Supplementary information

Proposal of a Stable B_3S Nanosheet as an Efficient Hydrogen Evolution Catalyst

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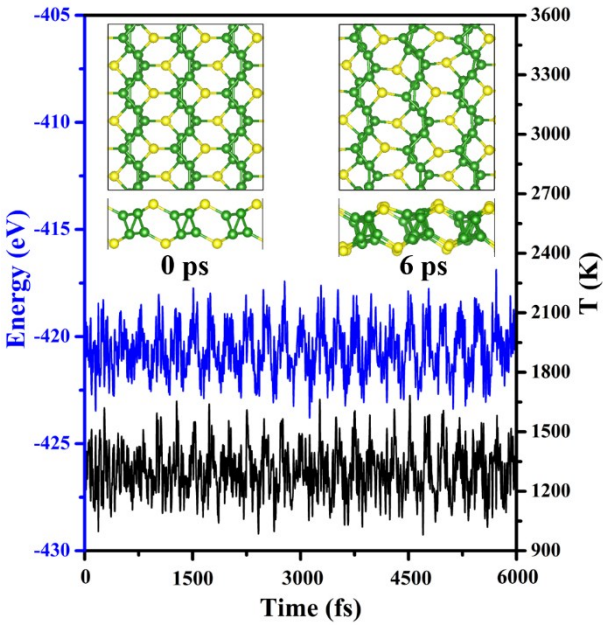

Figure S1. The fluctuation of total energy (blue) and temperature T (black) during the AIMD simulation at 1300 K. The insets are the top and side views of B_3S structure at the time of 0 and 6 ps, respectively.

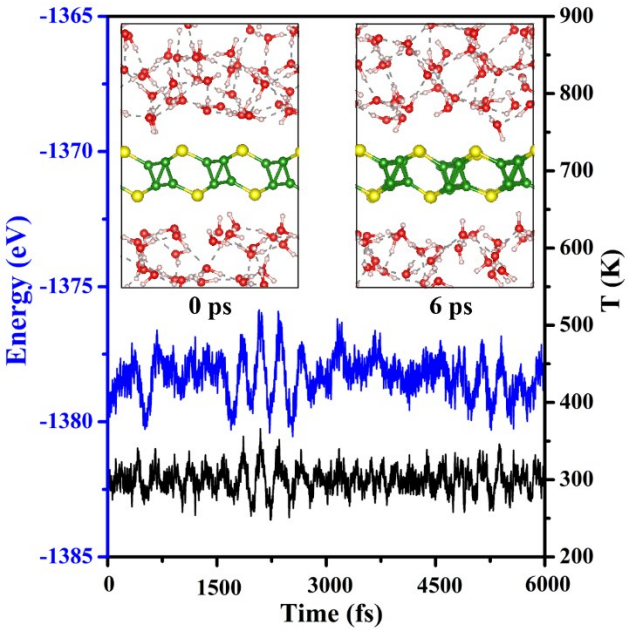

Figure S2. The fluctuation of total energy (blue) and temperature T (black) during 300 K AIMD in water environment. The insets are the side views of B_3S structure with 64 H_2O molecules at the time of 0 and 6 ps, respectively. Green, yellow, red and pale pink balls represent B, S, O and H atoms, respectively.

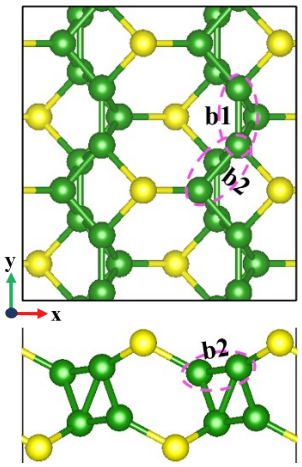

Figure S3. Two different B-B bridge sites (labelled as b1 and b2) on the B_3S surface that are possible for hydrogen adsorption. We find only the B-B bridge sites parallel to y-axis (b1) can stabilize atomic hydrogen, while a hydrogen atom initially placed on b2 site migrates to b1 site after structure optimization due to the steric repulsion of the surrounding S atoms.

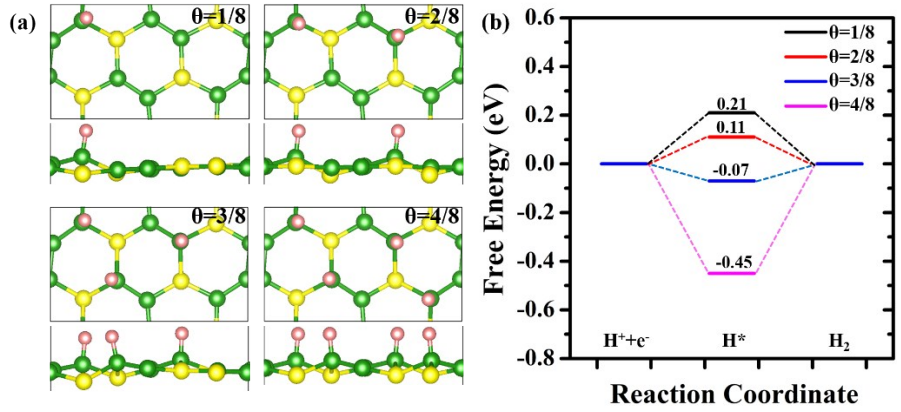

Figure S4. (a) The most stable configurations and (b) corresponding free energies of hydrogen adsorption on B_2S monolayer under different hydrogen coverages. Green, yellow and pink balls represent B, S and H atoms, respectively.