Physique Thorique, Ecole Polytechnique, France

Date submitted: 14 Nov 2016 Electronic form version 1.4