MAR05-2004-002116

Abstract for an Invited Paper for the MAR05 Meeting of the American Physical Society

Surface versus Bulk Coulomb Correlations in Photoemission Spectra of $SrVO_3$ and $CaVO_3$

ANSGAR LIEBSCH, Institute for Solid State Research, Research Center Jülich, 52425 Jülich, Germany

Photoemission is a key spectroscopy for the study of the electronic properties of strongly correlated materials. Spectra taken at low photon energies tend to show significantly stronger correlation features than high energy spectra, suggesting that Coulomb correlations near the surface are enhanced compared to the bulk. To investigate these differences the dynamical mean field theory is used in combination with the multi-orbital Quantum Monte Carlo method in order to evaluate quasiparticle spectra which can be compared directly with photoemission distributions. In the case of perovskites like SrVO₃ and CaVO₃, the planar character of the partially filled t_{2g} bands and the reduced coordination of surface atoms give rise to an effective narrowing of the surface density of states. As a result, the quasi-particle weight near E_F is reduced and the amplitude of the lower and upper Hubbard bands is enhanced, in agreement with experiment [1]. Preliminary results for VO₂ surfaces will also be discussed. [1] A. Liebsch, Phys. Rev. Lett. **90**, 96401 (2003); Eur. Phys. J. B **32**, 477 (2003).