DFT and Monte Carlo study of the magnetization versus temperature dependence of the $Zr(Fe_{1-x}Co_x)_2$ system

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Self-consistent field calculations for the $Zr(Fe_{1-x}Co_x)_2$ system were performed using the Korringa-Kohn-Rostoker method (SPR-KRR implementation). Following that the exchange integrals were obtained from the potential. KKR has been also used to obtain magnetic moments, out of which, using the Uppsala atomistic spin dynamics (UppASD), magnetization and susceptibility dependences on temperature were calculated for a whole range of concentrations. Utilised code allows for Monte Carlo simulations of the Heisenberg Hamiltonian. The lattice constants were optimized using the FPLO code. For both the SPR-KKR and FPLO codes the calculations were done using the GGA. The chemical disorder was treated using the coherent potential approximation (CPA).

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