Non-local core-hole screening in the O 1s XPS of low-dimensional cuprates

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Core-level XPS is well accepted as a powerful tool to investigate the electronic states of highly-correlated electron systems, such as cuprates and vanadates. Through the analysis of the XPS using cation core-levels, we can estimate the physical paramaters which characterize the electroni structure of the valence electron system. Moreover, in a previous paper[1], we demostrated that the detailed line shape of the leading edge in the Cu 2p XPS of cuprates provide direct information on the electronic structure near the Fermi energy. In contrast, the XPS using anion core-levels has not been used to investigate the electronic states directly. For instance, the O 1s XPS has often been used to check the surface contamination. However, the recent HAXPES experiments seem to indicate that the O 1s XPS also provides direct information on the bulk electronic states. In the present study, we extend our theory to the O 1s XPS of low-dimensional cuprates to study what information can be extracted from the O 1s XPS.

Figure 1 shows the O 1s XPS for electron-doped, undoped and hole-doped Cu_6O_{12} cluster models. In each case, the O 1s main structure is accompanied by a weak satellite about 10eV below. The line shape of the satellite depends on the doping. In a configuration-interaction picture, the main peak can be assigined to the $1s^1p^6$ electron configuration, while the satellie the $1s^1p^5C$ with C being an electron in the conduction band. In the undoped or electron-doped case, C resides in the upper Hubbard band (UHB). In the hole-doped case, C can reside in the Zhang-Rice singlet band as well as on the UHB. Thus the O 1s XPS observes the unoccupied states just above the Fermi energy.

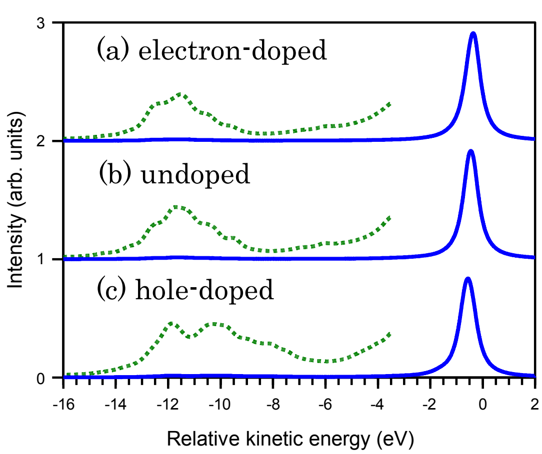

Fig.1: O 1s XPS for electron-doped, undoped and hole-doped Cu_6O_{12} clusters. The spectrum in the satellite region is enlarged 30 times.

[1] K. Okada and A. Kotani, J. Phys. Soc. Jpn., 74, 653 (2005)