Electronic Supplementary Information

DFT study and experimental evidence for the sonication-induced cleavage of molybdenum sulfide Mo_2S_3 in liquids

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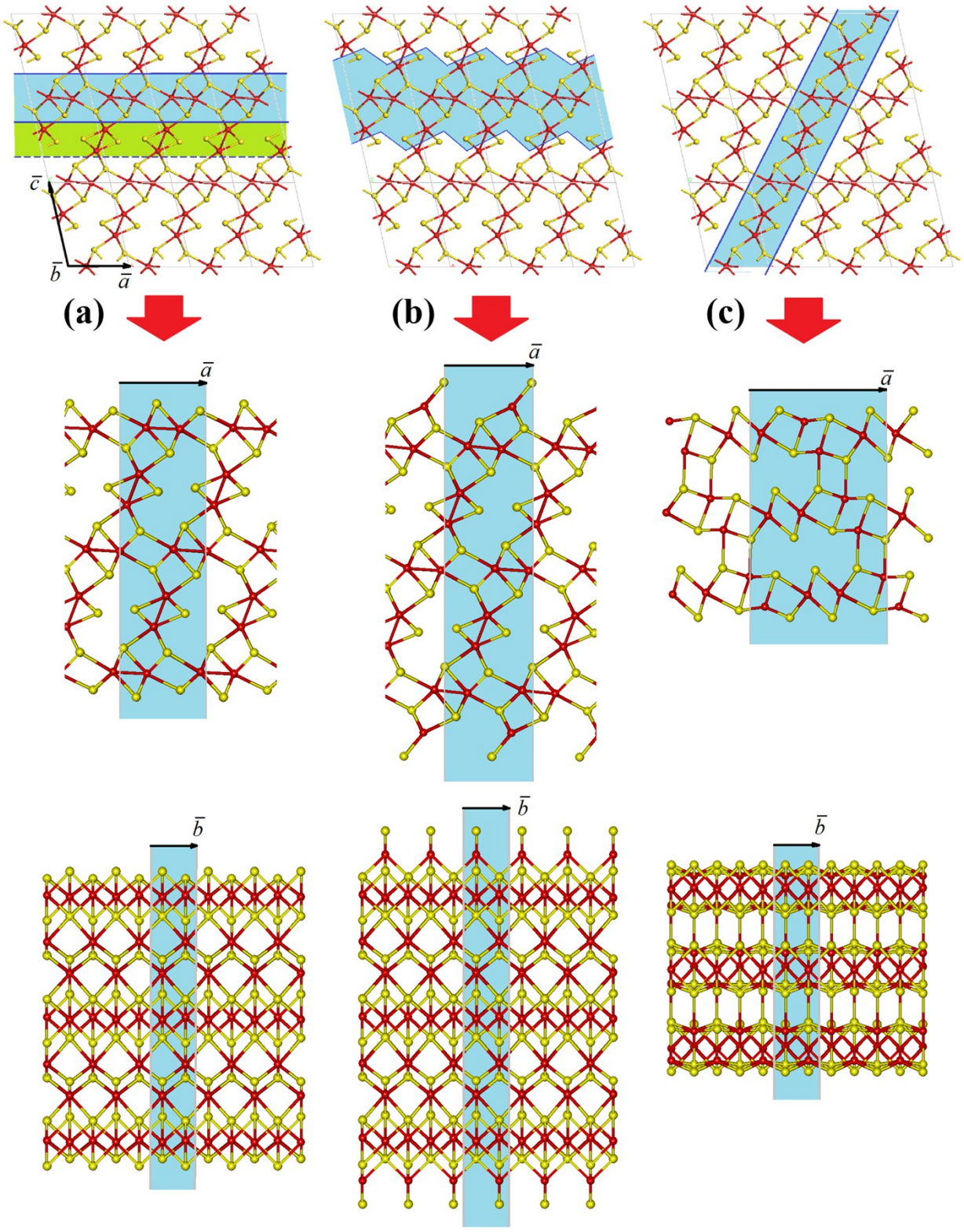

Fig. S1. Three possible methods of cleaving Mo_2S_3 crystal into nanosheets depending on the construction of a single "molecular" layer (*painted fields on the top*): (a) along the (001) plane with removal of unsaturated Mo and S atoms; (b) along the (001) plane and with tetrahedral coordination of surface Mo atoms; (c) along the $(\bar{1}01)$ plane. The models of triple layer nanosheets corresponding to every type of cleavage are visualized below in two main directions and with painted unit cell. Mo and S atoms are painted in red and yellow, respectively. Geometry of all structures is optimized using DFT method.

