Strain Engineering of Photocatalytic Materials

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Photocatalytic materials are pivotal for the implementation of disruptive clean energy applications like conversion of H_2O and CO_2 into fuels and chemicals driven by solar energy. However, efficient and cost-effective materials able to catalyze the chemical reactions of interest when exposed to visible light are scarce due to the stringent electronic conditions that they must satisfy. Chemical and nanostructuring approaches are capable of improving the catalytic performance of known photoactive compounds, however, the complexity of the synthesized nanomaterials and sophistication of the employed methods make systematic design of photocatalysts difficult. Here, we present the results of recent first-principles studies on semiconductor materials that have the potential to improve the rational and systematic engineering of photocatalysts[1,2]. First, we show that application of biaxial stress on binary oxides can modify their optoelectronic and catalytic properties in a significant and predictable manner. In particular, upon moderate tensile strains CeO_2 and TiO_2 become suitable materials for photocatalytic conversion of H_2O into H_2 and of CO_2 into CH_4 under sunlight. The band gap shifts induced by biaxial strain are qualitatively reproduced by a simple analytical model that only depends on structural and dielectric susceptibility variations. And second, we assess the water-splitting photocatalytic potential of piezoelectric materials that, despite may react to mechanical stimuli by noticeably adjusting their band gaps and band alignments, have been seldom investigated to date. In particular, we present a high-throughput screening of piezo-photocatalyst materials performed over ~1,000 piezoelectrics that relies on a simple electrostatic model and first-principles calculations. A number of overlooked binary and tertiary piezo-photocatalysts emerge as very promising from our analysis, among which SiC stands out due to its superb optoelectronic tunability under uniaxial strain and facile synthesis.

[1] Liu, Z., Shenoy, J. N., Menendez, C., Hart, J. N., Sorrel, C. C. & Cazorla, C**.** *Strain engineering of oxide thin films for photocatalytic applications*. Nano Energy **72**, 104732 (2020).

[2] Liu, Z. & Cazorla, C**.** *First-principles high-throughput screening of piezo-photocatalyst materials for water splitting under visible light*. Submitted (2021).