Supporting Information

Effect of CO and CO_2 on the desulfurization of H_2S using ZnO sorbent: A density functional theory study

Lixia Ling [a], Zhongbei Zhao [a], Baojun Wang *, [b], Maohong Fan *, [c], Riguang Zhang [b]

a) *College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, Shanxi, P.R. China E-mail: linglixia@tyut.edu.cn*

b) *Key Laboratory of Coal Science and Technology (Taiyuan University of Technology), Ministry of Education and Shanxi Province, Taiyuan 030024, Shanxi, People' Republic of China E-mail: wangbaojun@tyut.edu.cn*

c) *Department of Chemical and Petroleum Engineering, the University of Wyoming, Laramie, WY 82071, USA E-mail: mfan@uwyo.edu*

Table S1 The imaginary frequency of every transition state.

H_2S+CO		H_2S+CO_2	
Transition state	Imaginary frequency(cm^{-1})	Transition state	Imaginary frequency(cm^{-1})
TS1	-138.33	TS1*	-195.13
TS2	-936.01	TS2*	-235.71
TS3	-112.03	TS3*	-1095.74
TS4	-185.32	TS4*	-134.57
TS5	-298.51	TS5*	-345.24
		TS6*	-1685.37
		TS7*	-71.32
		TS8*	-1671.95

Table S2 Electronic total energy, enthalpy correction (H') and Gibbs free energy correction (G') of every species for R1 and R2 at different temperatures (K).

	E_{elec}($kJ·mol^{-1}$)	*H' (including ZPVE) (kJ·mol^{-1})*				*G' (including ZPVE) (kJ·mol^{-1})*			
		298.15	500	650	1000	298.15	500	650	1000
H_2S	-1048628.5	51.6	60.5	67.5	85.3	-15.8	-64.0	-102.2	-197.6
CO	-297524.7	21.4	27.3	31.9	43.1	-37.6	-79.2	-111.7	-191.6
COS	-1343129.4	31.0	39.9	47.1	64.9	-29.1	-72.3	-106.9	-193.8
H_2	-3073.2	34.8	40.7	45.0	55.3	-5.8	-35.0	-58.3	-116.3
CO_2	-495223.1	40.2	49.5	57.2	76.8	-1.0	-31.4	-56.7	-122.4
H_2O	-200695.2	64.7	71.6	77.0	90.6	6.6	-34.6	-67.2	-147.9

Table S3 Electronic total energy, enthalpy correction (*H*') and entropy (S) for the rate-determined step of forming COS at different temperatures (K).

		H' (including ZPVE) ($kJ·mol^{-1}$)			*S* ($J·mol^{-1}·K^{-1}$)		
	E_{elec}($kJ·mol^{-1}$)	298.15	500	1000	298.15	500	1000
IM4	-39478285.8	944.1	1384.5	2574.3	2358.6	3480.9	5124.8
TS4	-39478198.1	939.3	1378.7	2564.9	2396.7	3516.2	5155.2
IM6*	-39675956.4	964.0	1406.7	2606.0	2369.4	3497.3	5154.1
TS6*	-39675814.0	949.9	1391.6	2588.4	2363.7	3488.9	5142.3