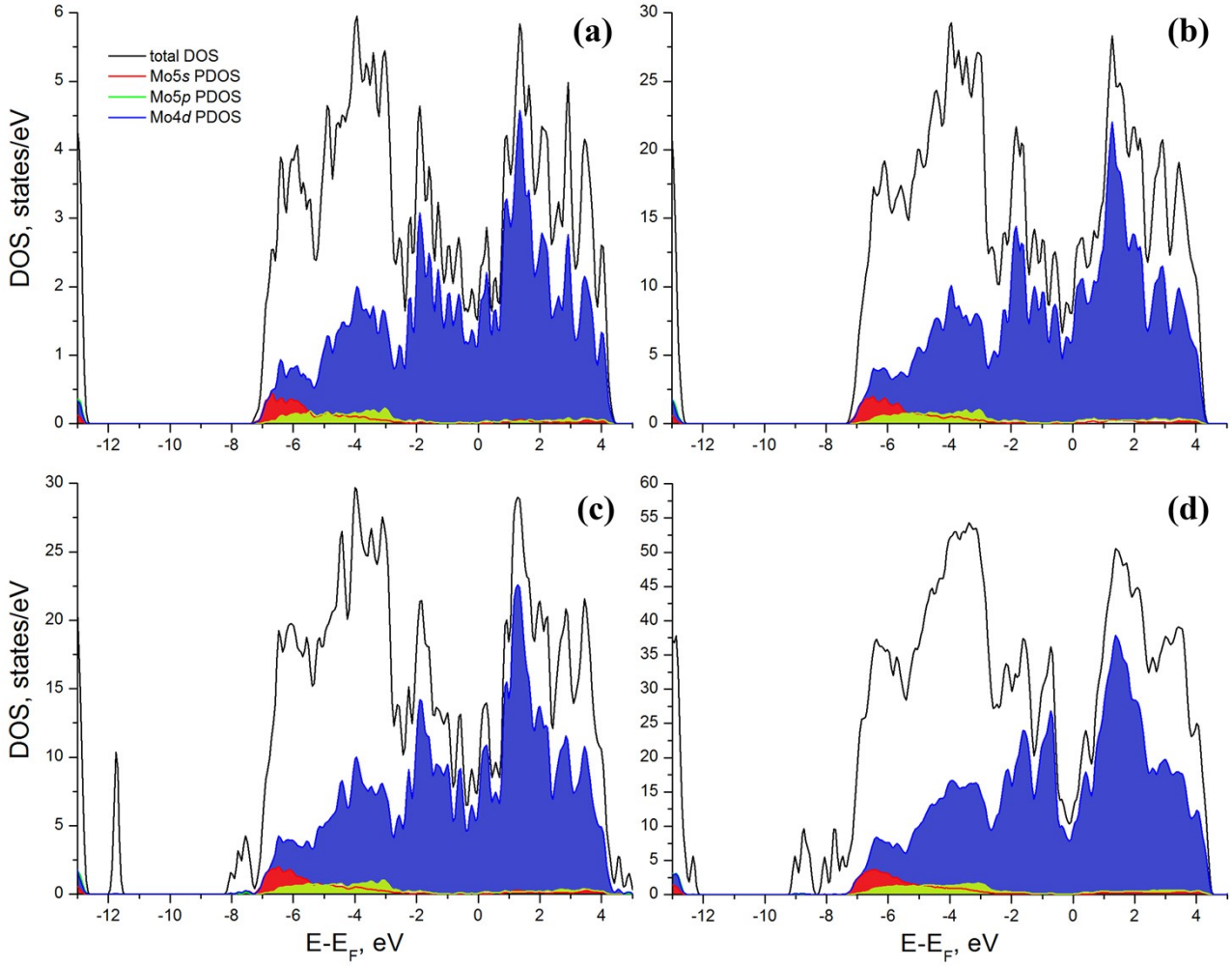

Fig. S2. Total and partial Mo densities of states for the bulk Mo_2S_3 (a), the clean $Mo_2S_3(\bar{1}01)$ five-layer nanosheet (b) and the same nanosheet with H_2O (c) or DMSO molecules (d) anchored to Mo atoms. DFT calculations.

