Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Enhancing the Solar Energy Conversion Efficiency of Solution-Deposited Bi_2S_3 Thin Films by Annealing in Sulfur Vapor at Elevated Temperature

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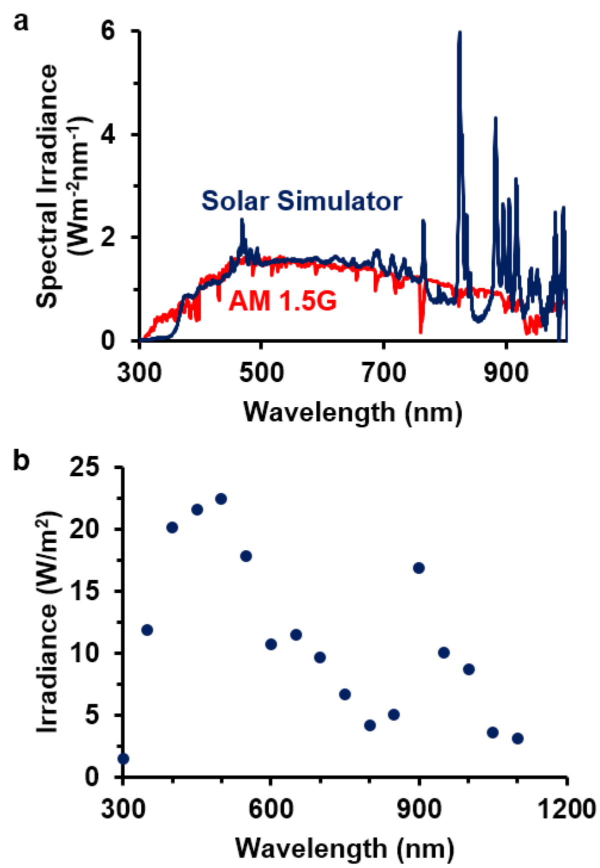

Figure S1. Spectral output of illumination sources used in this work measured with calibrated spectrometers. (a) Spectral irradiance of the class-AAA Solar Simulator (81.7 mW/cm^2 overall intensity), compared to the air mass 1.5 global (AM1.5G, ASTM-G173-3) standard. (b) Irradiance of Xe lamp with monochromator, used for incident photon-to-current conversion efficiency (IPCE) measurements.

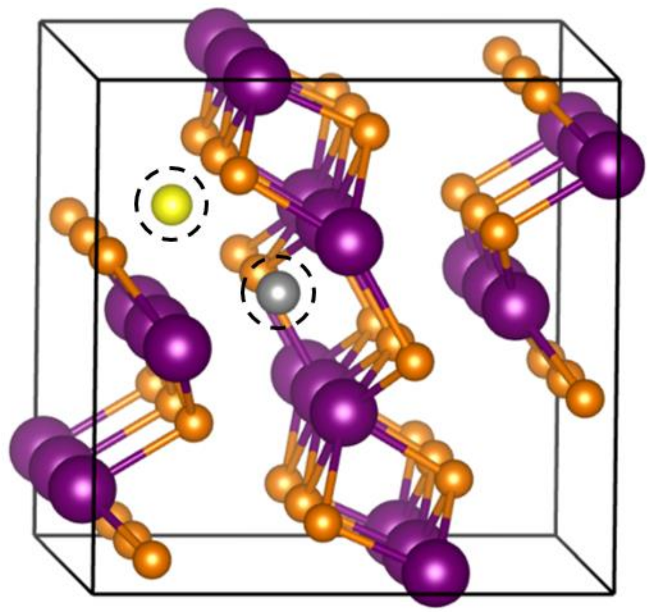

Figure S2. The crystal structure of a 60-atom Bi_2S_3 supercell with purple balls showing Bi atoms and orange balls showing S atoms. The yellow ball shows the interstitial sites for S_i, O_i, and H_i. The grey ball shows the vacancy site for S_v and the substitution sites for O_S and H_S.

