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Nature of the bandgap in In_2O_3 revealed by first-principles calculations and X-ray spectroscopy ARON WALSH, JUAREZ L.F. DA SILVA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO 80401, USA, CHRISTOPH KÖRBER, ANDREAS KLEIN, Darmstadt University of Technology, Darmstadt, Germany, L.F.J. PIPER, ALEX DEMASI, K.E. SMITH, Department of Physics, Boston University, Boston, MA 02215, USA, G. PANACCIONE, Laboratorio TASC, INFM-CNR, Area Science Park, 34012 Trieste, Italy, P. TORELLI, CNR-INFM-S3, Via Campi 213/A, I-41100 Modena, Italy, D.J. PAYNE, A. BOURLANGE, R.G. EGDELL, Chemistry Research Laboratory, Mansfield Road, Oxford OX1 3TA, UK — The origin of weak absorption 1 eV below the onset of strong optical absorption in In2O3 has previously been attributed to the presence of an indirect fundamental bandgap or surface band bending. We demonstrate conclusively that this is not the case. Through the application of bulk and surface sensitive X-ray spectroscopic techniques, we reveal that the valence band edge is found much closer to the bottom of the conduction band than expected on the basis of the widely quoted bandgap of 3.75 eV. First-principles theory shows that the upper valence bands of In2O3 exhibit small dispersion and the conduction band minimum is positioned at Γ; however, direct optical transitions give minimal dipole intensity until 0.8 eV below the valence band maximum. Our results set an upper limit on the fundamental bandgap of 2.9eV.

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