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Supporting Information

Theoretical investigation of H_2S removal on the $\gamma\text{-}Al_2O_3$ surfaces of different hydroxyl coverage

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

	D100		
	H_2S , $E_{ad}(kJ/mol)$	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%