

### Electronic Supplementary Information

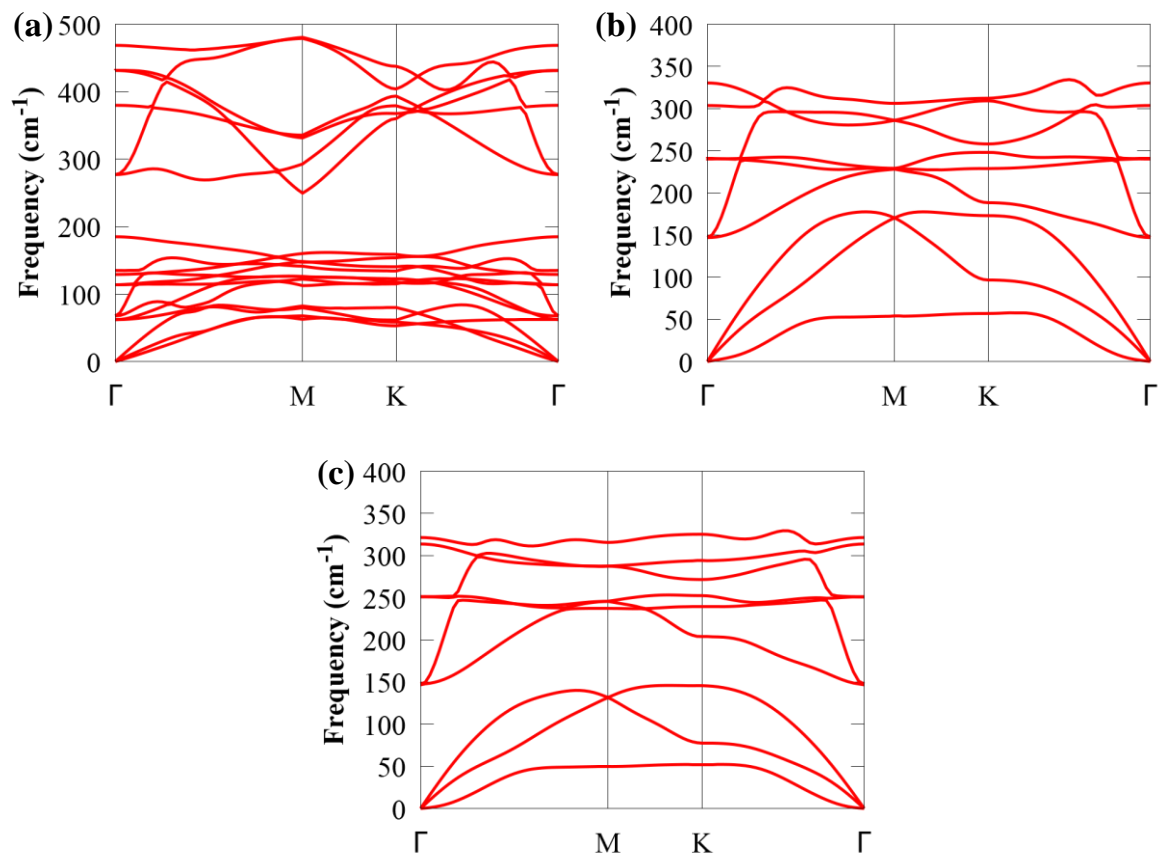
Two-dimensional layered Type-II  $MS_2/BiOCl$  ( $M = Zr, Hf$ ) van der Waals heterostructures: A promising photocatalysts for hydrogen generation

