Supporting Information

Constrained Growth of MoS_2 Nanosheets within a Mesoporous Silica Shell and Its Effects on Defect Sites and Catalyst Stability for H_2S Decomposition

Kelvin Mingyao Kwok[1,2], Sze Wei Daniel Ong[2], Luwei Chen[2]*, Hua Chun Zeng[1]*

[1] *NUS Graduate School for Integrative Sciences and Engineering and Department of Chemical and Biomolecular Engineering, Faculty of Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260*

[2] *Department of Heterogeneous Catalysis, Institute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1 Pesek Road, Jurong Island, 627833, Singapore*

*Emails: chen_luwei@ices.a-star.edu.sg
chezhc@nus.edu.sg

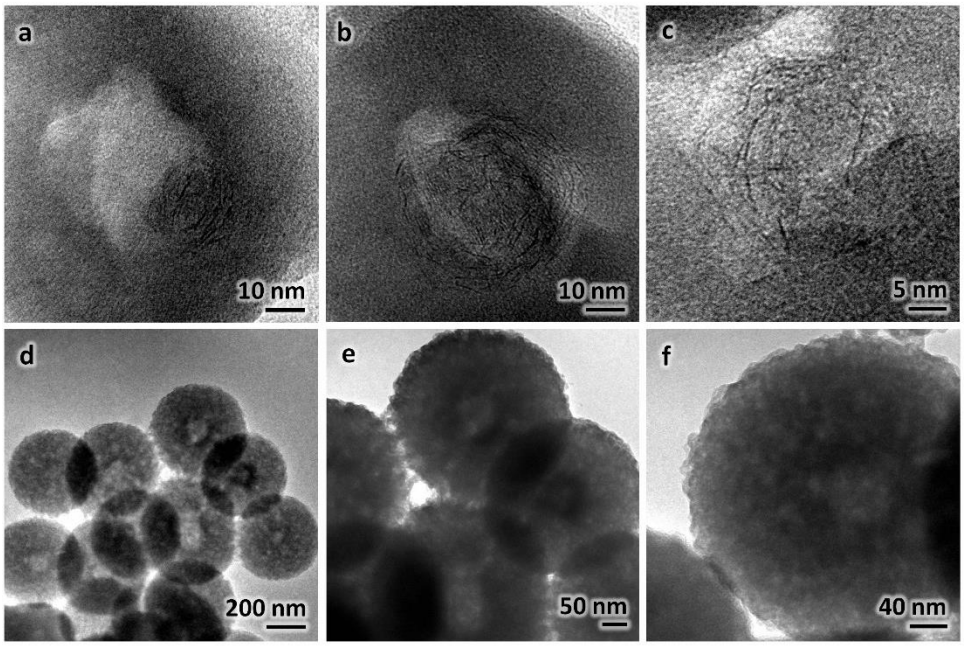

Figure S1. TEM images of MoS_2@SiO_2 synthesized from 100 mg of MoO_2@SiO_2 and 150 mg of thioacetamide in 40 mL of deionized water at a-c) 200°C for 12 h, and d-f) 170°C for 24 h.

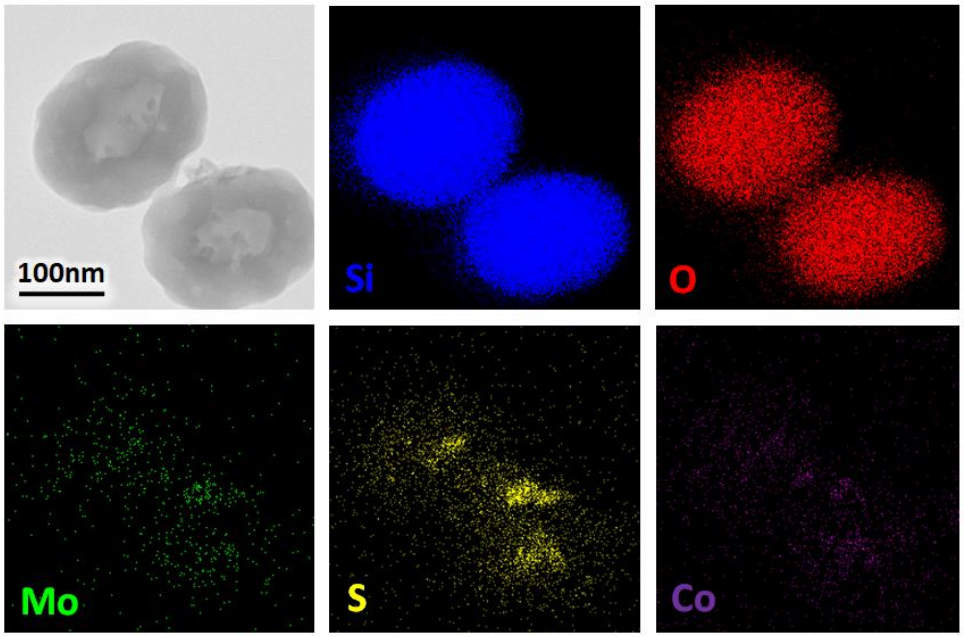

Figure S2. FETEM-EDX mapping images of MoS_2-Co@SiO_2 sample. Synthesis conditions: 100 mg of MoO_2@SiO_2, 20 mg of cobalt(II) acetate tetrahydrate, and 150 mg of thioacetamide in 40 mL of deionized water at 200°C for 24 h.

