Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Atomic reconstruction and oxygen adsorption behavior of pyrite (100) surface: A DFT study

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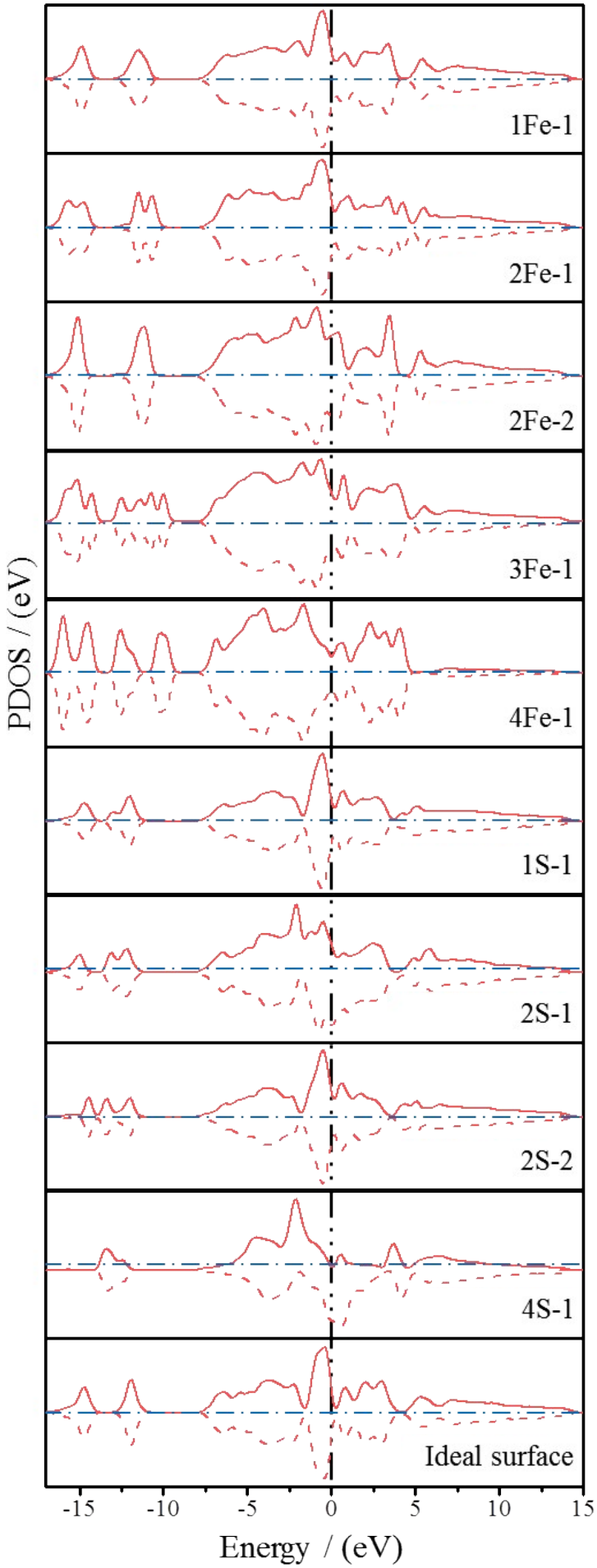

Fig S1 DOS of the atom on reconstructed surface(The solid line represents the spin up, and dotted line represents the spin down)