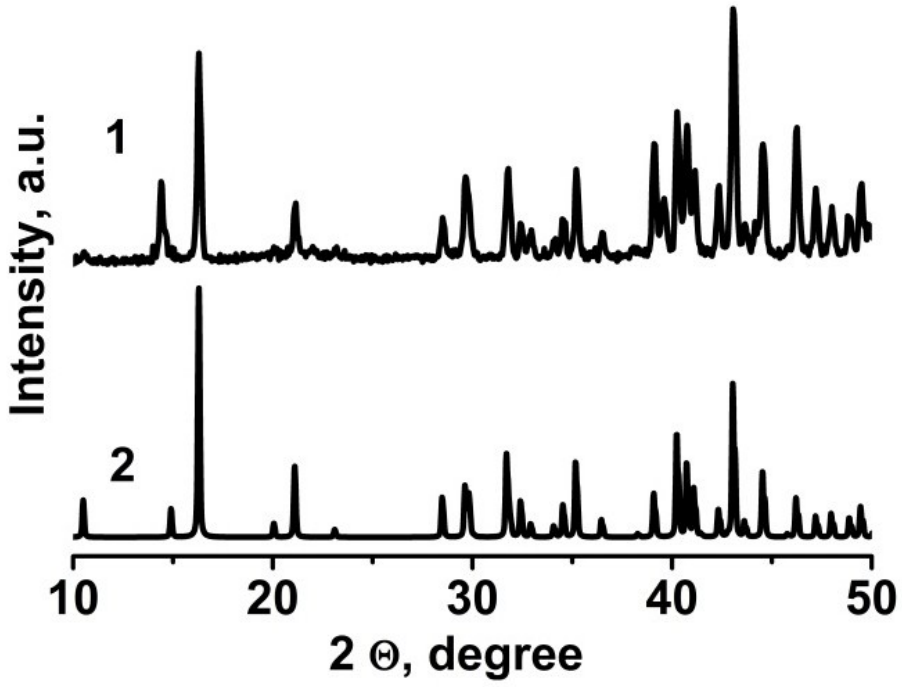

Fig S3. XRPD data of the bulk Mo_2S_3 sample (line 1) compared with the theoretical X-ray diffraction pattern of Mo_2S_3 (line 2) (73453-ICSD card).