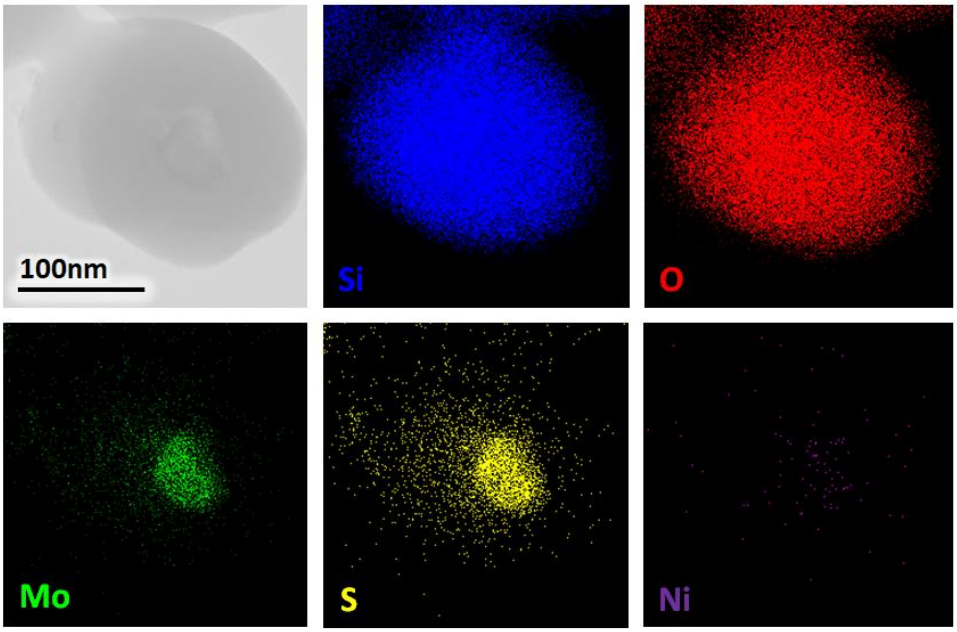

Figure S3. FETEM-EDX mapping images of MoS_2-Ni@SiO_2 sample. Synthesis conditions: 100 mg of MoO_2@SiO_2, 20 mg of nickel(II) acetate tetrahydrate, and 150 mg of thioacetamide in 40 mL of deionized water at 200°C for 24 h.

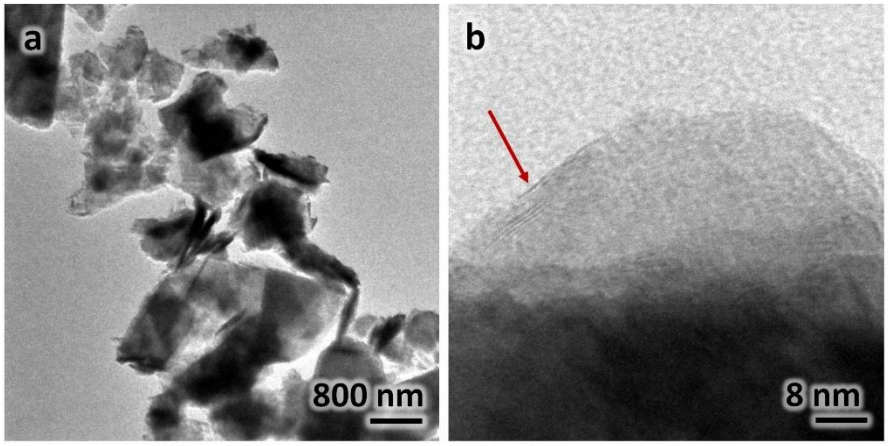

Figure S4. TEM images of bulk MoS_2 obtained commercially from Sigma Aldrich.

