JUM@P '11: Joint Users' Meeting at PSI 2011



Contribution ID: 121

Type: Talk

Cluster-Based Numerical Simulations for X-ray Spectroscopies in Correlated Materials

Friday, 16 September 2011 09:10 (30 minutes)

In this talk I will present an efficient scheme for calculating various x-ray spectroscopies using a combination of cluster exact diagonalization and ab-initio codes. These multi-orbital calculations include multiplet, charge-transfer, hybridization, and core-hole interactions all on the same footing, and are able to reproduce fairly well representative spectra on several transition metal oxide materials. Focus will be placed on x-ray absorption, resonant inelastic light scattering (RIXS), and the dielectric response S(q,w) of Fe- and Cu-based materials. As an example, the differences between RIXS and S(q,w) will be highlighted, with a specific focus on low energy magnon excitations.

Please specify the session

RIXS

Please specify poster or talk

Talk

Primary author: DEVEREAUX, Thomas P (Stanford University)Presenter: DEVEREAUX, Thomas P (Stanford University)Session Classification: Resonant Inelastic and Elastic X-ray Scattering

Track Classification: Resonant Inelastic and Elastix X-ray Scattering