Electronic Supplementary Material (ESI) for RSC Advances.

A First principle study of H_2S adsorption and decomposition on Ge (100) surface

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Table S1. Calculated lattice constant of bulk Ge with different pseudo- potentials.

Parameters	**Pseudo- potentials**		
	PAW-GGA	**PAW-PBE**	**US-GGA**
lattice constant (Å)	5.79	5.76	5.77
deviation (%) [a]	2.33	1.9	2.0

[a] The definition of deviation is $\frac{|\text{calaulated value} - \text{experimental value}|}{\text{experimental value}} \times 100\%$, in which the experimental value is 5.43 Å.

Table S2. The total energy (E in eV) and barriers for the respective transition states (E_b in eV) for the adsorption of H_2S on a clean Ge(100) surface calcaulted at different functionals and different cutoff energy values. .

	US(300 eV)		**US(450 eV)**		**PBE(300eV)**	
System	**E**	**E_b**	**E**	**E_b**	**E**	**E_b**
H_2S_{ad}	-351.3594		-351.3914		-306.4971	
$LM1_{III}$	-351.9863		-351.8528		-306.7356	
$TS1_{III}$	-351.3099	0.050	-351.2892	0.102	-306.3369	0.1602
$LM1_{II}$	-351.7965		-351.9285		-306.7278	
$TS1_{II}$	-350.9179	0.441	-350.9026	0488	-305.9288	0.5683
$LM1_{I}$	-351.9425		-351.7829		-306.6394	
$TS1_{I}$	-350.8532	0.506	-350.8605	0.530	-305.7885	0.7086

Table S3. Calaulated dimer bond length (d_D) and dimer tilting angle (θ) for a clean Ge(100) surface, compared with results from other calculations and experimental data.

	method	**d_D (Å)**	**θ (deg)**
Ge(100)-4x2	US-this work	2.54	20.7
	LDA[34]	2.41	19.0
	X-ray[35]	2.44	21.0
	STM[36]	2.51	19.7

