Supplementary material for

"First-principles investigation of H_2S adsorption and dissociation on titanium carbide surface"

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Table S1. The activation energy (E_{act} in eV) for H_2S dissociation on the surfaces of TiC, metal oxides of CeO_2, YSZ and various noble metals of Ir, Ni, Pd, Pt.

	E_{act} (eV)
TiC(001) (In this work)	
$H_2S \rightarrow SH + H$	0.34/0.32
$SH + H \rightarrow S + H + H$	1.32/1.48
$SH \rightarrow S + H$	1.16
$CeO_2(111)$[1]	
$H_2S \rightarrow SH + H$	0.19
$SH + H \rightarrow S + H + H$	0.69
YSZ(111)[2]	
$H_2S \rightarrow SH + H$	0.17
$SH \rightarrow S + H$	0.34
Ir(111)[3]	
$H_2S \rightarrow SH + H$	0.16
$SH \rightarrow S + H$	0.05
Ni(111)[3]	
$H_2S \rightarrow SH + H$	0.21
$SH \rightarrow S + H$	0.01
Pd(111)[3]	
$H_2S \rightarrow SH + H$	0.22
$SH \rightarrow S + H$	0.01
Pt(111)[3]	
$H_2S \rightarrow SH + H$	0.07
$SH \rightarrow S + H$	0.03
Pt/graphene[4]	
$H_2S \rightarrow SH + H$	0.27

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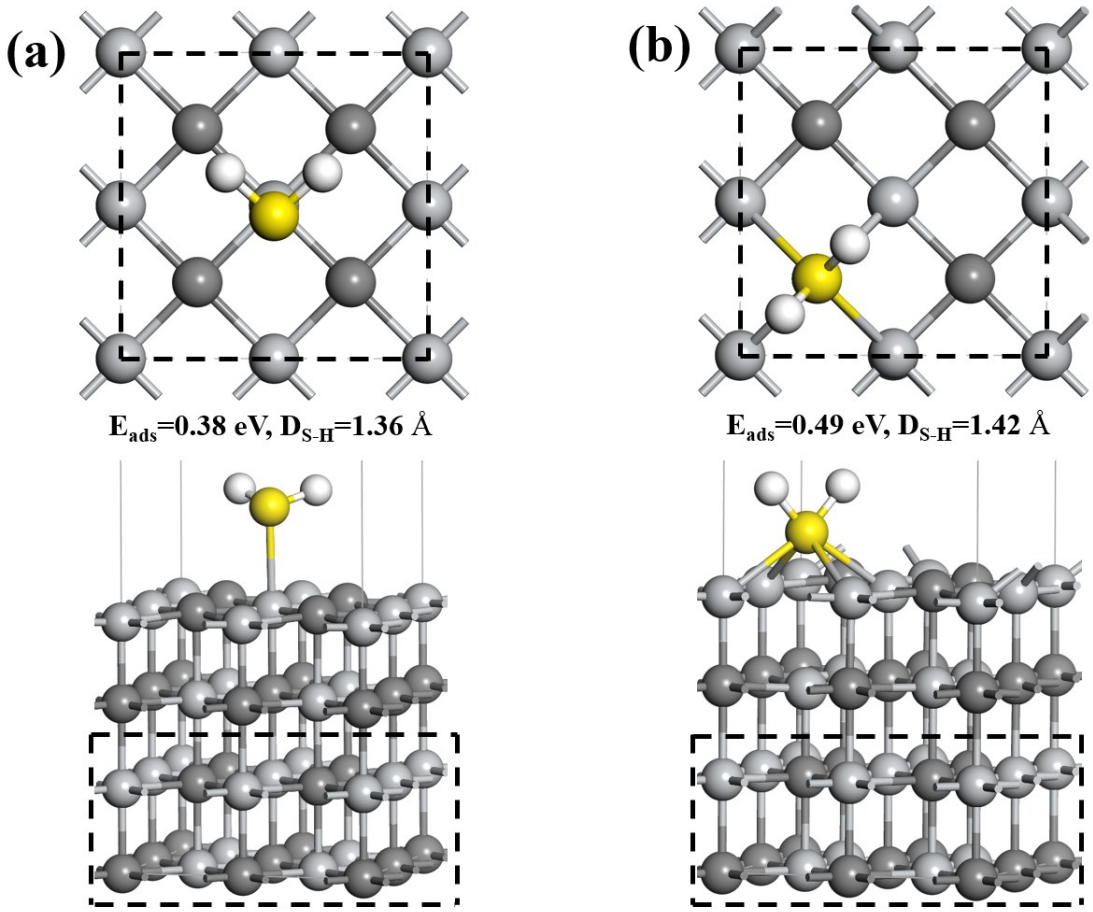

Fig. S1. Optimized structures for H_2S adsorbed on (a) the pure TiC(001), (b) the defective TiC(001) surface with a carbon vacancy (V_C-TiC(001)). The adsorption energies (E_{ads} in eV) and the S–H distances (D_{S-H} in Å) are shown in the figure. Color code: the black, light gray, yellow and white spheres denote the C, Ti, S and H, respectively.