

Supporting Information

Analysis of the interfacial characteristics of BiVO₄/metal oxide heterostructures and its implication on their junction properties

Yannick Hermans^{ab}, Sebastián Murcia-López^c, Andreas Klein^a, Roel van de Krol^d, Teresa Andreu^c, Joan Ramón Morante^c, Thierry Toupance^b and Wolfram Jaegermann^a

^a *Institute of Material Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany.*

^b *Université de Bordeaux, Institut des Sciences Moléculaires, ISM UMR 5255 CNRS, 351 Cours de la Libération, F-33405 Talence Cédex, France.*

^c *Department of Advanced Materials for Energy, Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre, 1, 08930 Sant Adrià de Besòs, Catalonia, Spain.*

^d *Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, Berlin 14109, Germany.*

Supplementary methods

Overlayer sputter conditions

Please find the exact experimental conditions of the sputtered NiO, CoO_x and ITO thin films in Table S1.

Table S1: Magnetron sputtering deposition parameters for NiO, CoO_x and ITO thin films

	NiO	CoO _x	ITO
T _{sub} (°C)	RT	RT	400
Pr (Pa)	0.5	0.5	0.5
O ₂ /Ar ratio (%)	20	10	0
P (W)	40 (DC)	40 (RF)	25 (RF)
Flux (sccm)	20	20	6.6
d (cm)	8.0	8.5	9.6
R (nm min ⁻¹)	3	1.3	5

In above table T_{sub} is substrate temperature, RT is room temperature, Pr stands for pressure, P is the power applied to the sputter target, d stands for the target-to-substrate distance and R stands for the deposition rate of the film.

Overlayer thickness calculation

The thickness of the deposited films was estimated from the difference in attenuation of the Bi4f and V2p_{3/2} core level emission. Since the kinetic energy of the photoelectrons from the Bi4f emission is higher than for the V2p_{3/2} emission the Bi4f photoelectrons are attenuated less because of the higher inelastic mean free path of these photoelectrons. The thickness of a thin film growing on top of the BiVO₄ substrate can then be evaluated, under the assumption that the surface V/Bi ratio does not change during film growth, according to following formula:

$$t = \frac{\ln\left(\frac{I_V \times I_{Bi0}}{I_{Bi} \times I_{V0}}\right) \times \lambda_V \times \lambda_{Bi}}{\lambda_V - \lambda_{Bi}}$$

where t: film thickness; I_V: integrated V2p_{3/2} core level intensity at film thickness t; I_{Bi}: integrated Bi4f core level intensity at film thickness t; I_{V0}: integrated V2p_{3/2} core level intensity at zero film thickness; I_{Bi0}: integrated Bi4f core level intensity at zero film thickness; λ_V: electron effective attenuation length of V2p_{3/2} photoelectrons; λ_{Bi}: electron effective attenuation length of Bi4f photoelectrons

The electron effective attenuation lengths were calculated using the “NIST Electron Effective-Attenuation-Length Database”, based on the density, number of valence electrons and band gap of the deposited film.

Supplementary figure

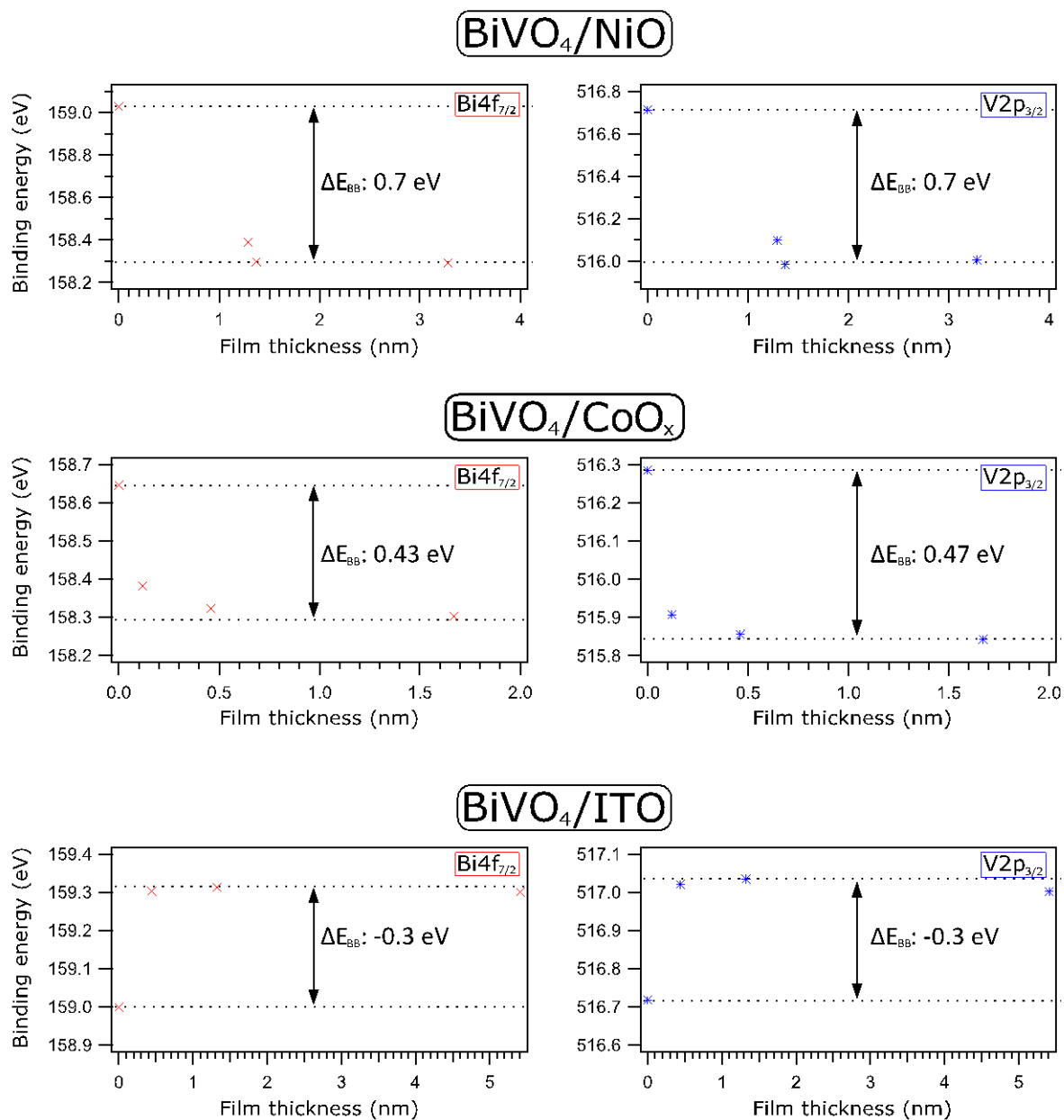


Figure S1: Evolution of Bi4f_{7/2} and V2p_{3/2} core level binding energy with respect to overlayer thickness for the BiVO₄/NiO, BiVO₄/CoO_x and BiVO₄/ITO interface experiments. Total band bending (ΔE_{BB}) values are denoted in the graphs.