Realistic Modelling of Materials with Strong Electronic Correlations

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Various electronic and structural properties of materials with strongly correlated electrons will be discussed and explained which were computed within LDA+DMFT, a combination of ab initio band structure methods and the dynamical mean-field theory. In particular, I will present recent results on (i) the correlated band structure of the charge-transfer insulator NiO, (ii) the magnetic moment collapse-driven Mott transition in MnO, (iii) the correlation-induced structural relaxation in the paramagnetic Jahn-Teller system $KCuF_3$, and (iv) kinks in the effective dispersion of correlated electron materials such as $SrVO_3$.

9.7 cm

13.4 cm

Subject category :

1. Strongly Correlated Electrons and High Temperature Superconductivity

Presentation mode :
invited

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