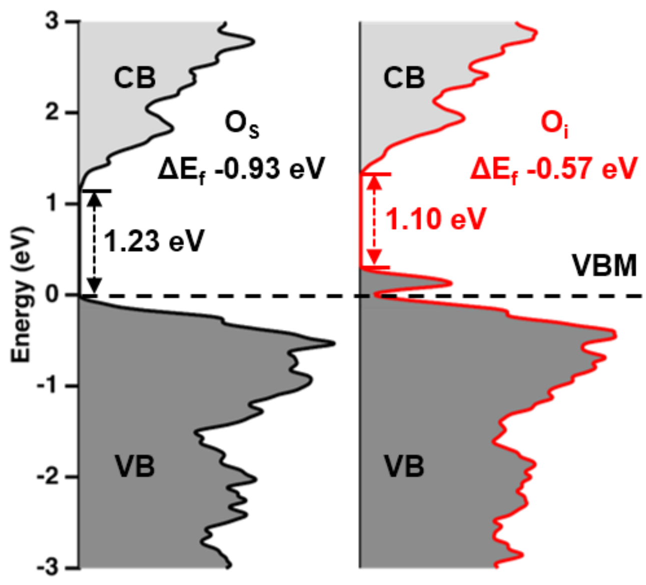

Figure S3. DFT-calculated density of states (DOS) and formation energies of Bi_2S_3 containing oxygen substitution of sulfur (O_S) and oxygen interstitial (O_i).

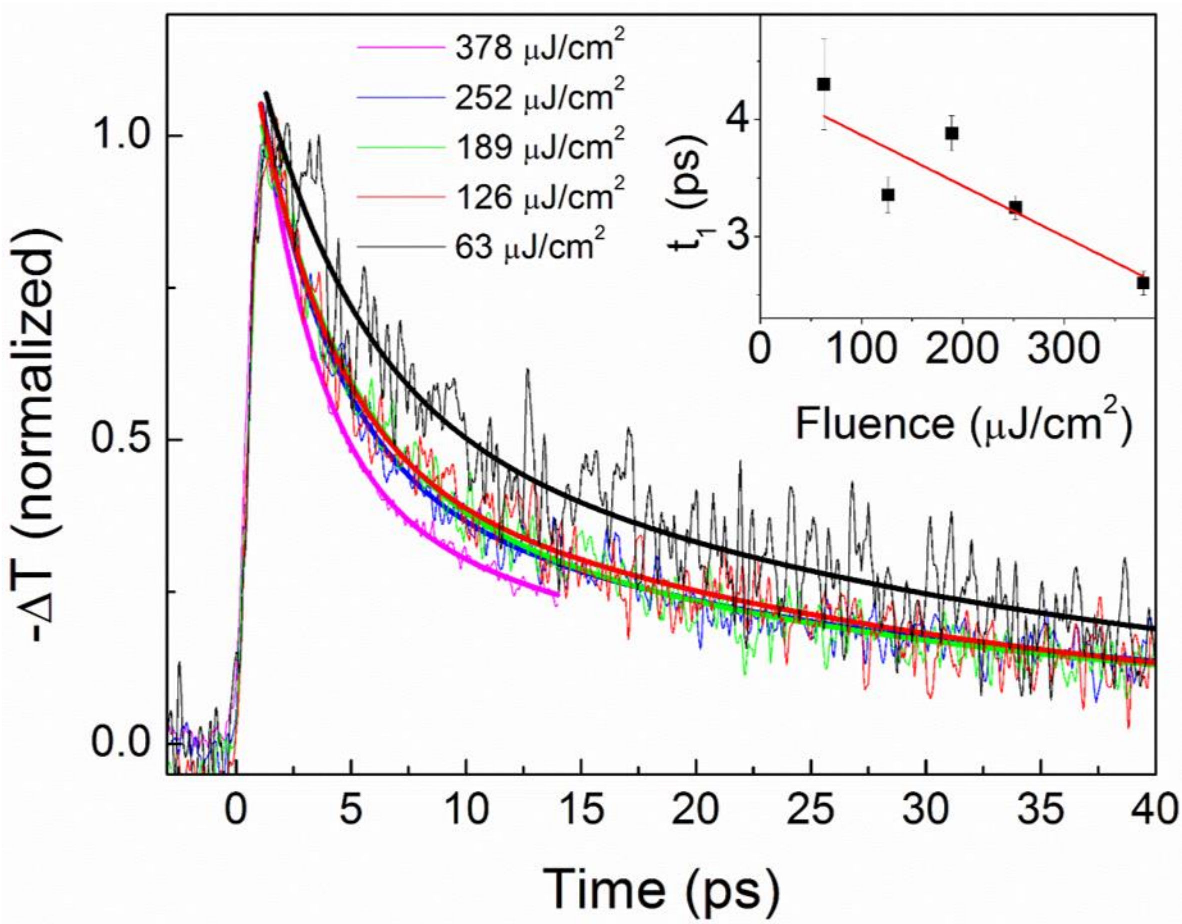

Figure S4. Normalized transient THz photoconductivity for S-annealed film at different excitation fluence values. Inset shows fluence dependence of the fast decay component.