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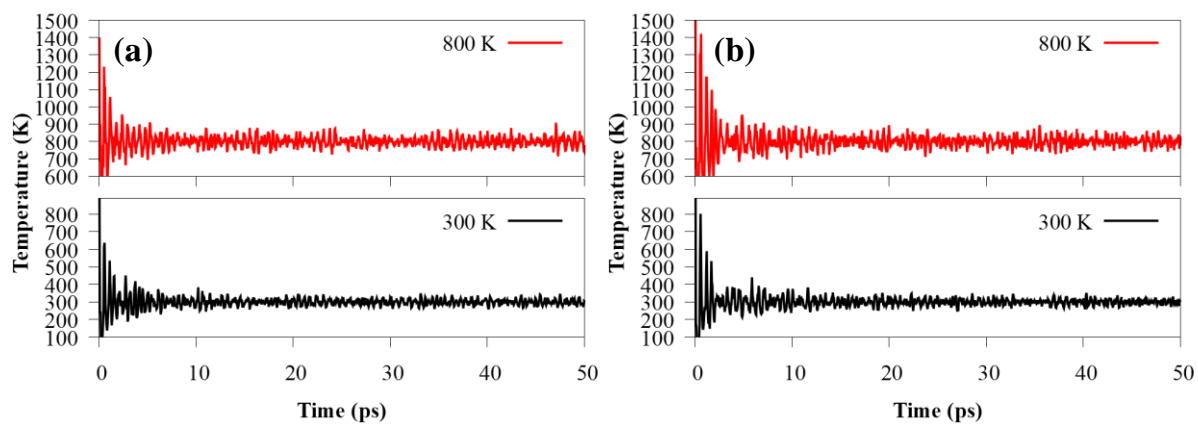
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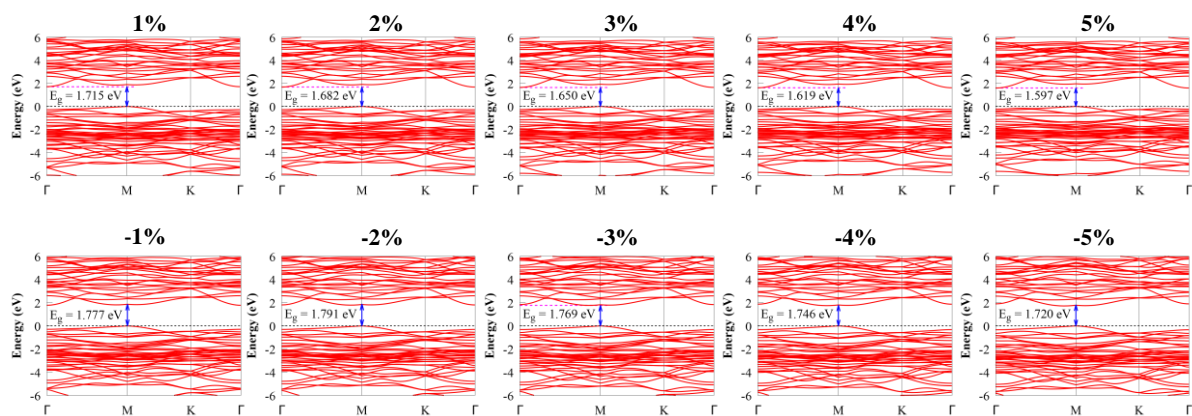
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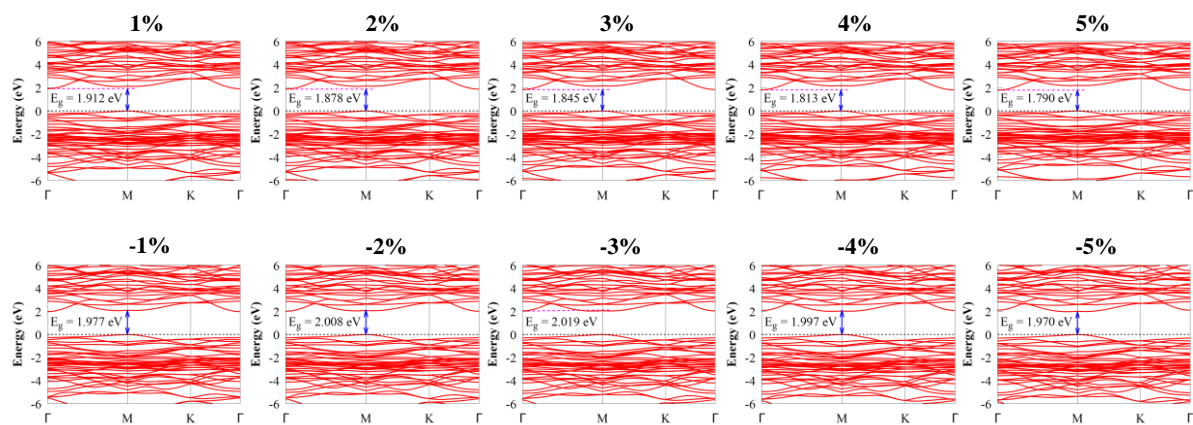
**Figure S1.** The phonon dispersion curve of (a) BiOCl, (b) ZrS<sub>2</sub> and (c) HfS<sub>2</sub>



**Figure S2.** Temperature fluctuation of (a) ZrS<sub>2</sub>/BiOCl and (b) HfS<sub>2</sub>/BiOCl at 300 K and 800 K.



**Figure S3.** The band structure versus strain for ZrS<sub>2</sub>/BiOCl heterostructures



**Figure S4.** The band structure versus strain for HfS<sub>2</sub>/BiOCl heterostructures