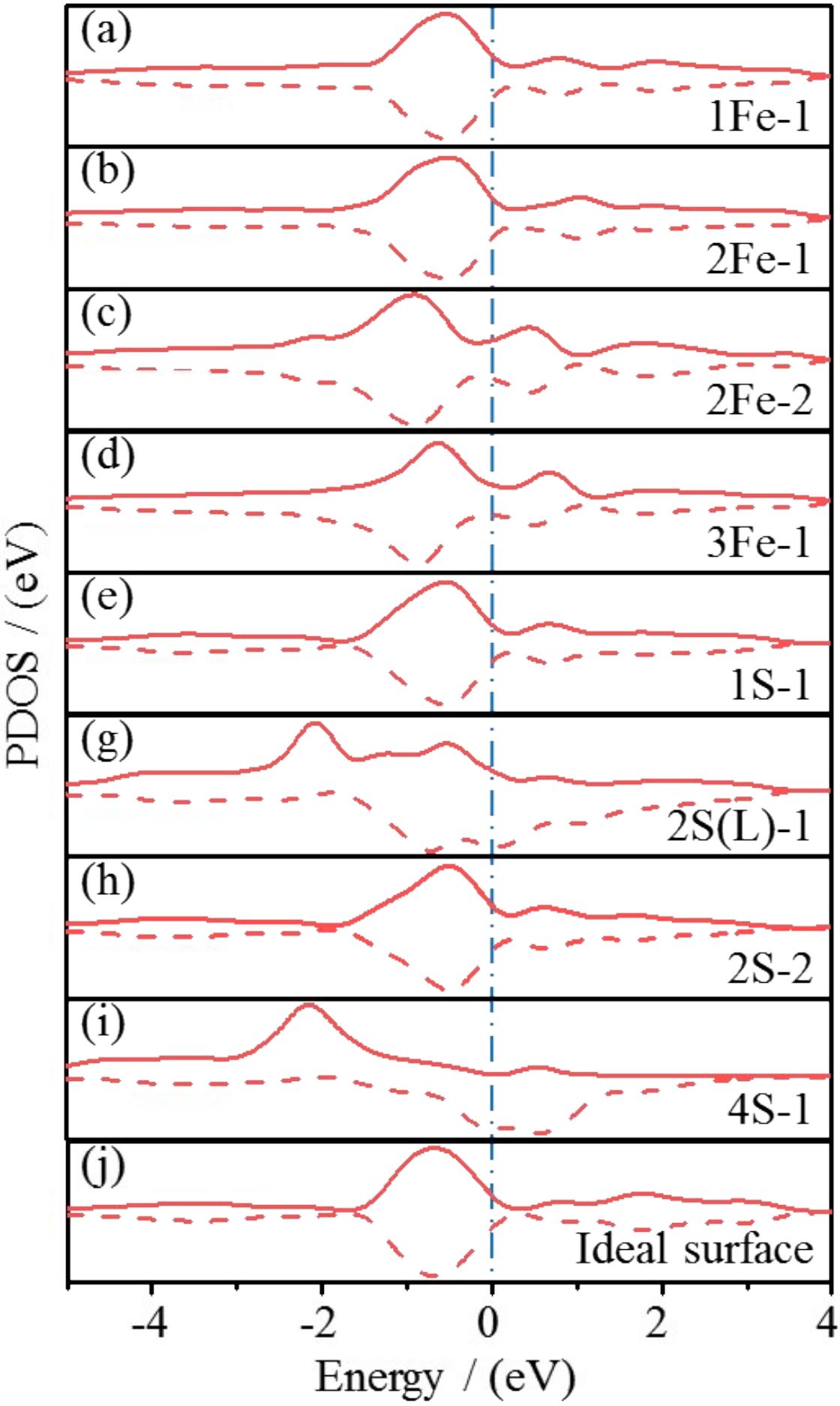

Fig S2 PDOS of d-band of Fe atom on reconstructed surface(The solid line represents the spin up, and dotted line represents the spin down)

Table S1 Mulliken charge of S and Fe atom on reconstructed surface (*e*)

Configuration	S	Fe
1Fe-1	-0.07	0.14
2Fe-1	-0.05	0.18
2Fe-2	-0.07	0.23
3Fe-1	-0.04	0.26
4Fe-1	0.00	0.00
1S-1	-0.09	0.11
2S-1	-0.13	0.18
2S-2	-0.11	0.13
4S-1	-0.25	0.28

