

## Cluster perturbation theory for transition metal oxides

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We propose a many-body method for band-structure calculations for strongly correlated electron systems and apply it to transition metal oxides with NiO as an example. The method may be viewed as an application of cluster perturbation theory to a realistic model of a transition metal oxide whereby the Coulomb interaction within the transition metal d-shells is treated by exact diagonalization and the hopping between different atoms (as described by an LCAO-parameterization of an LDA bandstructure) is treated by cluster perturbation theory. We find good agreement between the calculated single-particle spectrum and angle resolved photoemission experiments in NiO.

9.7 cm

13.4 cm

### **Subject category :**

7. Computations of Electronic Structures

### **Presentation mode :**

oral

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