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Core-level Photoemission Study for Cuprates with a Dynamical Mean-Field Approach Considering Realistic Crystal Structure ATSUSHI HARIKI, TAKAYUKI UOZUMI, Department of Mathematical Sciences, Graduate School of Engineering, Osaka Prefecture University — Recently, remarkable experimental progress reveals some characteristic spectral features in the $2p_{3/2}$main line of Cu 2p core-level X-ray photoemission spectra (XPS)[1]. The structures show strong material dependence and drastic changes for electron or hole doping. Van Veenendaal et al., pointed out that the main line shape is strongly affected by the so-called nonlocal screening which is accompanied by a formation of a Zhang-Rice singlet (ZRS) in the XPS final state[2]. On the other hand, Taguchi et al., shows these features are reproduced by introducing an phenomenological extended impurity model[1]. We consider that this topic on 2pXPS of cuprates still remain controversial. In this study, we propose another approach based on the dynamical mean field theory(DMFT) considering the realistic crystal structure. Many-particle effects including the ZRS is appropriately embedded in the hybridization function of a single impurity Anderson model through the DMFT self-consistent cycle. Our approach reproduces experimental results and shows that the Cu $2p_{3/2}$ main line is closely related with the quasi-particle structure near the Fermi energy.

[1] M.Taguchi et al.,Phy.Rev.Lett.95(2005)177002 [2] M.A.van Veenendaal and G.A.Swatzky Phys.Rev.Let70(1993)2459

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