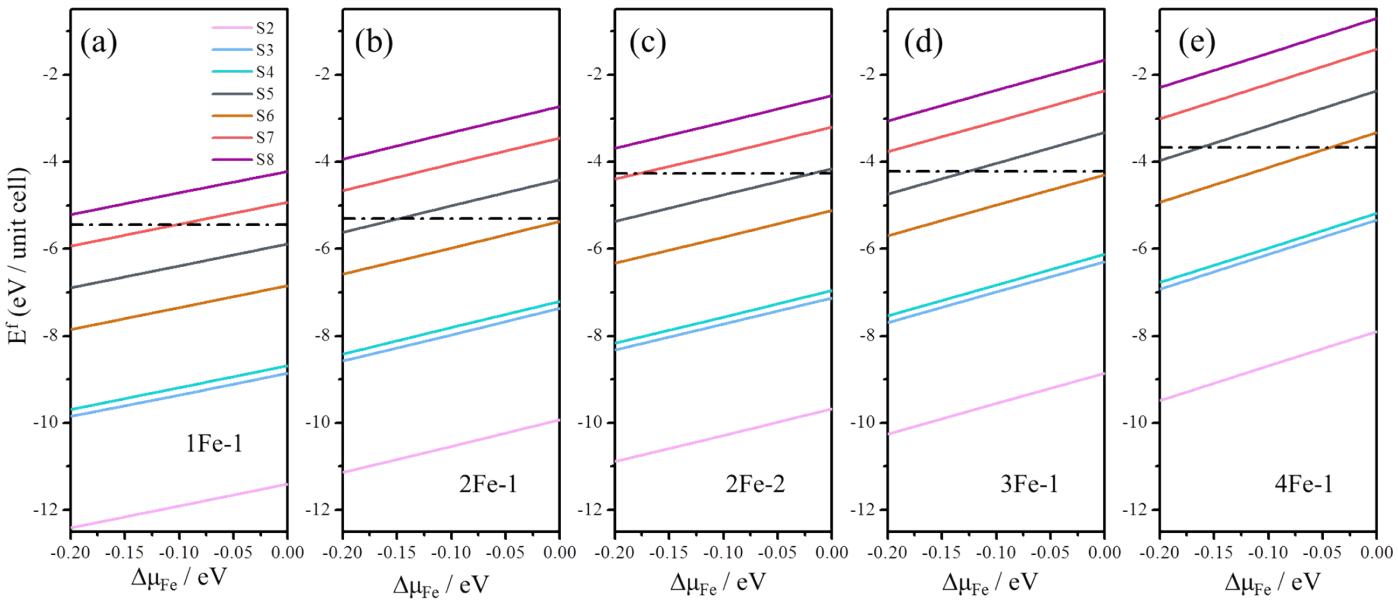

Fig. S3 Formation energies E^f (in eV / unit cell) for surfaces with different configuration when FeS as equilibrium phase and S_2 molecules serve as the reference potential energy of S atom (dashed lines represents the binding energy)

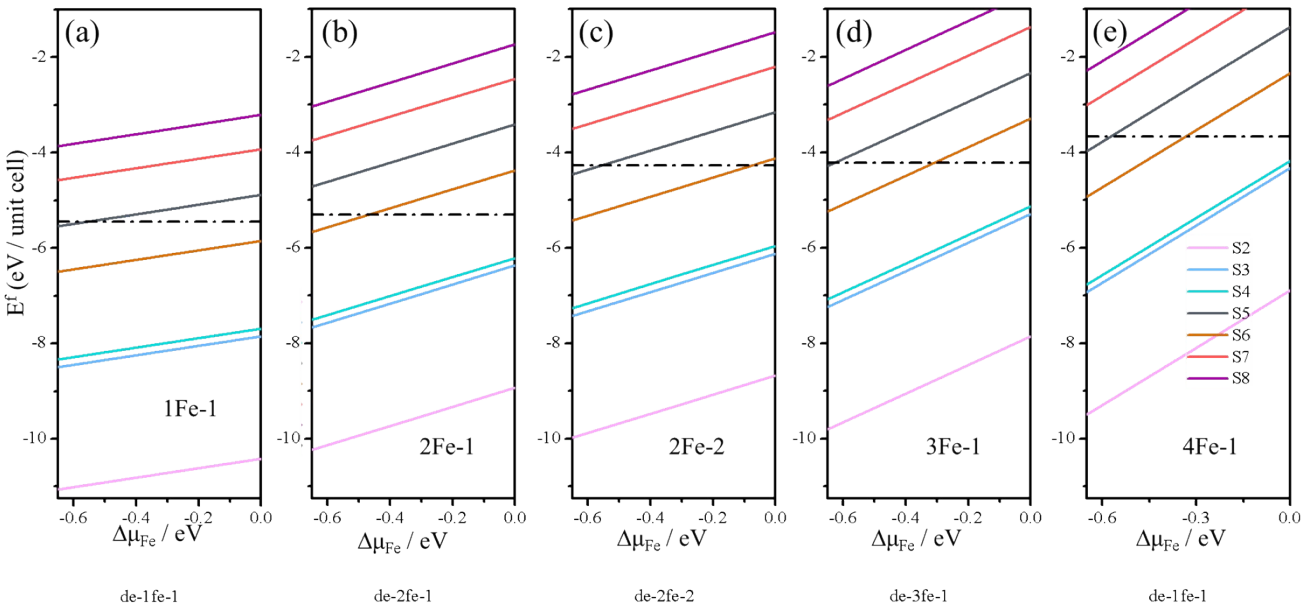

Fig. S4 Formation energies E^f (in eV / unit cell) for surfaces with different configuration when FeS_2 as equilibrium phase and S_8 molecules serve as the reference potential energy of S atom (dashed lines represents the binding energy)

