

Interface effects in the electronic structure of TiO₂ deposited on MgO, Al₂O₃ and SiO₂ substrates

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Abstract

We report the Ti 2*p* x-ray absorption (XAS) and resonant photoemission (RPES) spectra of one equivalent TiO₂ monolayer grown on MgO, Al₂O₃ and SiO₂ substrates. The Ti 2*p* XAS spectra of these monolayers were compared to atomic multiplet calculations projected in different octahedral crystal fields. The comparison indicates that the crystal field splitting and the Ti 3*d* – O 2*p* hybridization is reduced with the increasing covalent character of the substrates. The analysis of the RPES spectra provides the Ti 3*d* contributions to the valence band in these systems. These were compared to configuration interaction calculations of a TiO₆ cluster for different Ti 3*d* – O 2*p* hybridizations. The Ti 3*d* states in the valence band shift to lower binding energies with the increase of the covalent character of the substrates. These effects are consistent with the reduction of the effective Ti 3*d* – O 2*p* interactions, which, in turn, is due to the formation of Ti – O – M (M=Mg, Al, Si) cross-linking-bonds with a more covalent element.