1C/2002S2-002, 2005S2-002

Systematic tight-binding analysis of ARPES spectra of transition-metal oxides

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Introduction

3*d* transition-metal (TM) oxides have attracted a lot of interest in these decades because of their intriguing physical properties such as metal-insulator transition, colossal magnetoresistance, and ordering of spin, charge, and orbitals [1]. In order to understand the properties of these systems, the determination of band dispersions by angle-resolved photoemission spectroscopy (ARPES) has been highly required. Recent technological development has made it possible to grow high-quality single-crystal thin films using the pulsed laser deposition method, and a setup has been developed for their film growth followed by *in-situ* photoemission measurements [2]. We have analyzed the ARPES data recently accumulated for various 3*d* TM oxides of perovskite structures [$SrTiO_3$ [3], $SrVO_3$ [4], $La_{1-x}Sr_xMnO_3$ [5], $Pr_{1-x}Ca_xMnO_3$ [6] and $La_{1-x}Sr_xFeO_3$ [7]] by a nearest-neighbor tight-binding (TB) model [8], and obtained a systematic variation of the electronic structure of the periodic lattice of 3*d* TM atoms. We compared the obtained parameter values with those obtained by fitting the local-density-approximation (LDA) band structure to the same TB model and those from configuration-interaction (CI) cluster-model theory.

Experiment and calculation

All the ARPES measurements presented in this report were performed using a photoemission spectroscopy system combined with a laser molecular beam epitaxy chamber at beamline BL-1C of the Photon Factory, KEK [2]. Details of the experimental conditions for the respective materials were described in Refs. [3-7]. The LDA band-structure calculations were performed using the linearized augmented plane wave method implemented in the WIEN2K package. We assumed a cubic paramagnetic state. In the CI cluster-model calculations [1], we considered a TMO_6 octahedral cluster.

Results and Discussion

Figure 1 shows the comparison of the variation of $|(pd\sigma)|$ [panel (a)] and ε_d (the effective energy level of TM 3*d* orbitals relative to that of O 2*p* orbitals) [panel (b)] in ARPES, LDA, and CI theory. As seen from Fig. 1 (a), the values of $(pd\sigma)$ are similar in all the three estimates, meaning that as for the strength of *p*-*d* hybridization the values from the local CI cluster-model theory can describe the band structures of periodic systems. The behaviors of ε_d are not similar among the three estimates as shown in Fig. 1. The values of ε_d in the LDA calculation are a little smaller than those in ARPES due to the tendency of LDA to underestimate the binding energies of the O 2*p* bands. The values of ε_d from CI theory are much smaller than those from ARPES except for the case of Ti. We attribute this difference to the effective nature of the "*d* bands"

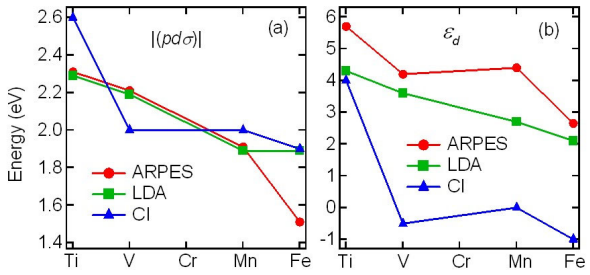

Fig. 1: Transition-metal dependences of the *p*-*d* transfer integral $|(pd\sigma)|$ (a) and the effective *d* level ε_d relative to O 2*p* (b) deduced from ARPES, LDA calculation, and CI theory.

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