Supporting information

Surfactant-free Synthesis of SingleCrystalline SnS_2 and Effect of Surface Atomic Structure on the Photocatalytic Property

Mengyi Li[1], Enzuo Liu[1, 2], Huilin Hu[1], ShuxinOuyang[1, 2], Hua Xu[1, 2], Defa Wang[1, 2 *]

[1]*TU-NIMS Joint Research Center, and Tianjin Key Laboratory of Composite and Functional Materials, School of Materials Science and Engineering, Tianjin University, 92 Weijin Road, Nankai District, Tianjin 300072, China*

[2]*Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), 92 Weijin Road, Nankai District, Tianjin 300072, China*

S1. Calculation of Surface Energy

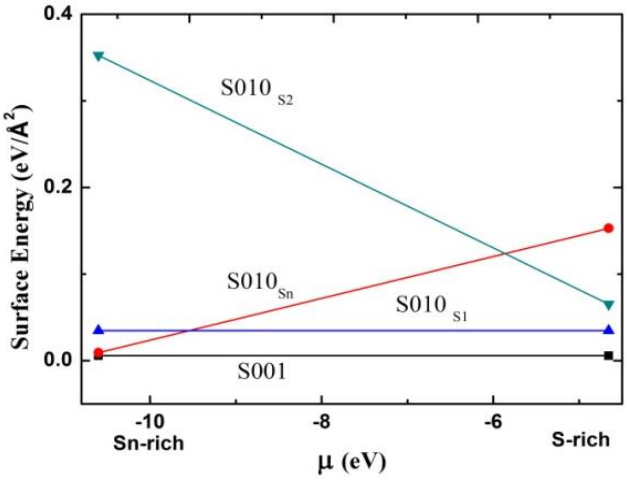

FIGURE S1: Surface energy changes of S001, $S010_{S1}$, $S010_{S2}$ and $S010_{Sn}$ facets with the condition from Sn-rich to S-rich.

The surface energy (γ) of each facet was calculated by the following formula:

$$\gamma=\frac{Eslab-nEbulk-mE0}{2A},$$

*Correspondence should be addressed to Defa Wang; E-mail: defawang@tju.edu.cn

Where E_{slab} is the total energy of the slab, n is the total number of SnS_2 unit cells contained in the slab model, E_{bulk} is the energy per unit cell of SnS_2, m is obtained by subtracting n Sn atoms and 2n S atoms from the number of Sn and S atoms in the surface slab. E_0 is the chemical potential of the extra atom species. The calculated surface energies are 0.0065 and 0.034 eV/$Å^2$ for S001 and $S010_{S1}$ facets, respectively.

"The result shows that compare to the {010} surface, the {001} surface owns lower surface energy, meaning that the {001} facet is more stable than the {010} surface."