Supporting Information

Analysis of the interfacial characteristics of $BiVO_4$/metal oxide heterostructures and its implication on their junction properties

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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	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 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 $BiVO_4$ 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

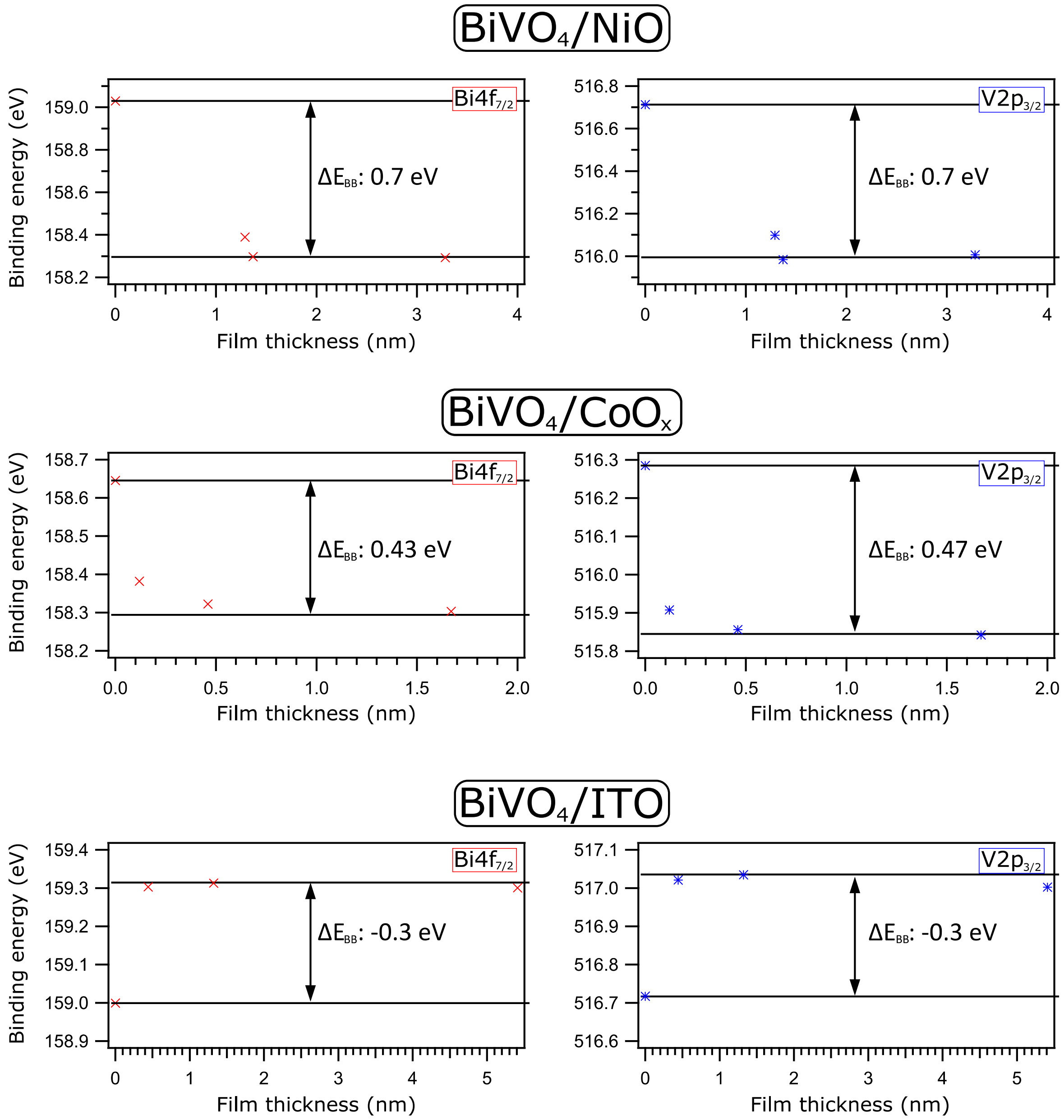

Figure S1: Evolution of Bi4f$_{7/2}$ and V2p$_{3/2}$ core level binding energy with respect to overlayer thickness for the BiVO$_4$/NiO, BiVO$_4$/CoO$_x$ and BiVO$_4$/ITO interface experiments. Total band bending (ΔE_{BB}) values are denoted in the graphs.