Supporting Information

Cu_2O/Cu_2S Microstructure Regulation Towards High Efficiency Photocatalytic Hydrogen Production And Its Theoretical Mechanism Analysis

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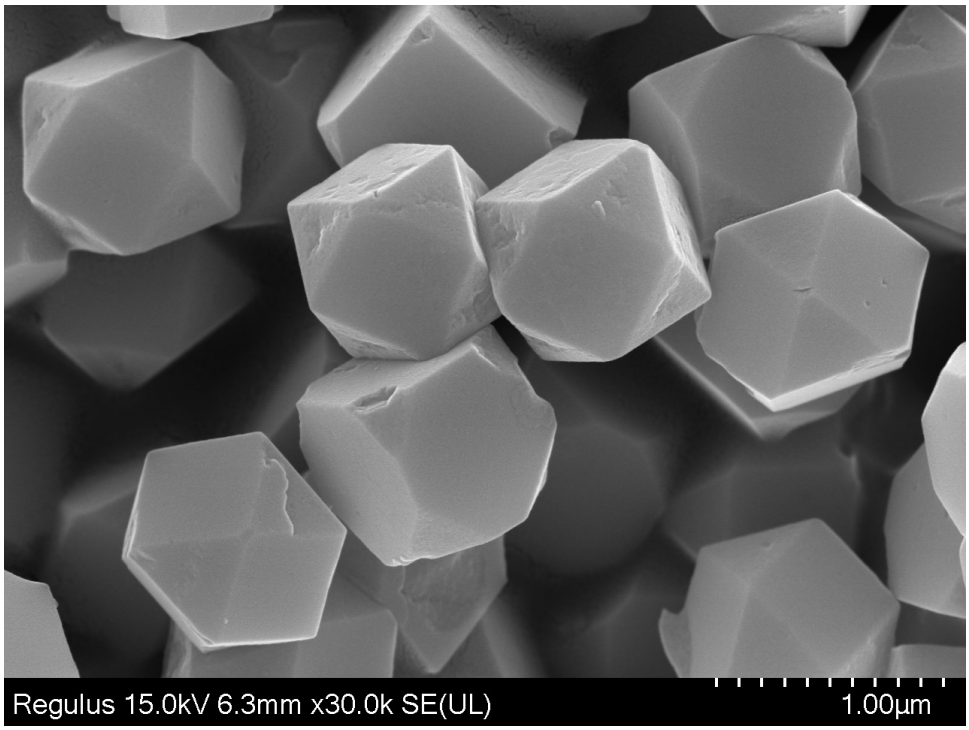

