Realistic Modeling of Materials with Strong Electronic Correlations

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Abstract:
Several characteristic properties of materials with strong electronic correlations will be described and microscopically explained within LDA+DMFT, a combination of ab initio band structure methods and the dynamical mean-field theory [1]. In particular, I will discuss

- the strong spectral transfer in (Sr,Ca)VO_3 leading to a characteristic three-peak structure of the spectral function [2],
- the correlated band structure of the charge-transfer insulator NiO [3],
- the correlation-induced structural relaxation in the paramagnetic Jahn-Teller system $KCuF_3$ [4],
- a generic mechanism explaining the appearance of kinks in the effective dispersion of correlated electron materials [5].

References:
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