Electronic structure of the Mott–Hubbard compound $SrVO_3$ studied by resonant photoemission spectroscopy

Gunwoo Kim[a], Chihiro Inoue[a], Masaaki Higashino[a], Daiki Ootsuki[b], Hiroshi Kumigashira[c], Shigeki Miyasaka[d], and Teppei Yoshida[a]

[a] *Graduate School of Human and Environmental Studies, Kyoto University, Sakyo-ku, Kyoto, Kyoto, 606-8501, Japan*
[b]*Research Institute for Interdisciplinary Science, Okayama University, 3-1-1, Tsushima-naka, Tsushima, Kita-ku, Okayama 700-8530, Japan*
[c]*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan*
[d]*Department of Material Science, Graduate School of Science, University of Hyogo, Ako, Hyogo 678-1297, Japan*

Keywords: Vanadium Oxides, Resonant photoemission, Mott-Hubbard system.

$SrVO_3$ (SVO) is a Mott–Hubbard correlated metal in which strong on-site Coulomb repulsion U_{dd} splits the V $3d$ spectral weight into an itinerant coherent (quasiparticle) part and a localized incoherent (Hubbard-band) part. To elucidate the effects of strong electron correlations in many-electron systems, it is essential to investigate the coherent and incoherent components, which have been studied both experimentally [1] and theoretically [2]. In this context, Mossanek *et al.* [3] studied the influence of O $2p$–V $3d$ hybridization on the coherent and incoherent parts; their cluster-model calculations indicated that an O $2p$ contribution to the incoherent feature is crucial to reproduce photoemission spectra [4].

In this work, we investigated the electronic structure of SVO by performing resonant photoemission spectroscopy (RPES) at the V L-edge and the O K-edge, together with local-density-approximation (LDA) calculations. Figure 1 shows V L-edge RPES spectra and the LDA partial density of states (PDOS). By tuning the photon energy from $h\nu = 510.46$ to 519.46 eV, we observe a resonant enhancement of the spectral intensity. A comparison between the spectrum at $h\nu = 519.46$eV and the LDA PDOS reveals correlation-induced features that cannot be reproduced by LDA: a coherent feature (~ 0.17 eV) and an incoherent feature (~ 1.7 eV). In addition, a structure associated with O $2p$ states appears at ~ 3.7 eV, while features at ~ 5.8 and ~ 7.1eV are attributable to O $2p$–V $3d$ hybridized states. At higher binding energies, *LVV* Auger emission and shallow-core-level features are observed.

Figure 2(a) presents O K-edge RPES measured in the photon-energy range around the O K-edge. With increasing photon energy, a *KVV* Auger feature shifts toward higher binding energy (orange dashed line). Figures 2(b) and 2(c) compare the O K-edge x-ray absorption spectrum (XAS) with constant-initial-state (CIS) spectra taken at selected binding energies. The CIS spectra taken at the O $2p$ band and at O $2p$–V $3d$ hybridized-state binding energies closely follow the near-edge XAS peaks, whereas the CIS spectra taken at the coherent and incoherent energies do not. This behavior suggests that the coherent and incoherent features near Fermi level E_F have negligible O $2p$ character.

Finally, as shown in Fig. 2(d), we reproduced the *KVV* Auger line shape extracted from RPES using the Cini–Sawatzky formalism [5-6] combined with the LDA O $2p$ PDOS, yielding an estimate of the O $2p$ on-site Coulomb energy $U_{pp} = 5.6$ eV. While previous work [3] neglected U_{pp} and consequently inferred an O $2p$ contribution near E_F, our results indicate that a non-negligible U_{pp} suppresses O $2p$ states near E_F.

In this presentation, we will report the values of $U_{dd}(U_{pp})$ estimated from V L-edge (O K-edge) RPES and discuss characteristics of the electronic structure of SVO.