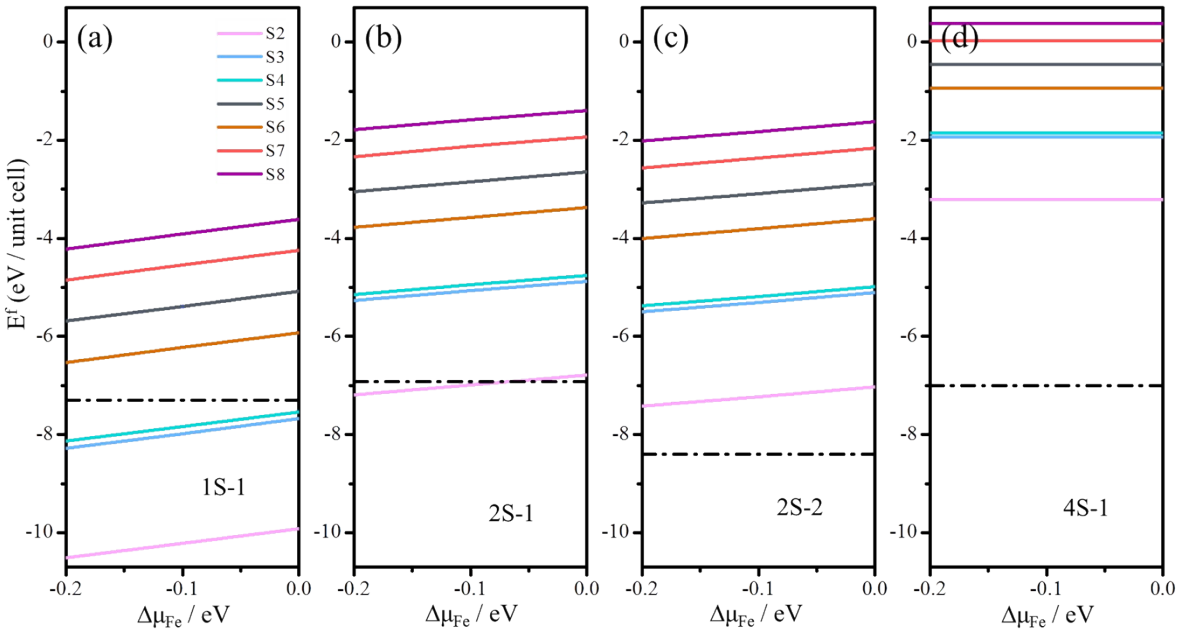

Fig. S5 Formation energies E^f (in eV / unit cell) for surfaces with different configuration when FeS as equilibrium phase and S_2 molecules serve as the reference potential energy of S atom (dashed lines represents the binding energy)

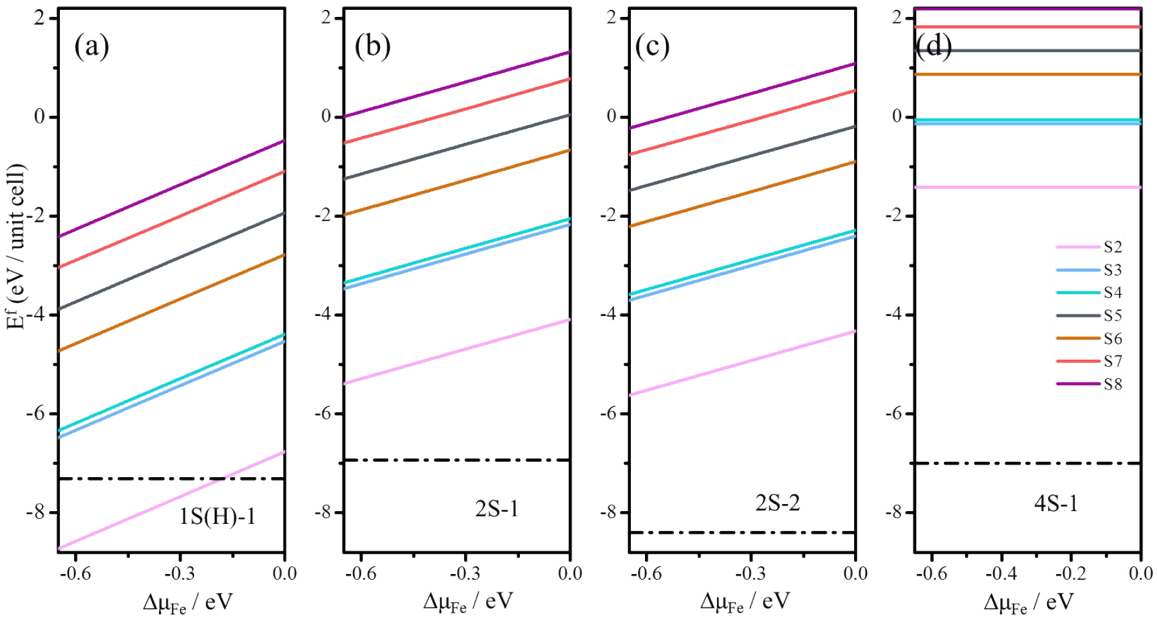

Fig. S6 Formation energies E^f (in eV / unit cell) for surfaces with different configuration when FeS_2 as equilibrium phase and S_8 molecules serve as the reference potential energy of S atom (dashed lines represents the binding energy)