

Supplementary Information for:

Adsorption and Desulfurization Mechanism of Thiophene on Layered FeS (001), (011) and (111) Surfaces: A DFT-D2 Study

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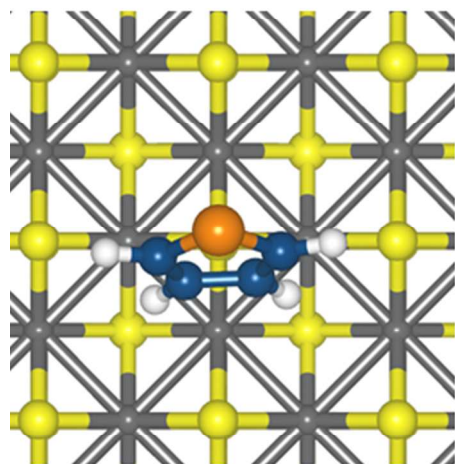
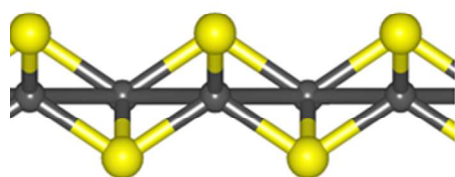
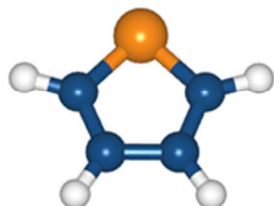
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This supporting information contains the detailed information on all other conformations of thiophene adsorption configurations and structural parameters on stoichiometric (S⁰) FeS (001), (011) and (111). It contains three Figures and one Table.

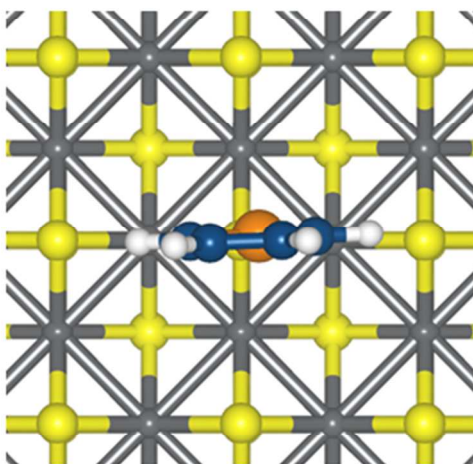
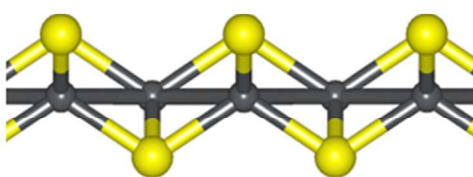
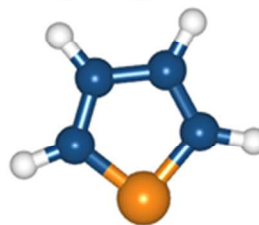
Figure S1: Optimized adsorption structures of a thiophene on stoichiometric (S^0) FeS(001) surface, in side (top) and top (bottom) views. (Colour scheme: Fe = grey, S_{slab} = yellow, C = blue, S_{molecule} = orange).

(b) Slant-H



$$E_{\text{ads}} = -0.19 \text{ eV}$$

(c) Upright-S



$$E_{\text{ads}} = -0.13 \text{ eV}$$

Figure S2: Optimized adsorption structures of a thiophene on stoichiometric (S^0) FeS(011) surface, in side (top) and top (bottom) views. (Colour scheme: Fe = grey, S_{slab} = yellow, C = blue, S_{molecule} = orange).

