## VIENNA COMPUTATIONAL MATERIALS LABORATORY

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## Strongly correlated alloys and dynamical mean field theory

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For the physical description of the transition metal alloys both strong interactions and disorder have to be accounted for, and hence it is highly desirable to have a method that can treat, on equal footing, disorder and partially filled strongly interacting d states of transition metals. Combination of two techniques, the coherent potential approximation for disorder and the dynamical mean-field theory for correlated electrons which share an effective medium interpretation of the system of interest, allows one to investigate different physical properties of real alloys. The magnetic properties of Fe-Ni alloy and structural phase transition in Fe-Mn alloy are investigated as a function of temperature and concentration. Comparison of the coherent potential approximation and dynamical mean-field theory calculations agrees well with experimental data.