Non-local Correlation Effects in Crystals

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Dynamical mean field theory (DMFT)in combination with the first-principle LDA-scheme (LDA+DMFT) is an optimal starting point to go beyond static density functional approximation and include effects of spin and orbital fluctuations in the local self-energy correction.
In order to go beyond the local approximation we formulate a general multiorbital dual-fermions scheme that include a full vertex of impurity problem as a effective interactions in non-local action.
The possibilities to includes the interaction vertex in the DMFT calculations within the continuous time QMC-scheme as well as k-dependence approximation beyond DMFT will be discussed.