ELECTRONIC SUPPLEMENTARY INFORMATION

DFT Investigation of NH_3 Physisorption on $CuSO_4$ Impregnated SiO_2

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Table S-1 Energy of complexation (for reaction SSQ + CS → SSQ·CS) of optimized $SiO_2/CuSO_4$ complexes with variable final position of the Cu^{2+} and SO_4^{2-} ions. See Fig. S-1 for the corresponding geometries.

$SiO_2/CuSO_4$ Structure	Total Energy (kJ/mol)
SSQ•CS	-213.4
SSQ•CS(II)	-167.9
SSQ•CS(III)	-209.1
SSQ•CS(IV)	-165.7

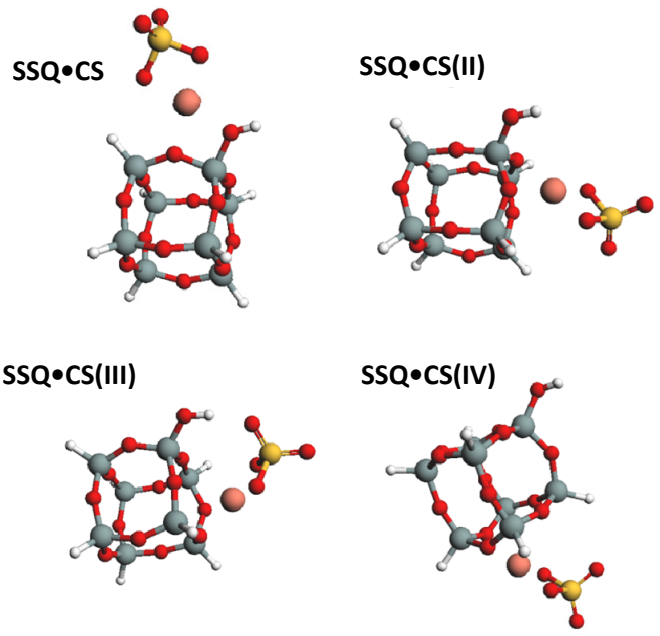

Fig. S-1 3D Optimized geometries of various configurations of SSQ•CS.

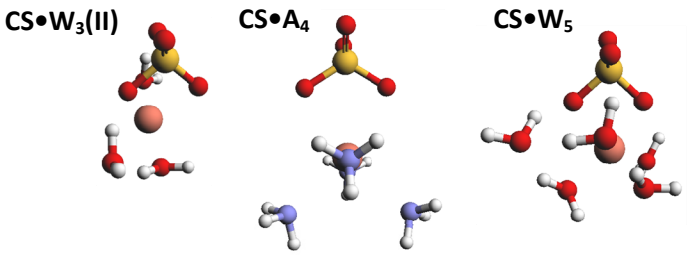

Fig. S-2 Structures demonstrating the influence of hydrogen bonding in $CuSO_4$ complexed with (from left to right) 3 H_2O, 4 NH_3, or 5 H_2O.