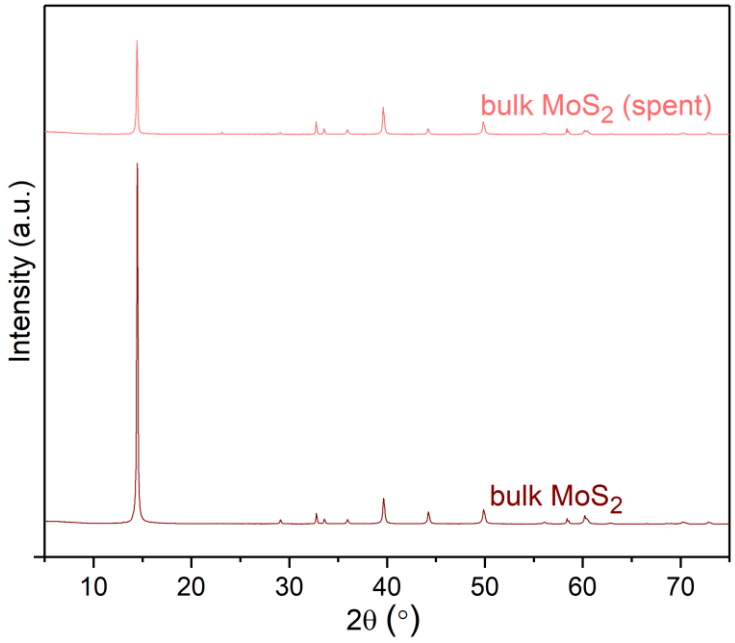

Figure S5. XRD patterns of fresh and spent bulk MoS_2 catalysts.

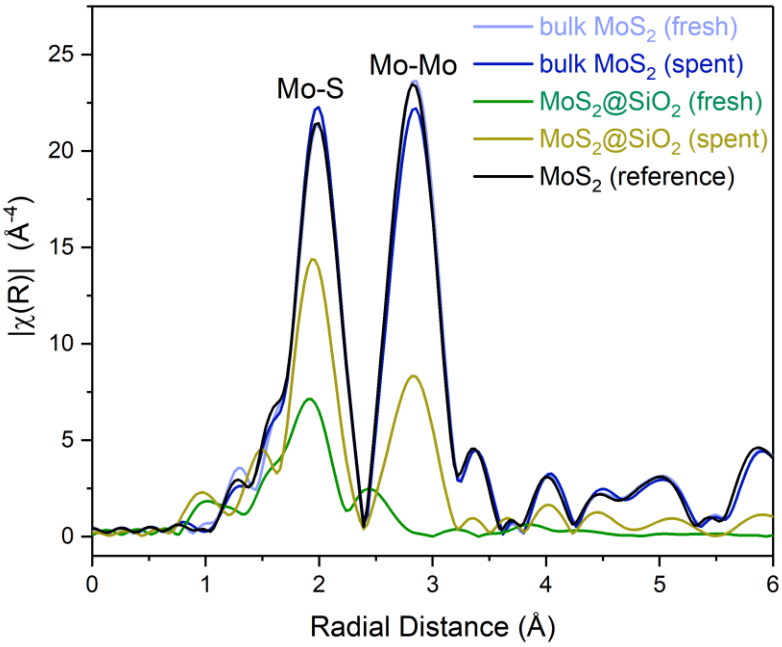

Figure S6. Fourier-transforms of Mo *K*-edge EXAFS for fresh and spent bulk MoS_2 and MoS_2@SiO_2 catalysts.

Figure S7. Solid sulfur collected after H_2S decomposition, collected at the bottom of the reaction tube.

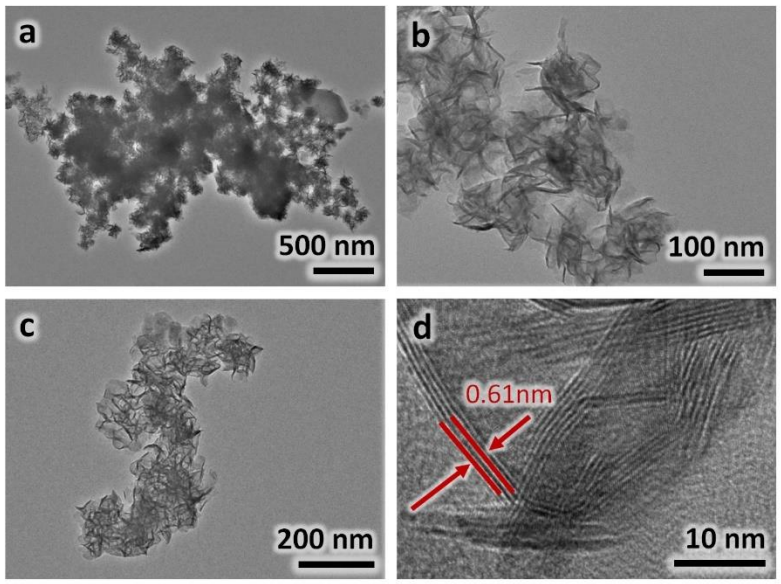

Figure S8. TEM images of a spent MoS_2-NP catalyst after H_2S decomposition reaction (500–800°C, total reaction time 12 h).