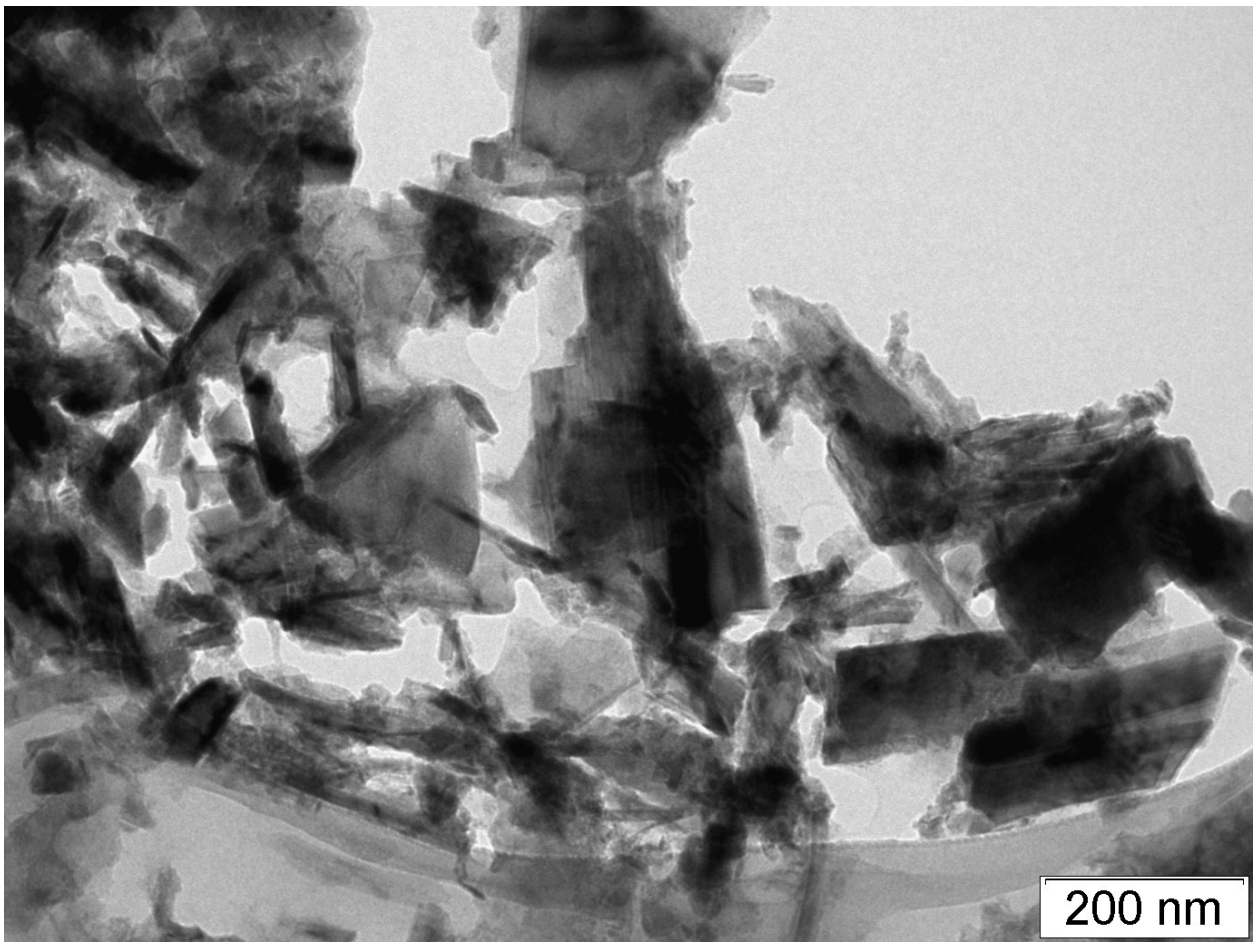

Fig. S4. HRTEM overview of the Mo_2S_3 nanostructures in colloids from the ethanol-water dispersion