Fig.S1 SEM image of Cu_2O sample

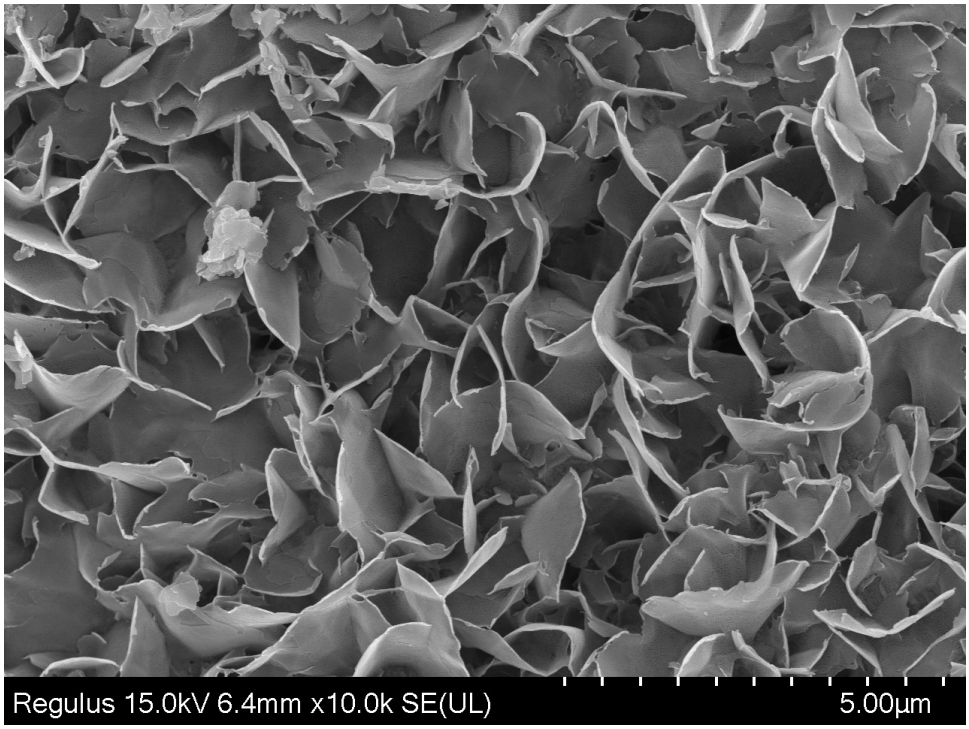

Fig.S2 SEM image of Cu_2O/Cu_2S-1 sample

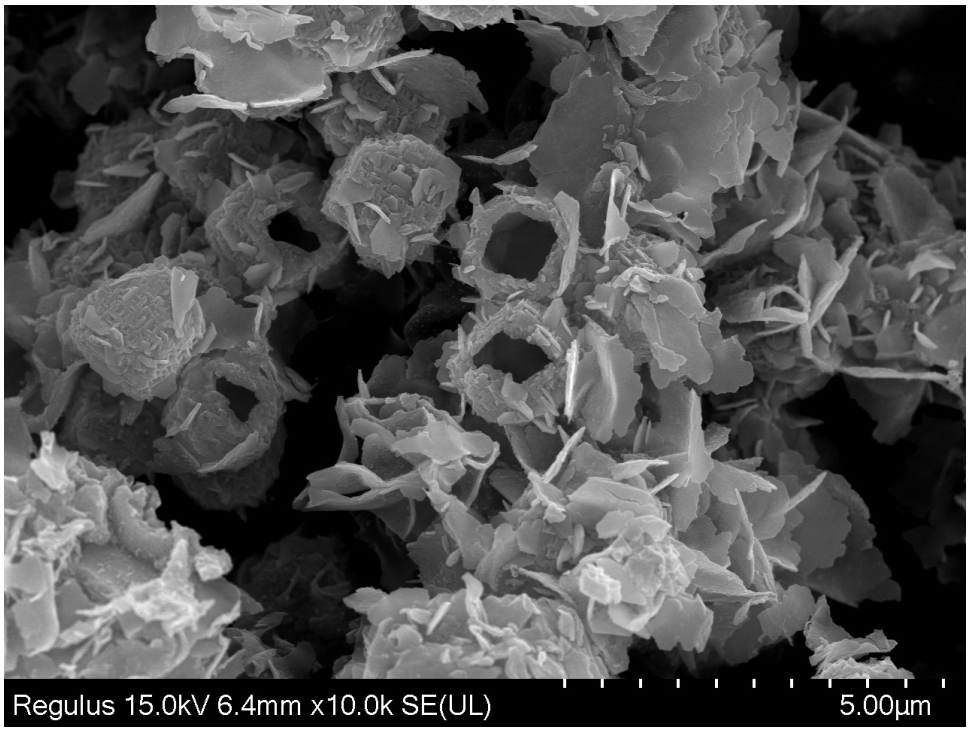

Fig.S3 SEM image of Cu_2O/Cu_2S-2 sample

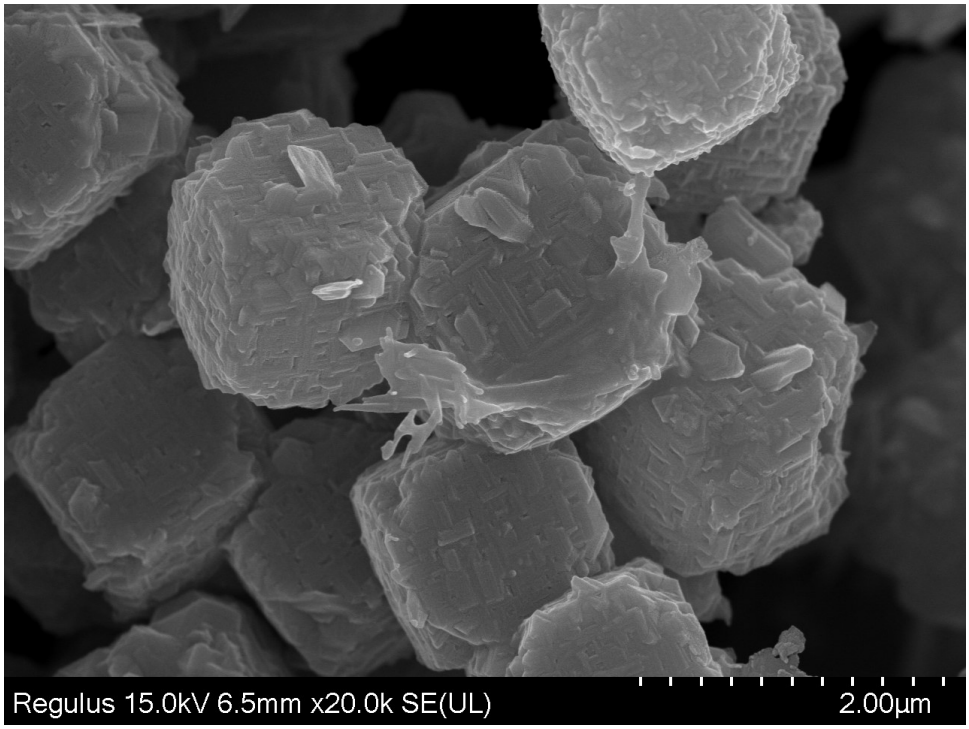

Fig.S4 SEM image of Cu_2O/Cu_2S-3 sample

All DFT computations were performed utilizing the Perdew-Burke-Ernzerhof (PBE) flavor of spin-polarized DFT with generalized gradient approximation (GGA), as integrated in the software of Vienna ab initio simulation program (VASP). To treat valence electrons, a plane waves basis set with a kinetic energy cutoff of 400 eV was adopted. The convergence criteria for energy and force were set at 10^{-5} eV and 0.02 eV/Å, respectively. The k-point densities used for Brillouin zone sampling in electronic calculations were 9×9×1. A grimme of DFT-D3 method was adopted in all calculations. To avoid inaccuracies due by periodic effects, a 15 Å vacuum layer was placed along the z-axis of the plane to simulate the slab surface.