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Site specific valence band structure of SrTiO₃ determined with X-ray standing waves JORG ZEGENHAGEN, SEBASTIAN THIESS, TIEN-LIN LEE, ESRF, France, FRANCOIS BOTTIN, CEA/DIF, France — Structure and chemical composition define the properties of materials, notably band structure and electronic characteristics of solids. Ab initio calculations deliver frequently reliably predictions, which are, however, difficult to verify, in particular in view of the direct relationship between atomic and electronic structure. Combining the x-ray standing wave (XSW) technique with X-ray photoelectron spectroscopy (XPS) is a unique tool in this sense. It is used here to identify unambiguously parts of the valence band of SrTiO₃, which can be assigned to Sr, Ti, or O-sites of the lattice. The XSW/XPS measurements were performed in UHV at the ID32 insertion device beamline at the ESRF using a (001) oriented, atomically clean SrTiO₃ crystal. Traversing the (111) and (112) Bragg reflections and recording the valence band for different standing wave positions within the lattice unit cell, the site specific contributions could directly be identified. Obtained experimental results are in very good agreement with theory, by utilizing as adjustable parameters the X-ray absorption cross sections of the valence electrons.

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