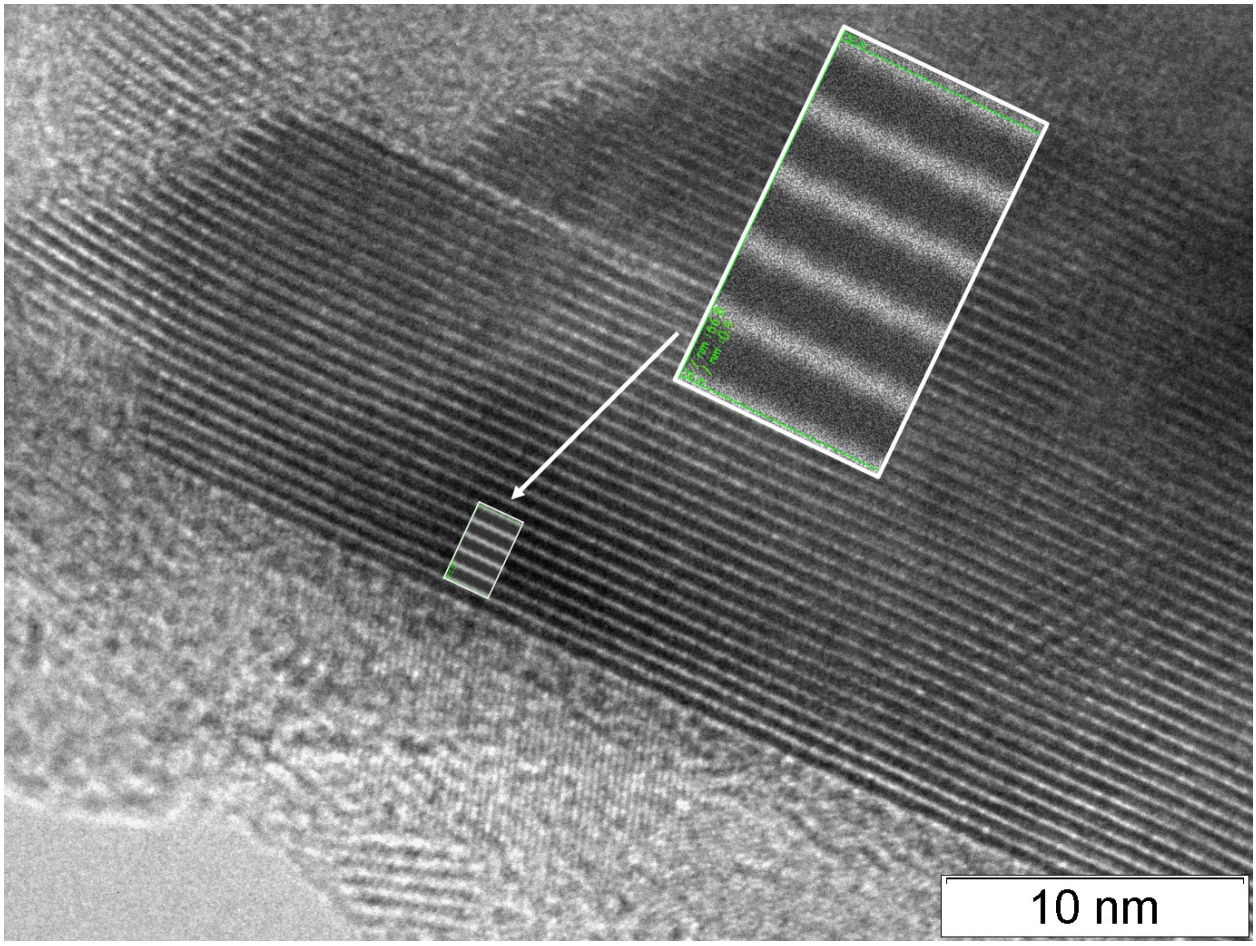

Fig. S5. HRTEM image of Mo_2S_3 particle obtained from the dispersion in ethanol-water, showing its layer structure (inset is simulated image with lattice fringes (-101), corresponding zone axis: [101] of the crystal (parameters are: d / nm = 66.8, t / nm = 0.9, where d – defocusing of microscope, t - thickness of the crystal).

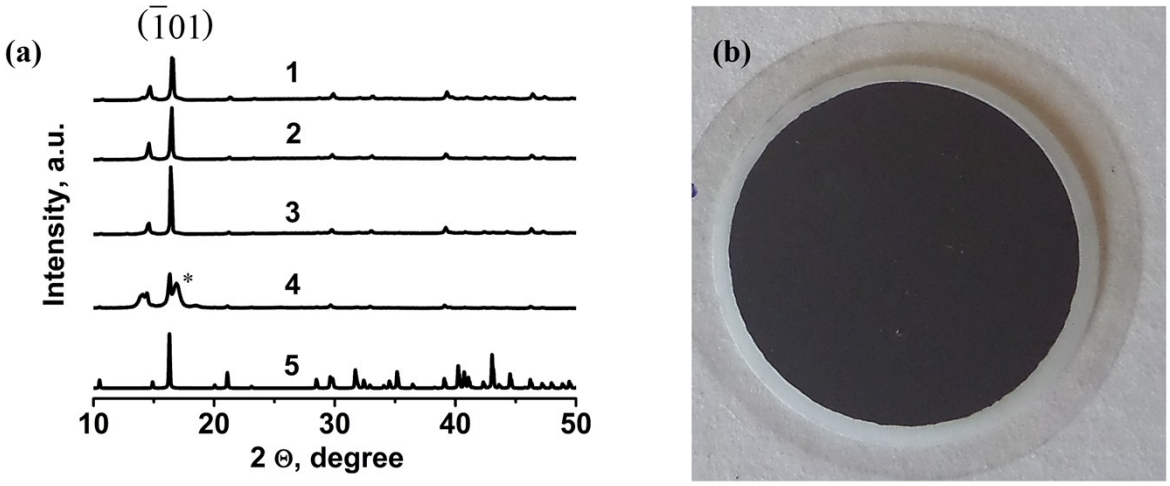

Fig. S6. (a) – XRPD data for films obtained by filtering the dispersions in ethanol-water mixture (1), i-PrOH (2), NMP (3), DMSO (4) compared with the theoretical X-ray diffraction of Mo_2S_3 (5) (73453-ICSD card). Symbol (*) indicates the reflection of filter material. (b) – photograph of film prepared from DMSO dispersion by filtration.

