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### Site-specific Valence Photoemission Spectroscopy of Hematite ( $\alpha\text{-Fe}_2\text{O}_3$ )

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Beamline(s): X24A

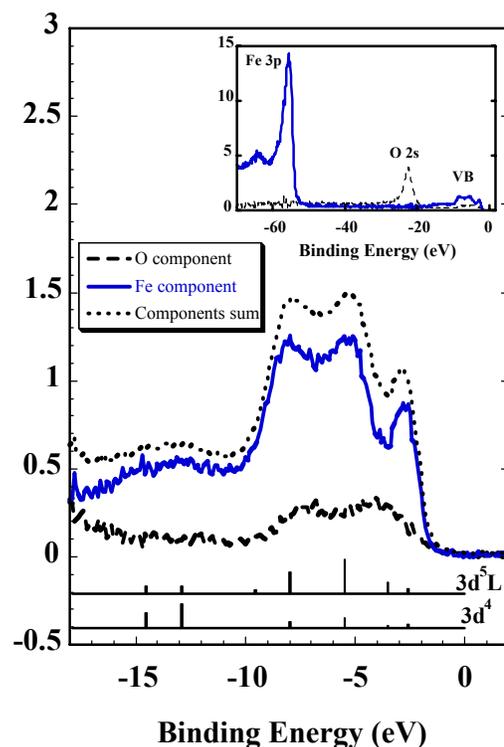
**Methods and Materials:** The crystallographic site-specific valence band electronic structure of hematite ( $\text{Fe}_2\text{O}_3$ ) was studied by x-ray standing wave (XSW) induced photoemission. Using the X24A Beamline at the National Synchrotron Light Source, the XSW was generated by Bragg diffraction from the  $(10\bar{1}4)$  planes in the back reflection geometry from  $\alpha\text{-Fe}_2\text{O}_3(0001)$  single crystal at an incident photon energy of  $\sim 2300$  eV. By fine tuning the incident photon energy with respect to the 0.5 eV wide  $(10\bar{1}4)$  reflectivity, we were able to controllably position the XSW antinodes with respect to the  $(10\bar{1}4)$  diffraction planes.

**Results:** By choosing two photon energies that gave the maximum contrast for the Fe and O photoemission signals, we were able to separate out the Fe and O photoemission spectra (See Fig. 1). This includes the Fe 3d and O 2p components of the valence band. The extended binding energy region of the spectra (shown in the inset) clearly demonstrates the ability of this technique to elementally decompose the spectra. In the valence band region of the spectra, the O component has two peaks with binding energy at 4.0 and 7.2 with the average position at 16 eV above the O 2s. (This is similar to finding for  $\text{Al}_2\text{O}_3$  which has little overlap between the cation and O valence states [2].) The Fe component consists of four peaks extending 18 eV below the Fermi level with maxima at 2.7, 5.3, 8.0, and 12.4 eV. Our Fe 3d-derived final state spectrum is similar to the three peaks obtained by Fe 3p resonance photoemission [1]. However, our method excludes the contribution from a hybridized O 2p component, and the unresolved broad feature at 5 to 8 eV in the resonance photoemission measurement was resolved into two peaks in our spectrum. Our results show good agreement with a theoretical configuration interaction cluster calculation for the Fe 3d derived final states which includes  $d^4$  and  $d^5L$  photoemission final states [3].

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#### References:

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**Fig. 1**  $\text{Fe}_2\text{O}_3$  photoemission spectra separated into Fe and O components by selectively aligning the antinode (and then node) of the X-ray standing wave with the  $(10\bar{1}4)$  Fe atomic planes. The vertical lines at bottom show positions and relative intensities of the  $3d^5L$  and  $3d^4$  final states predicted in Ref. 3.