Electronic structure calculations for correlated materials

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Materials with strong Coulomb correlations are challenges for electronic structure calculations. During the last years new methods for their description have been developed. The combination of dynamical mean field techniques with density functional theory allows for the calculation of electronic properties of materials from first principles, taking into account the effect of arbitrarily strong Coulomb interactions.

We will give an introduction to dynamical mean field theory and its use within electronic structure calculations. For illustration, results on transition metal compounds and iron oxypnictides will be described. Finally, we will close by discussing the current limitations and perspectives of how to go beyond current LDA+DMFT techniques.