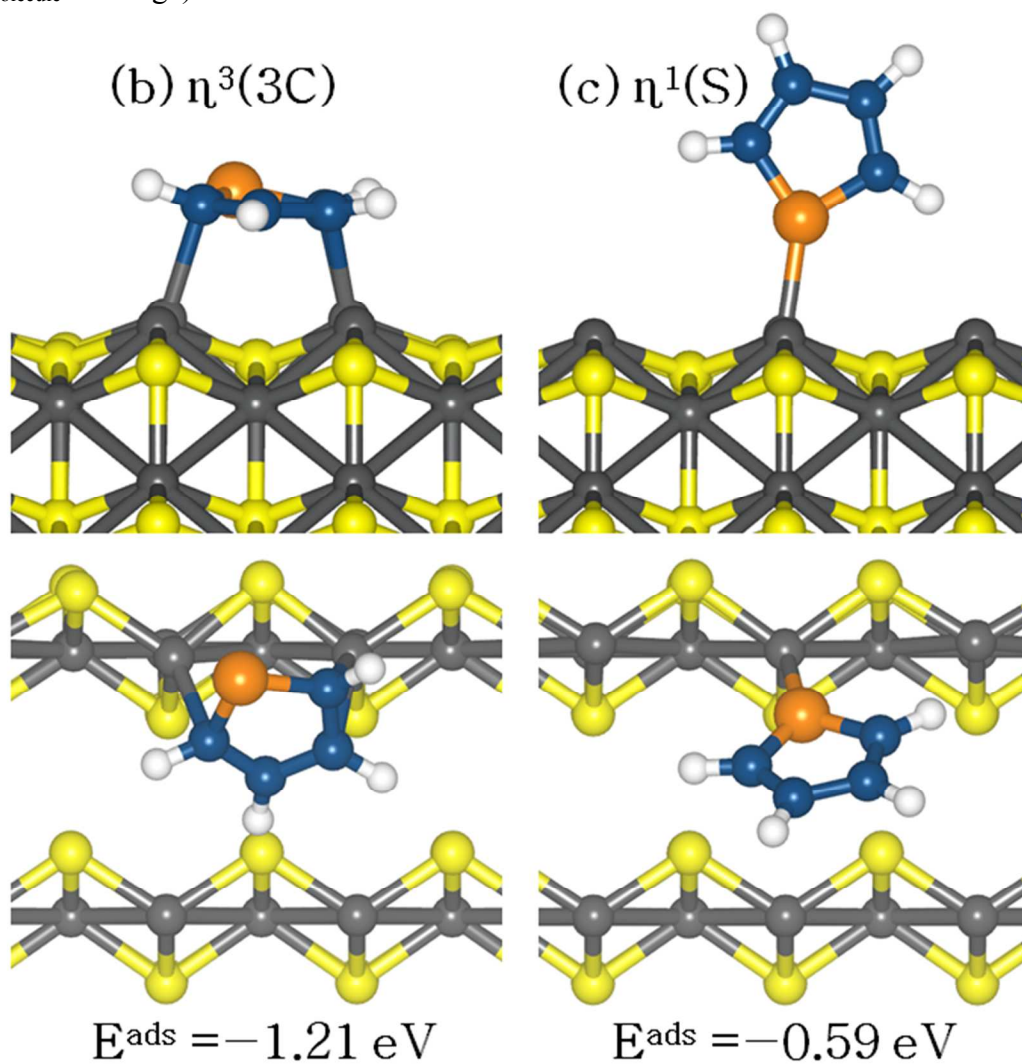


Figure S2: Optimized adsorption structures of a thiophene on stoichiometric (S^0) FeS(111) surface, in side (top) and top (bottom) views. (Colour scheme: Fe = grey, S_{slab} = yellow, C = blue, S_{molecule} = orange).

