

Seminar Schedule

Prof. Ansgar Liebsch

(Research Center Juelich, Germany)

Date: Feb. 3 (Mon.) 14:00 ~

Room: Seminar room, 2nd floor, prefab bldg

“ Quasi-particle spectra of perovskites:
Enhanced Coulomb correlations at surfaces ”

Abstract

Photoemission spectra of the perovskites Sr,CaVO₃ (Sekiyama et al, Maiti et al), SrRuO₃ (Fujioka et al) and La,CaVO₃ (Maiti et al) indicate that Coulomb correlations are more pronounced at the surface than in the bulk. To investigate this effect we use the Dynamical Mean Field Theory and multi-orbital Quantum Monte Carlo method to evaluate the quasi-particle self-energy, starting from a realistic layer-dependent density of states. The reduced coordination number of surface atoms causes a significant narrowing of the surface density of those subbands which hybridize in planes normal to the surface, leading to stronger surface correlations than in the bulk, in agreement with experiment. We also discuss the possibility of a separate surface metal-insulator transition in La,CaVO₃ and of an orbital-selective metal-insulator transition in Sr,Ca₂RuO₄.

連絡先 :
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