

Supplementary materials

Figures

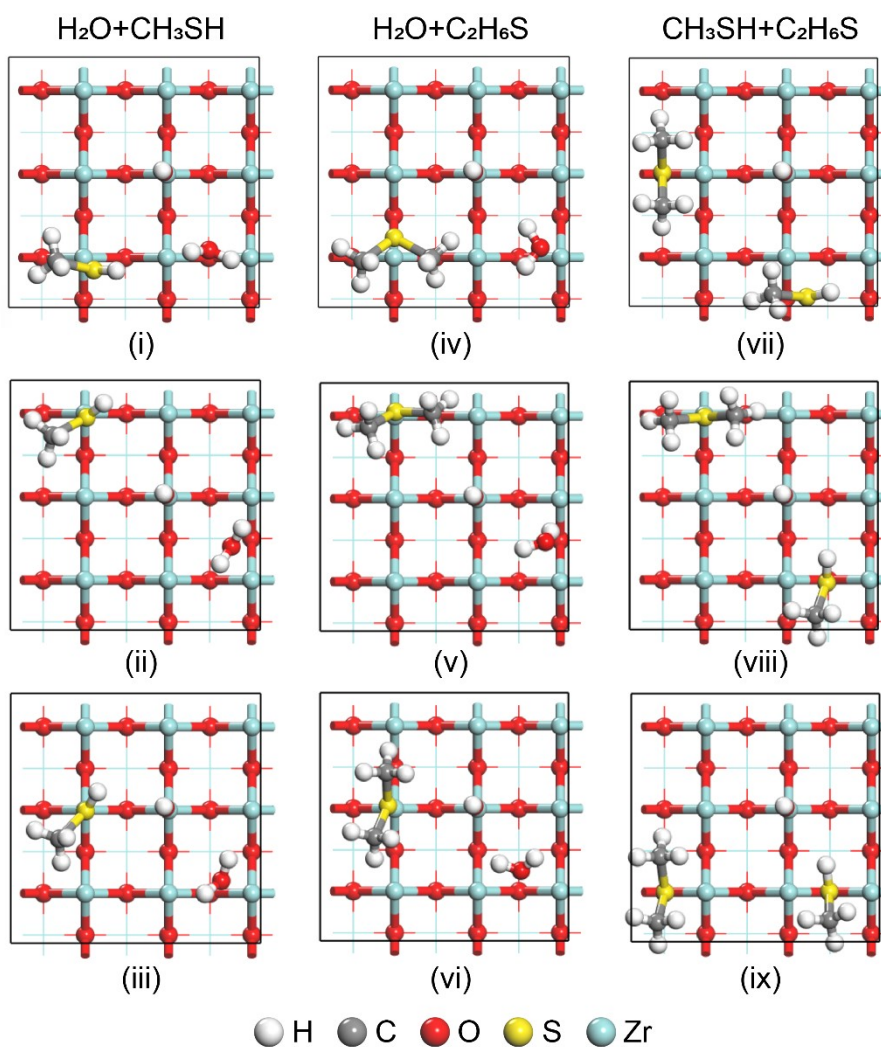


Fig. S1. Optimised adsorption configuration for two-gas molecules adsorption over hydroxyl-modified ZrO₂

Tables

Table S1 Adsorption energy of two-gas molecules adsorption over hydroxyl-modified

ZrO ₂	
Adsorptive geometries	Adsorption energy (kJ/mol)
(i)	-219.78
(ii)	-172.14

(iii)	-185.03
(iv)	-173.37
(v)	-134.25
(vi)	-151.72
(vii)	-148.04
(viii)	-118.22
(ix)	-129.46
