Electronic Supporting Information
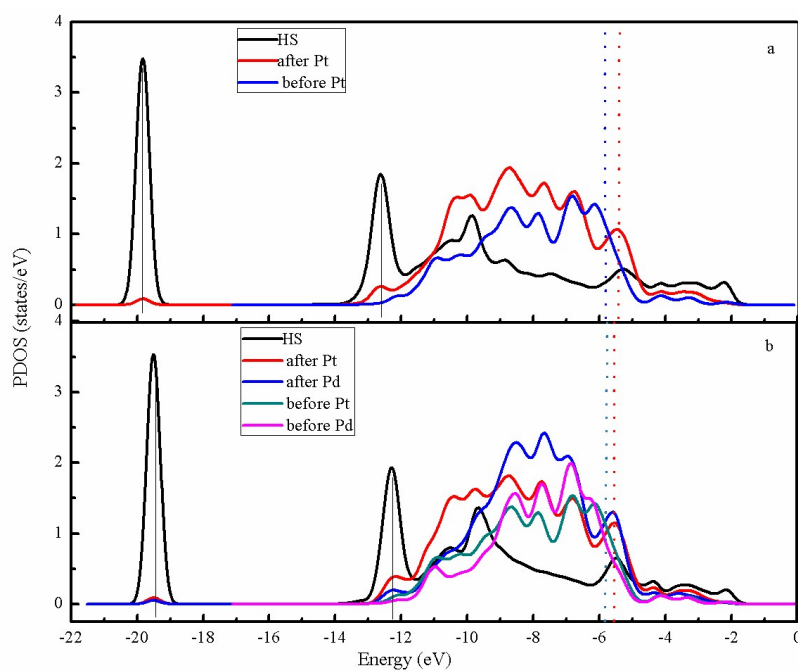

Fig. S1. PDOS of HS adsorption on Pt-1Pd(111): (a) HS at the B_1 site, (b) HS at the B_2 site.

S + H → HS
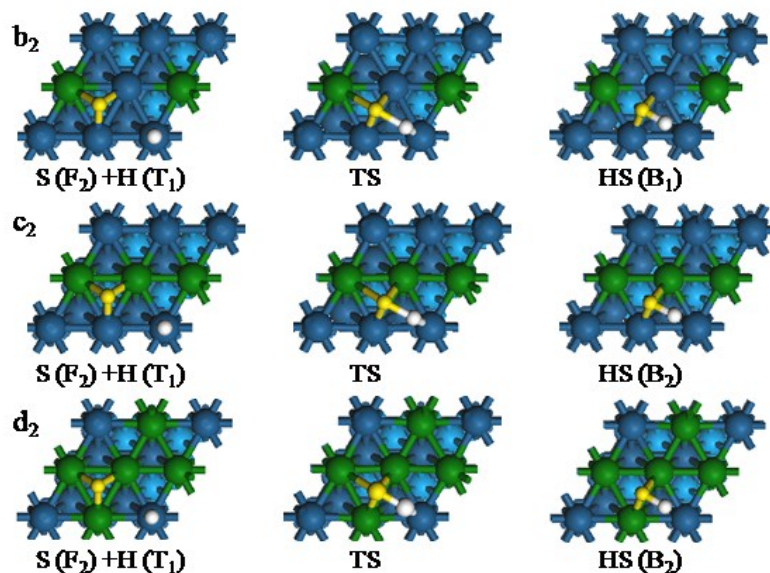

Fig. S2 The structures of the initial, transition and final states for S+H→HS path(II) reaction. (b_2) On Pt-1Pd(111), (c_2) On Pt-2Pd(111), (d_2) On Pt-3Pd(111).

HS+H→H$_2$S

b$_2$

HS(B$_2$)+H(T$_1$)　　　　TS　　　　H$_2$S(T$_1$)

c$_2$

HS(B$_2$)+H(T$_1$)　　　　TS　　　　H$_2$S(T$_1$)
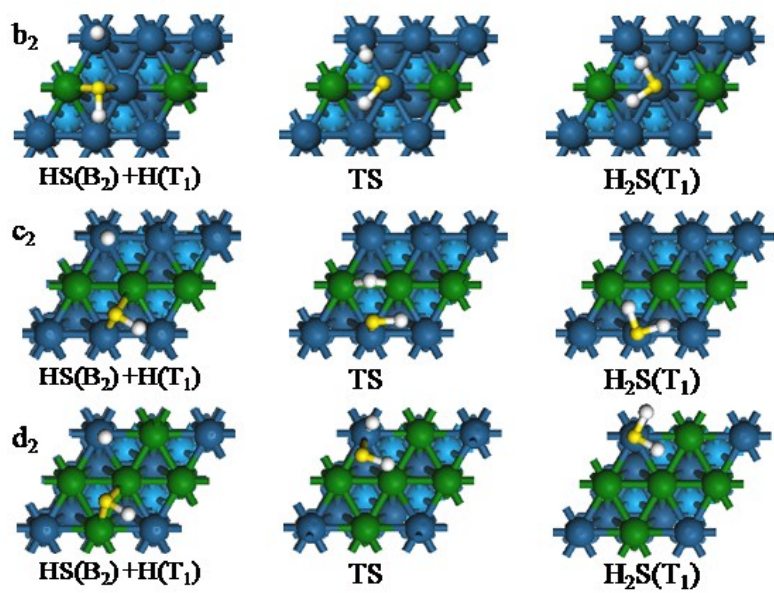
d$_2$

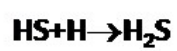
HS(B$_2$)+H(T$_1$)　　　　TS　　　　H$_2$S(T$_1$)

Fig. S3 The structures of the initial, transition and final states for HS+H→H$_2$S path(II) reaction. (b$_2$) On Pt-1Pd(111), (c$_2$) On Pt-2Pd(111), (d$_2$) On Pt-3Pd(111).

Table S1. The imaginary frequency of the transition states in the different reaction

reaction	imaginary frequency(cm^{-1})
Pt	
$S + H \rightarrow HS$	-991
$HS + H \rightarrow H_2S$	-361
Pt-1Pd	
$S(F_1) + H \rightarrow HS$	-908
$HS (B_1) + H \rightarrow H_2S$	-598
$S(F_2) + H \rightarrow HS$	-1089
$HS (B_2) + H \rightarrow H_2S$	-167
Pt-2Pd	
$S(F_1) + H \rightarrow HS$	-911
$HS (B_1) + H \rightarrow H_2S$	-133
$S(F_2) + H \rightarrow HS$	-876
$HS (B_2) + H \rightarrow H_2S$	-296
Pt-3Pd	
$S(F_1) + H \rightarrow HS$	-875
$HS (B_1) + H \rightarrow H_2S$	-397
$S(F_2) + H \rightarrow HS$	-853
$HS (B_2) + H \rightarrow H_2S$	-997
Pt-4Pd	
$S + H \rightarrow HS$	-740
$HS + H \rightarrow H_2S$	-1233
Pd	
$S + H \rightarrow HS$	-750
$HS + H \rightarrow H_2S$	-1017