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Dynamical Mean-Field Approach to Core-Level Spectroscopy of NiO and its Insulating Character ATSUSHI HARIKI, TAKAYUKI UOZUMI, Department of Mathematical Sciences, Graduate School of Engineering, Osaka Prefecture University — Core-level X-ray photoemission spectroscopy (XPS) is a powerful tool to investigate electronic structure of strongly correlated electron systems, such as $3d$ transition metal oxides. In the Ni$2p$XPS of NiO, a characteristic double-peak structure has been observed in the $2p_{3/2}$ main line, [1] which is considered to be related with the insulating property of NiO. However, previous studies contradicts each other for the spectral assignment of the double peaks. [1,2] Thus, a further investigation about the microscopic origin of the double peaks from a different viewpoint is required. In this talk, we investigate the double-peak structure using a framework, which was recently proposed in our research group, based on the dynamical mean-field theory (DMFT) under realistic crystal structure. We show that, besides the so-called nonlocal screening indicated by Van Veenendaal et al., [2] the antiferromagnetic ordering of NiO plays a crucial role of the formation of the double peaks. We conclude from the spectral analysis that the lowest first ionization state of NiO is given by an electron removal from the Zhang-Rice doublet band.

[1] M. Taguchi et al.: Phys. Rev. Lett. **100** (2008) 206401.
[2] M. A. van Veenendaal and G. A. Sawatzky: Phys. Rev. Lett. **70** (1993) 2459.

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