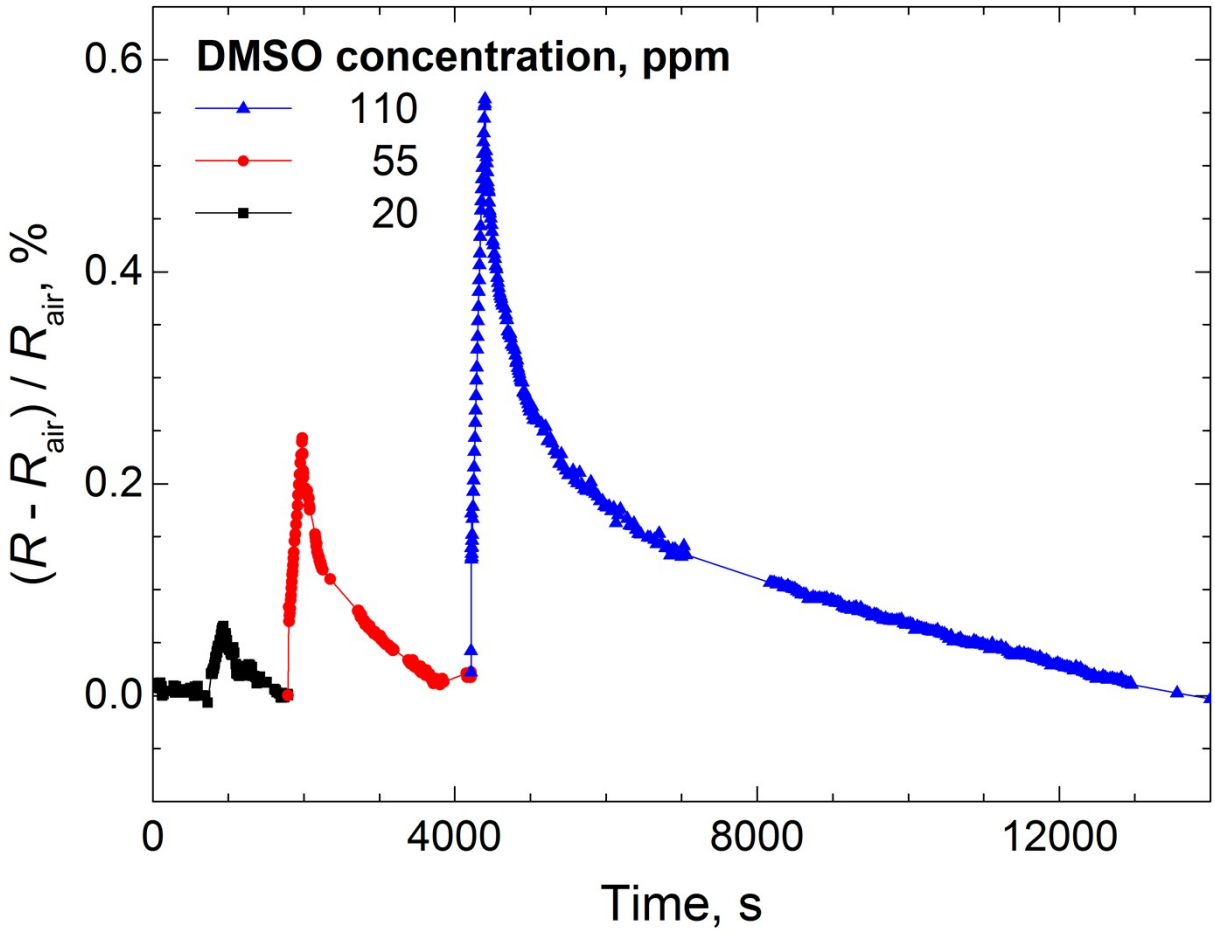

Fig. S7. Time dependence of electrical resistance of the Mo_2S_3 thin film sample in the presence of DMSO during the whole experimental time range. The dependence shows that the resistance was completely recovered in about 14000 s.