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International Conference on

Nanomaterials and Nanochemistry

November 29-30, 2017 | Atlanta, USA

Potential of strained SnO_2 as a photo-catalyst for water splitting process

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Photocatalytic water splitting technology has recently received extensive attention as a promising method to produce hydrogen, which has generated an urgent need to find alternative photocatalytic materials for such technique. In the present study, the electronic and photocatalytic properties of SnO_2 under uniaxial strain have been examined, based on density functional theory (DFT), showing that under tensile strain the band gap energy decreases, while an opposite behavior is demonstrated in the case of compression. Band edge alignments of unstrained SnO_2 shows that the VBM is more positive than the redox potential of O_2/H_2O (1.23V) while the CBM for pH = lies above the redox potential of $H+/H_2$ (0V), which mean that the pure SnO_2 cannot be used for hydrogen evolution reaction (HER). Applying compressive strain, the CBM edge position decreases gradually as the strain percent increases, in other hand under tensile strain the CBM edge position could be corrected for pH ≥ 10 which clearly reveals the ability of mechanical strain to modulate the band structure and the photocatalytic properties of SnO_2 in order to improve its suitability as a photo-catalyst for water splitting.

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