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# The valence band structure the ZnO(10$\bar{1}$0) surface studied by ARPES

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## Introduction

The energetic position and the dispersion width of the anion-derived dangling-bond state on the ZnO(10$\bar{1}$0) surface have long been controversial issues.

The first theoretical attempt to describe the surface electronic structure of ZnO(10$\bar{1}$0) has been done by Ivanov and Pollmann utilizing the empirical tight-binding method (ETBM) [1]. Later, Wang and Duke have examined the band structure using a so-called $sp^3$ model in the framework of the ETBM [2]. These two approaches have concordantly shown that the O 2p dangling-bond band lies within the projected bulk bands. On the other hand, ab initio calculations by Schröer et al. have indicated that the dangling-bond state lies within the fundamental band gap [3], in sharp contrast to the results of the empirical approaches. So far, no experimental investigations on the two-dimensional band structure of ZnO(10$\bar{1}$0) have been reported.

In the present study, angle-resolved photoelectron spectroscopy (ARPES) measurements have been carried out to clarify the band structure of the O 2p dangling-bond state.

## Experiment

The ARPES measurements were performed at Beam Line 11C. Photoelectrons were collected by an electron energy analyzer of the 180 degrees hemispherical-sector type with an acceptance angle of ±1 degree. The total resolution was 0.25eV at photon energy of 22.5eV, whitch was estimated from the Fermi edge in the spectra of the Ta sample holder. The base pressure of the ultrahigh vacuum system was $2\times10^{-10}$ Torr. Measurements were carried out at room temperature.

## Result and Discussion

Figure shows the two dimensional band structure for ZnO (1010) obtained from the off-normal emission measurements along the $\bar{\Gamma}$ $\bar{X}$ and $\bar{\Gamma}$ $\bar{X}$' axes. Open circles show the O 2p dangling-bond state, and filled circles correspond to the positions of bulk-band related states. The O 2p dangling-bond state positions at 3.7eV at the $\bar{\Gamma}$ point and shifts downwards by 0.8eV and 0.5eV up to $\bar{X}$ point and $\bar{X}$' point, respectively.

In the figure, the gray area indicates the projected bulk band region given by the $sp^3$ model calculation [2]. The valence band maximum of the calculated projected bulk bands is aligned at 3.15±0.05eV, which is determined experimentally. It is clearly seen that the O 2p dangling-bond band locates within the projected bulk-band region in both the $\bar{\Gamma}$ $\bar{X}$ and $\bar{\Gamma}$ $\bar{X}$' axes. Namely, the state forms a surface resonance along these axes. This result is in good agreement with that given by the $sp^3$ ETBM (shown by red line) in terms of the energetic position and the dispersion width especially along the $\bar{\Gamma}$ $\bar{X}$ axis. However, the result of the ab initio calculations (blue line) does not reproduce the experimentally determined band. The present result settles the controversial issue about the energetic position of the O 2p dangling-bond state relative to the bulk bands.

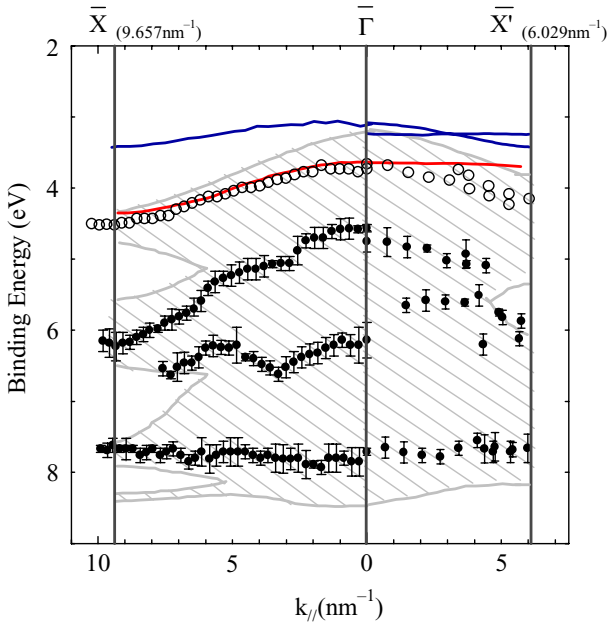


**Figure:** Valence band structure for ZnO (10$\bar{1}$0) surface along $\bar{\Gamma}$ $\bar{X}$ and $\bar{\Gamma}$ $\bar{X}$' axes. The red line indicates the O 2p dangling-bond band calculated by Wang and Duke [2]. The blue lines show the dangling-bond bands reported by Schröer et al [3].

## References

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