

Supporting Information

Theoretical investigation of H₂S removal on the γ -Al₂O₃ surfaces of different hydroxyl coverage

Table S1. The comparison of the calculated values at the different k-point mesh

	D100		
	H ₂ S, E_{ad} (kJ/mol)	HS+H, E_{ad} (kJ/mol)	TS1 _a , E_a (kJ/mol)
3×3×1	-32.52	-587.55	13.22
5×5×1	-32.35	-587.36	13.36
Deviation	0.52%	0.03%	1.05%