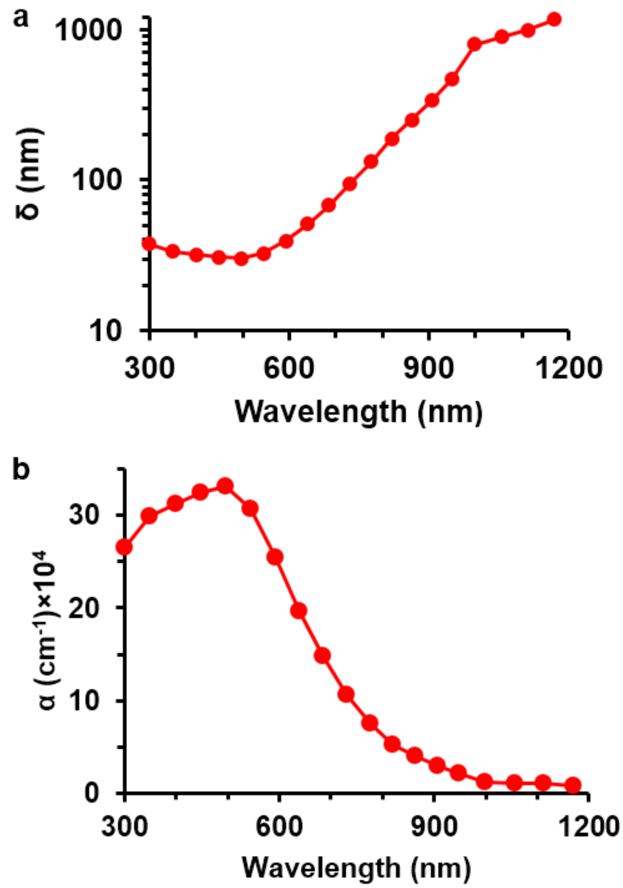

Figure S5. (a) Light absorption depths and (b) absorption coefficients of 10 layers of S-annealed Bi_2S_3 thin film.

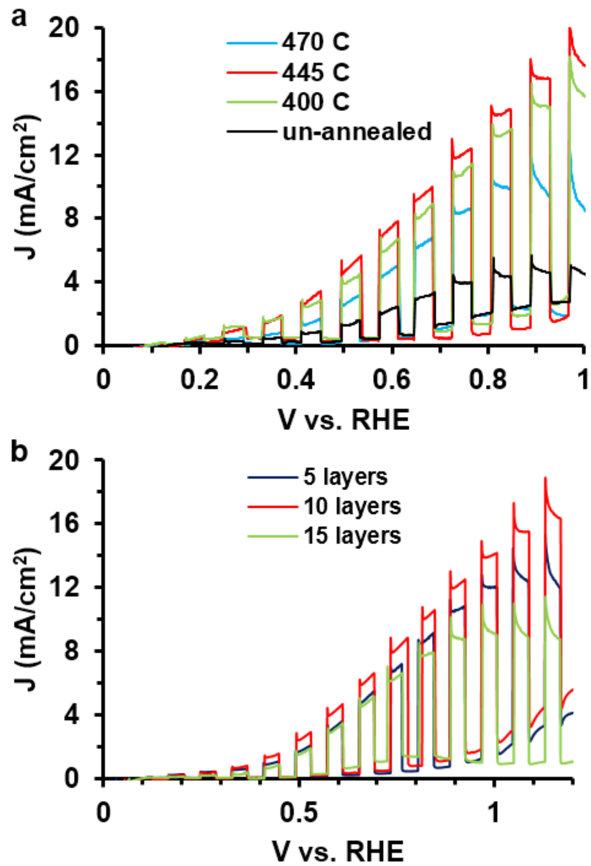

Figure S6. *J*-*V* measurements in 0.3 M Na_2S aqueous electrolyte. (a) 10 layers of Bi_2S_3 thin films without annealing and with sulfur vapor annealing at different temperatures. (b) Bi_2S_3 thin films with different thickness annealed at 445 °C in sulfur vapor.