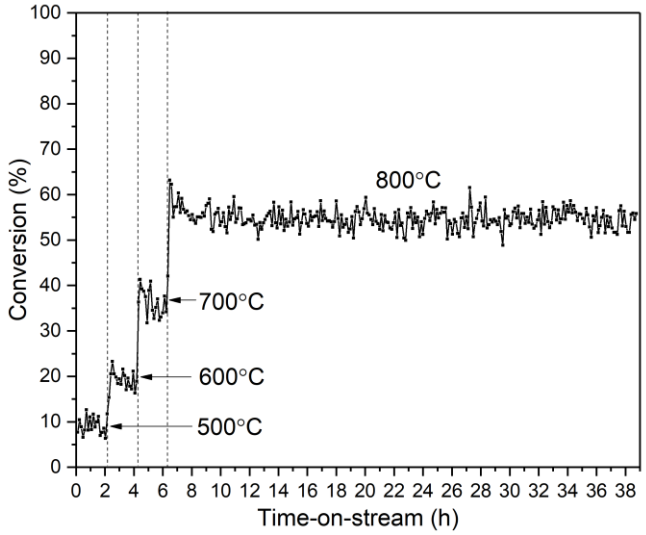

Figure S9. (a) Conversion of H_2S for the MoS_2@SiO_2 catalysts. Reaction conditions: 50 mg catalyst, 40 mL/min of 2500 ppm H_2S in N_2, 2 h of reaction at 500°C, 600°C, 700°C, and 800°C, respectively, after which another 30 h of test was applied (total time-on-stream: 38 h).

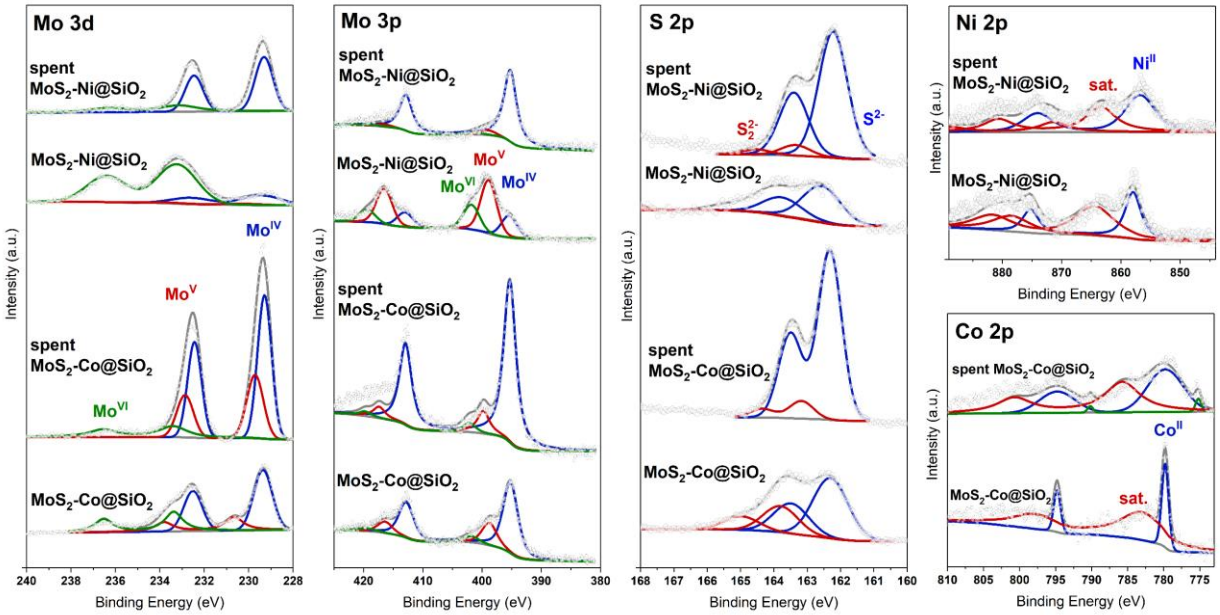

Figure S10. XPS spectra of the bulk MoS_2, MoS_2-NP, and MoS_2@SiO_2 samples and their spent catalysts after H_2S decomposition reaction.

Table S1. ICP-OES analysis results of the various MoS_2 catalysts. Pure MoS_2 (i.e. MoS_2-NP, bulk MoS_2) would have a theoretical Mo content of 59.9 wt%.

Catalyst	Metal content (wt%)
MoO_2@SiO_2	6.76% Mo
MoS_2@SiO_2	7.46% Mo
MoS_2-Co@SiO_2	7.17% Mo, 4.27% Co
MoS_2-Ni@SiO_2	7.54% Mo, 3.97% Ni