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The valence electronic structure of multiferroic $BiFeO_3$ from high energy X-ray photo-electron spectroscopy and first principles theory R. KNUT, Department of Physics and astronomy, Uppsala University, Uppsala, Sweden, S. FALEEV, DIPANJAN MAZUMDAR, O. MRYASOV, ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, O. KARIS, Department of Physics and astronomy, Uppsala University, Uppsala, Sweden, U ALABAMA TEAM, UPPSALA TEAM — BiFeO3 (BFO) is a multi-functional material with high ferroelectric and magnetic ordering temperature. Here we have investigated the electronic structure of (001) oriented 100nm rhombohedral BFO thin films using high energy X-ray photoelectron spectroscopy (XPS). By making use of the energy dependence of the relative cross sections for different states, we were able to selectively probe the elemental contributions to the valence band . At high energies, states with high main quantum number will have a higher relative probability for photo-ionization, i.e., the Bi 6s and 6p contributions in the valence region are enhanced relative to the Fe 3d and O 2p. We find that the Bi 6p states hybridize strongly with the valence band dominated by the Fe 3d and O 2p states, resulting in a splitting of the 3d states due to bonding and anti-bonding combinations with the Bi 6p. Our results thus suggest that a previously relatively ignored electronic interaction needs to be considered for BFO and related Bi-TMOs. Ab initio calculations indicate the importance of screened Coulomb correlations to describe Bi and Fe electronic states.

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