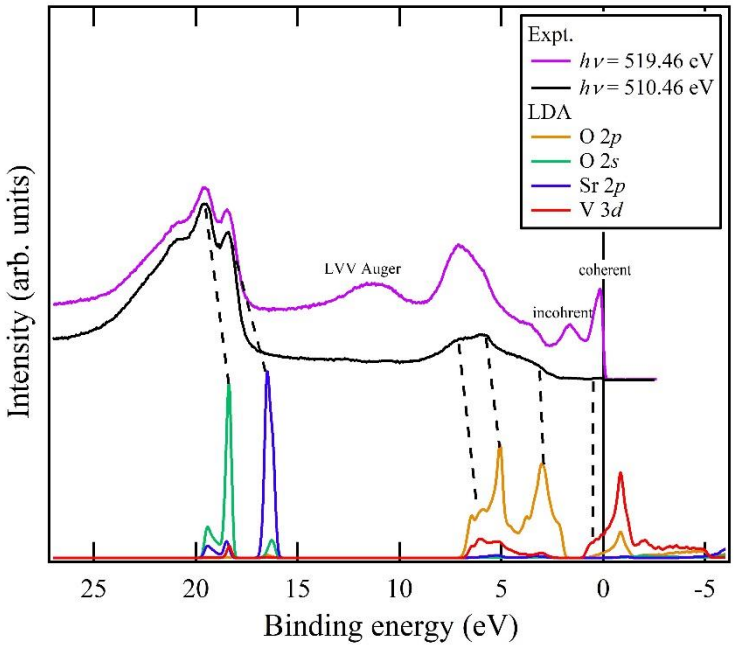

FIGURE 1. Comparison between V L-edge RPES spectra and the LDA-calculated PDOS of SVO.

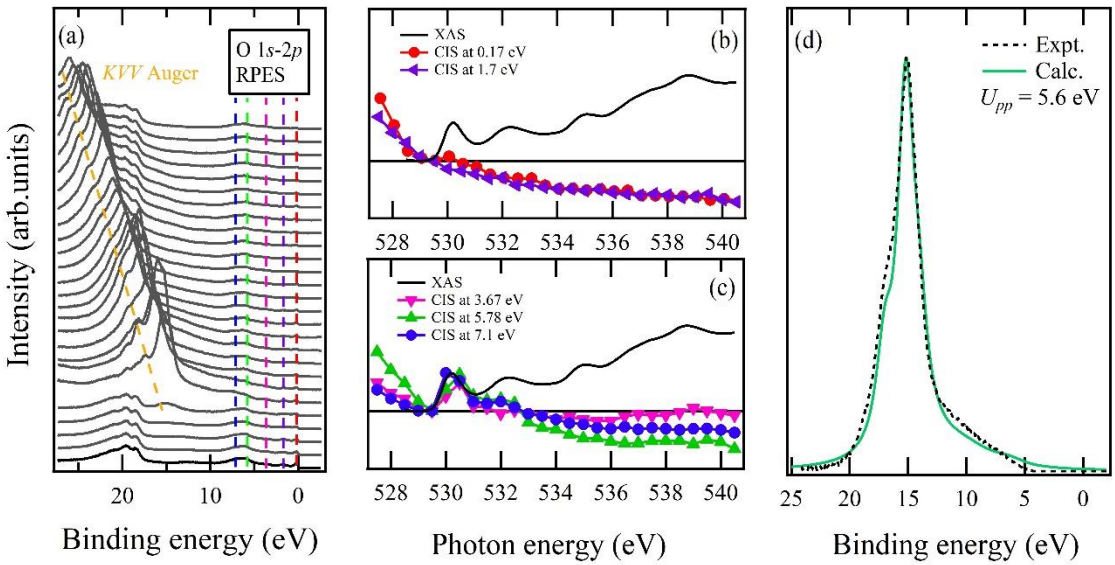

FIGURE 2. (a) O K-edge RPES spectra of SVO. (b), (c) Comparison of the O K-edge XAS spectrum with CIS spectra extracted from the RPES data in Fig. 2(a) at selected binding energies (indicated by vertical dashed lines). (d) Comparison of the *KVV* Auger line shape extracted from RPES with the Auger line shape calculated using the Cini–Sawatzky formalism combined with the LDA-calculated O $2p$ PDOS. The value of U_{pp} used in the calculation is 5.6 eV.

REFERENCES

1. S. Aizaki, T. Yoshida, K. Yoshimatsu, M. Takizawa, M. Minohara, S. Ideta, A. Fujimori, K. Gupta, P. Mahadevan, K. Horiba, H.Kumigashira, and M. Oshima, Phys. Rev. Lett. **109**, 056401 (2012).
2. I.A. Nekrasov, K. Held, G. Keller, D.E. Kondakov, T. Pruschke, M. Kollar, O.K. Andersen, V.I. Anisimov, and D. Vollhardt, Phys. Rev. B **73**, 155112 (2006).
3. R. J. O. Mossanek, M. Abbate, T. Yoshida, A.Fujimori, Y. Yoshida, N. Shirakawa, H. Eisaki, S. Kohno, P.T. Fonseca, and F.C. Vicentin, Phys. B **79**, 033104 (2009).
4. K. Morikawa, T. Mizokawa, K. Kobayashi, A. Fujimori, H. Eisaki, S. Uchida, F. Iga, and Y. Nishihara, Phys. B **52**, 13711 (1995).
5. M. Cini, Solid State Communications **20**, 605 (1976); **24**, 681-684 (1977); Phys. Rev. B **17**, 2788 (1978).
6. G. A. Sawatzky, Phys. Rev. Lett. **39**, 504 (1977).