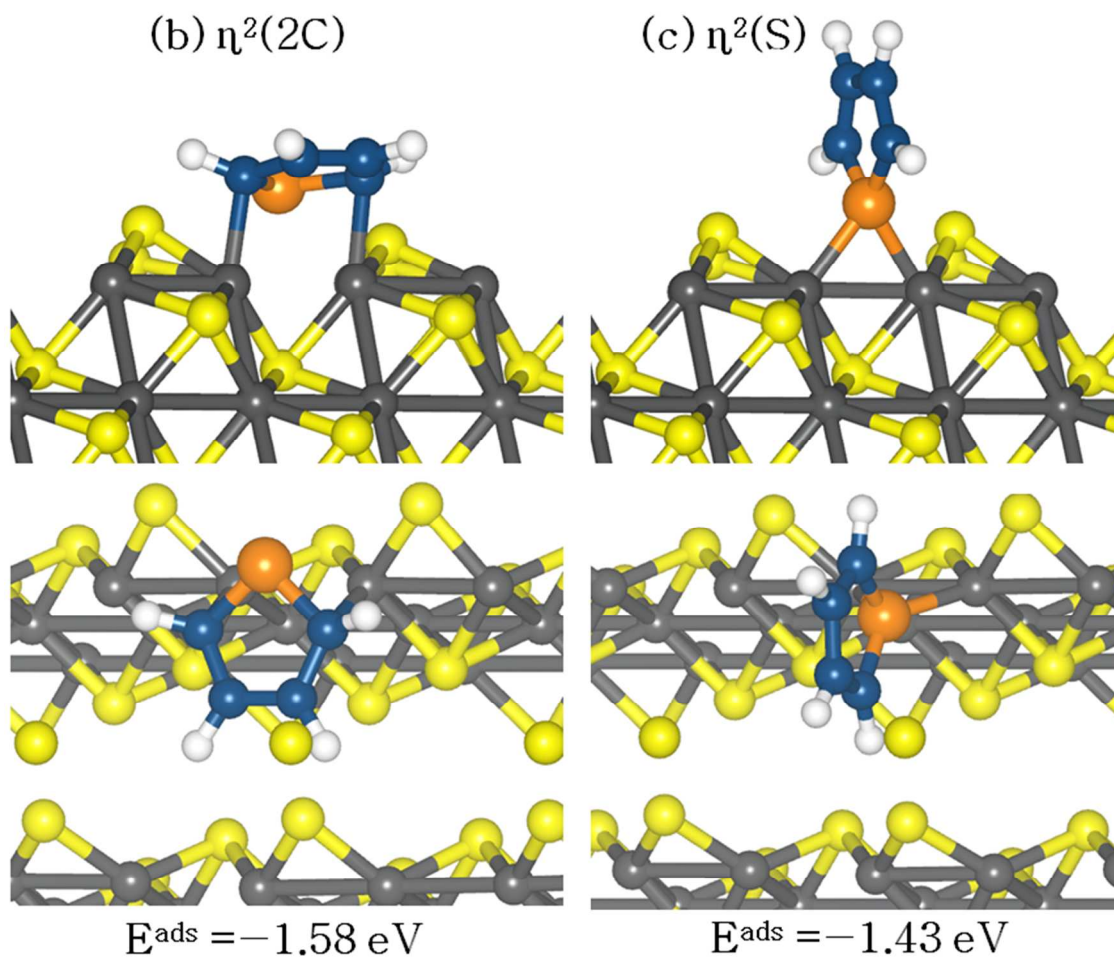


Table S1: Adsorption energies and structural parameters of thiophene adsorbed on stoichiometric FeS (001), (011) and (111) surfaces.

Parameters	FeS(001)		FeS(011)		FeS(111)	
	S-up	S-down	$\eta^3(3C)$	$\eta^1(S)$	$\eta^2(2C)$	$\eta^2(S)$
$E_{\text{ads}} / \text{eV}$	-0.19	-0.13	-1.21	-0.59	-1.58	-1.43
$\sum q / e^-$	0.00	0.00	0.28	0.10	0.36	0.18
$d(\text{C1-C2}) / \text{\AA}$	1.374	1.375	1.402	1.373	1.427	1.357
$d(\text{C2-C3}) / \text{\AA}$	1.425	1.423	1.417	1.425	1.373	1.444
$d(\text{C3-C4}) / \text{\AA}$	1.375	1.375	1.430	1.375	1.427	1.359
$d(\text{C1-S}) / \text{\AA}$	1.719	1.717	1.765	1.719	1.797	1.743
$d(\text{C4-S}) / \text{\AA}$	1.719	1.718	1.769	1.728	1.786	1.745
$d(\text{S-Fe}) / \text{\AA}$	---	---	---	2.255	2.412	2.194
$d(\text{C-Fe}) / \text{\AA}$	---	--	2.201	---	2.124	---
$d(\text{S}_{\text{Thio}}-\text{S}_{\text{surf}}) / \text{\AA}$	---	3.510	3.344		3.184	3.378
$d(\text{C}-\text{S}_{\text{surf}}) / \text{\AA}$	3.424	---	3.129		3.042	---
$d(\text{H}-\text{S}_{\text{surf}}) / \text{\AA}$	2.989	---	3.087		2.766	2.413