

Supplementary Information

Achieving Highly Efficient 2D SnC monolayer-based Photocatalyst for Water Splitting via a Synergistic Strategy of S-scheme Heterostructure Construction and Silicon Doping

Dinghua Yang, Xi Zhang, Ya Nie, Hongyu Zhu and Gang Xiang*

College of Physics, Sichuan University, Chengdu 610064, China

*Corresponding authors' email: gxiang@scu.edu.cn

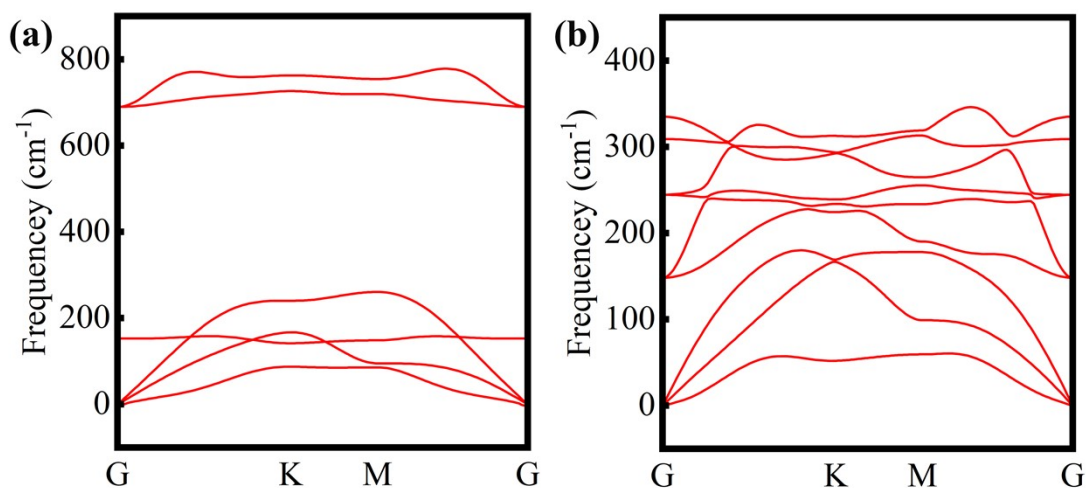


Fig. S1 The phonon spectra of (a) SnC ML and (b) ZrS₂ ML.

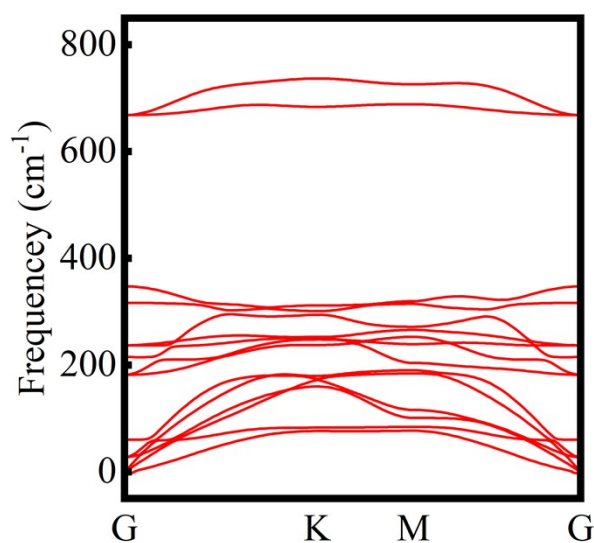


Fig. S2 The phonon spectrum of SnC/ZrS₂ HS.

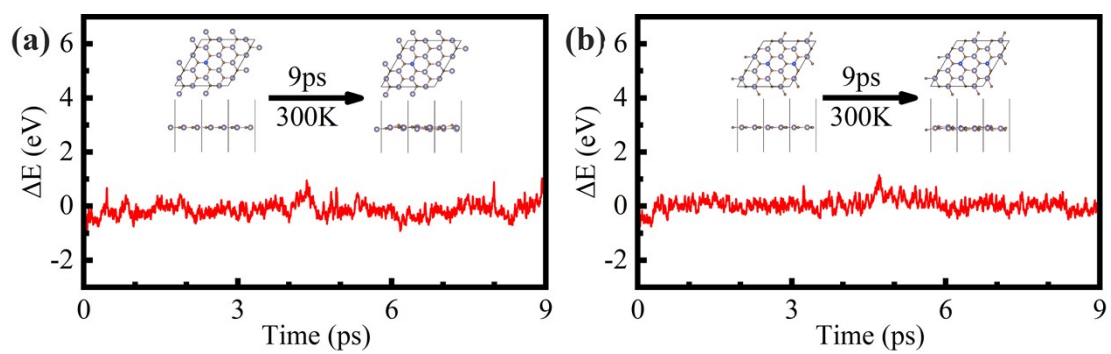


Fig. S3 *ab initio* molecular dynamics simulations at 300 K of (a) $\text{Sn}_{11}\text{Si}_1\text{C}_{12}$ and (b) $\text{Sn}_{10}\text{Si}_2\text{C}_{12}$.