

## Supplementary Information

### Theoretical Study on Adsorption and Dissociation of NO<sub>2</sub> Molecule on Fe(111) Surface

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**Table S1.** Convergence tests for adsorption energies with different number of layers.

site	number of layers	E <sub>ads</sub> (kcal/mol)
FeNO <sub>2</sub> (S-μ <sub>3</sub> -N,O,O')	6-layer model	-64.59
	9-layer model	-65.28

**Table S2.** Convergence tests for adsorption energies with constant  $k$ -point and varied cut-off energies.

site	$k$ -point	cut-off energy (eV)	$E_{\text{ads}}$ (kcal/mol)
FeNO <sub>2</sub> (S- $\mu_3$ -N,O,O')	4×4×1	400	-64.59
		450	-63.71
		500	-63.61
		550	-63.67
		600	-63.71
		650	-63.71
		700	-63.97
		750	-64.20
		800	-64.18

**Table S3.** Convergence tests for adsorption energies with constant cut-off energy and varied  $k$ -points.

site	cut-off energy (eV)	$k$ -points	$E_{\text{ads}}$ (kcal/mol)
FeNO <sub>2</sub> (S- $\mu_3$ -N,O,O')	400	4×4×1	-64.59
		5×5×1	-64.87
		6×6×1	-64.74
		7×7×1	-64.29
		8×8×1	-64.53