Supplementary Information for

Prediction of $(TiO_2)_x(Cu_2O)_y$ Alloys for Photoelectrochemical Water Splitting

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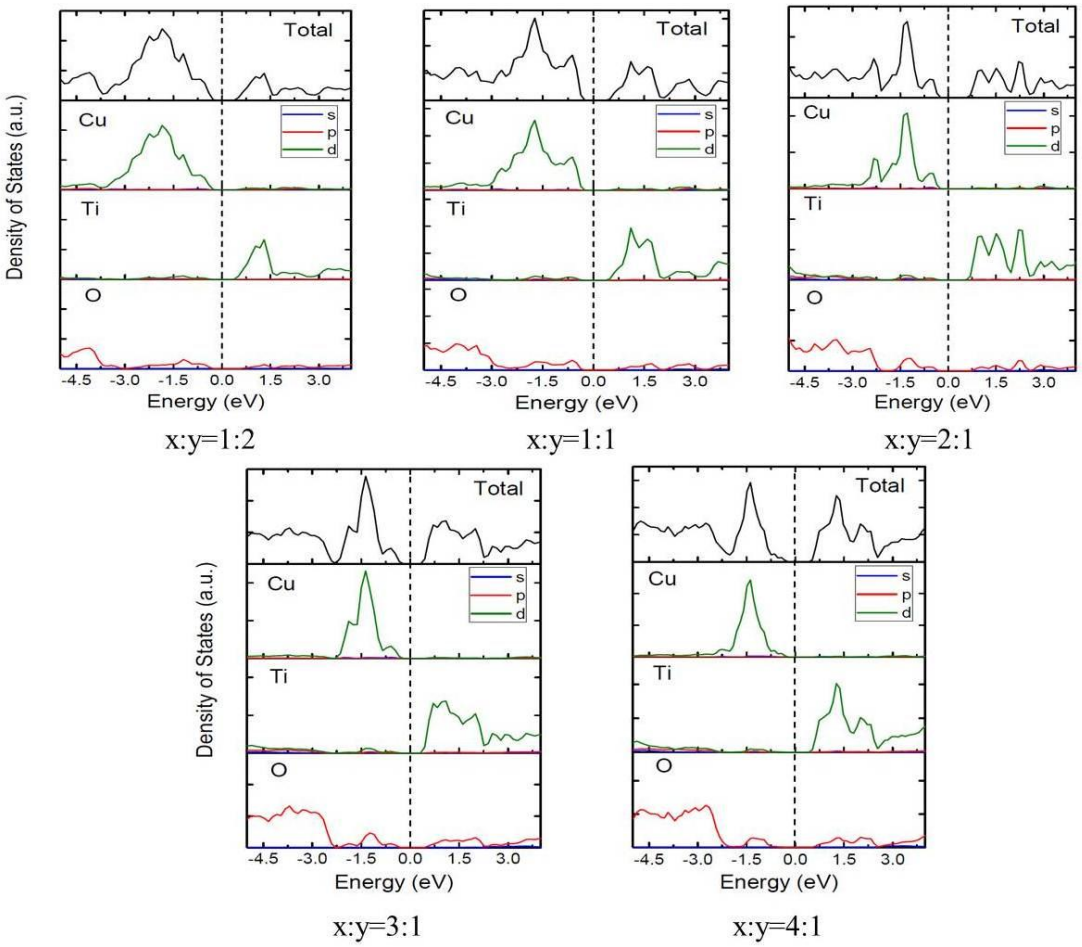
I. Partial density of states (PDOS) of $(TiO_2)_x(Cu_2O)_y$ alloys by the PBE functional

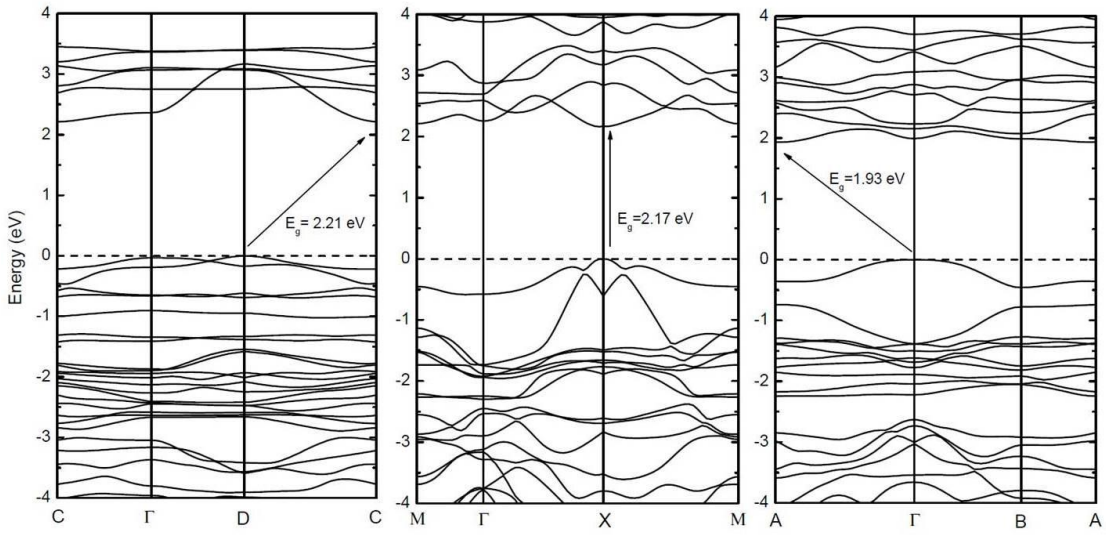


x:y=1:2 x:y=1:1 x:y=2:1

x:y=3:1 x:y=4:1

The energy levels of the VBMs are set to zero. The red lines represent the p states, while the blue ones and the green ones represent the s states and the d states, respectively.

II. Band structure of selected $(TiO_2)_x(Cu_2O)_y$ alloys from the HSE06 calculations



x:y=1:1 x:y=2:1 x:y=3:1

The VBMs are set to zero. The fractional coordinates of the k-points are as follows: Γ (0.0, 0.0, 0.0), A (0.4444, 0.4444, 0.5), B (0.5, 0.0, 0.5), C (-0.3333, 0.1333, 0.06667), D (0.0, 0.4667, 0.0), M (0.5, 0.5, 0.5), X (-0.2333, 0.35, 0.0).