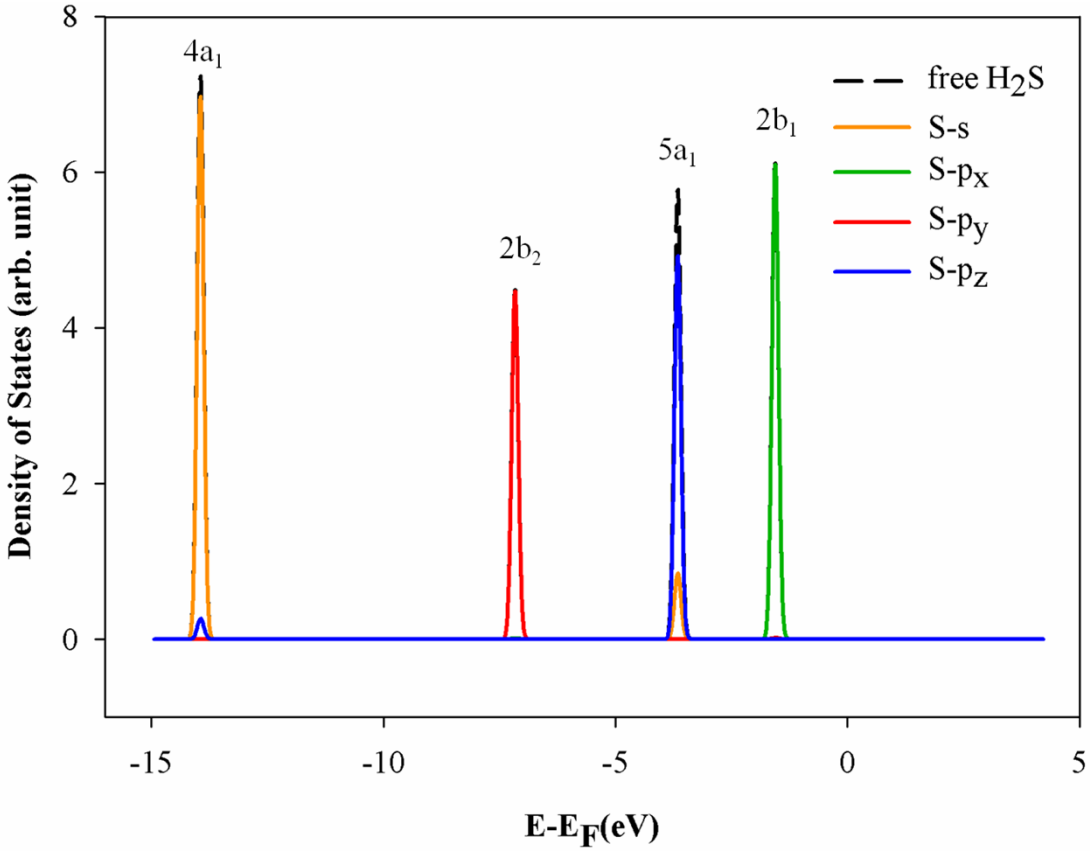

Figure S1. PDOS of gaseous H_2S.

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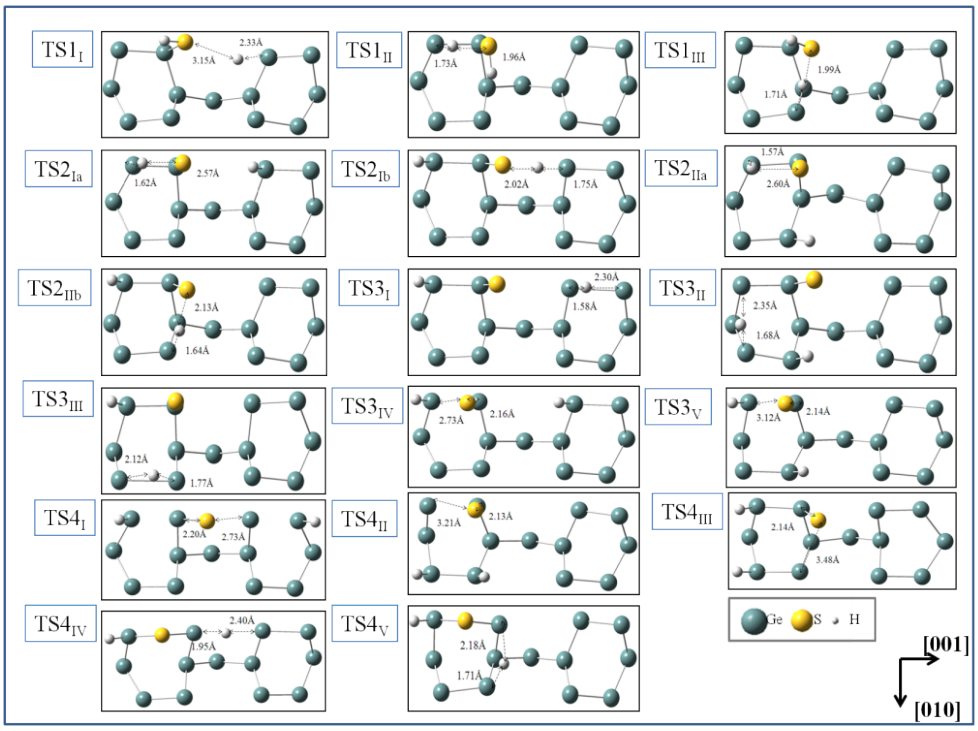

Figure S2. Top view of all transition states of the reactions for H_2S on Ge(100) surface. (a) $TS1_I$, (b) $TS1_{II}$, (c) $TS1_{III}$, (d) $TS2_{I\text{-}a}$, (e) $TS2_{I\text{-}b}$, (f) $TS2_{II\text{-}a}$, (g) $TS2_{II\text{-}b}$, (h) $TS3_I$, (i) $TS3_{II}$, (j) $TS3_{III}$, (k) $TS3_{IV}$, (l) $TS3_V$, (m) $TS4_I$, (n) $TS4_{II}$, (o) $TS4_{III}$, (p) $TS4_{IV}$, (q) $TS4_V$.