Supporting Information

A modelling in catalytically oxidative decomposition of carbon tetrachloride on ZnS nanocluster using density functional theory

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Table S1 Mulliken atomic charges for oxygen molecule adsorbed on the $(ZnS)_n$ clusters

	6	7	11	12	13		15		16	17	25	26
O1	-0.028	-0.070	-0.013	-0.018	-0.121	-0.063	-0.174	-0.016	-0.009	-0.069	-0.101	-0.019
O2	-0.034	-0.133	-0.070	-0.087	-0.131	-0.124	-0.274	-0.064	-0.010	-0.171	-0.127	-0.077

Table S2 Summary of the energies for the reaction of CCl_4 and O_2 on the $(ZnS)_{12}$ cluster[a]

Reaction step	ΔE_0	ΔH (298.15K)	ΔG (298.15K)
$A+O_2+CCl_4 \rightarrow B$	-18.42	-17.64	1.52
B→C-TS	26.82	27.47	26.33
B→D	19.10	20.01	21.18
D→E-TS	3.91	3.14	3.99
D→F	-75.52	-76.13	-74.14
F→G-TS	4.37	4.13	5.16
F→H	-44.46	-44.44	-45.50
H→I-TS	28.08	28.49	27.36
H→J	11.45	12.29	10.50
J→K-TS	38.43	37.70	39.28
J→L	35.76	30.93	29.30
L→M-TS	6.72	8.07	5.56
L→N	-96.16	-92.43	-94.52

[a] All the energies are in kcal/mol. ΔE_0 is the zero-point-corrected energy, ΔH and ΔG are the changes of the enthalpies and Gibbs free energies for the process specified.

Table S3 Summary of the energies for the reaction of CCl_4 and O_2 without the $(ZnS)_{12}$ cluster [b]

Reaction step	ΔE_0	ΔH (298.15K)	ΔG (298.15K)
a→b-TS1	37.19	37.76	38.00
a→c	30.65	31.95	31.49
c→d-TS2	1.39	0.68	-0.22
c→e	-38.58	-38.57	-35.47
e→f-TS3	10.99	10.06	9.23
e→g	-26.79	-28.00	-29.70
g→h-TS4	81.32	80.86	77.49
g→i	39.43	38.78	32.26
i→j-TS5	10.65	13.42	9.38
i→k	-93.72	-90.24	-93.02

[b] All the energies are in kcal/mol. ΔE_0 is the zero-point-corrected energy, ΔH and ΔG are the changes of the enthalpies and Gibbs free energies for the process specified.

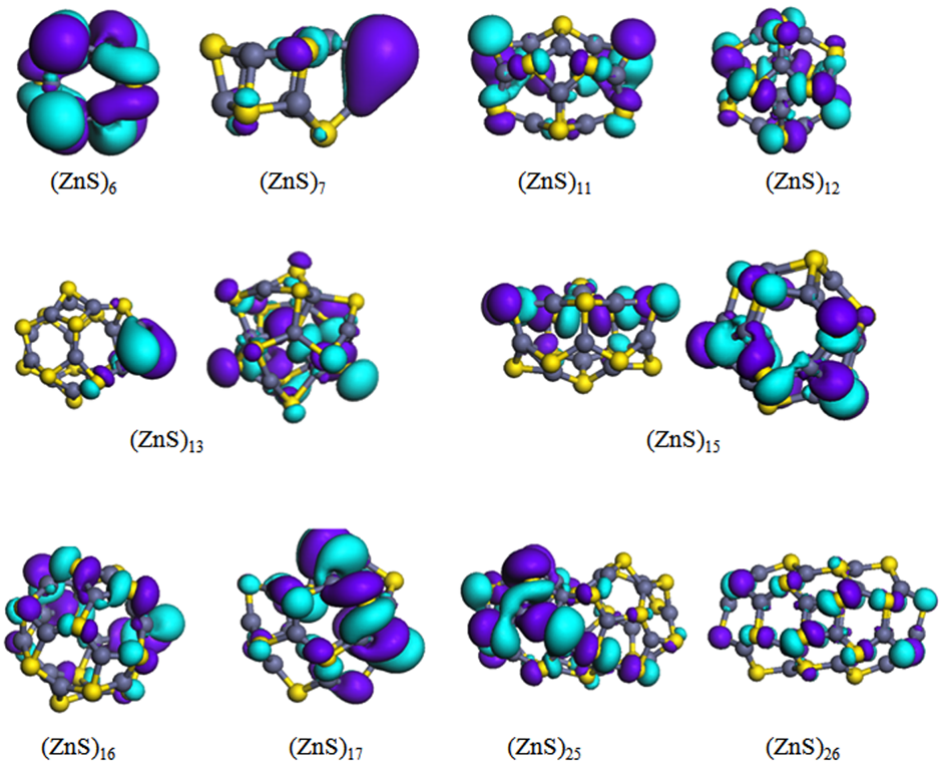

Figure S1 The highest occupied molecular orbital (HOMO) of (ZnS)n nanoclusters

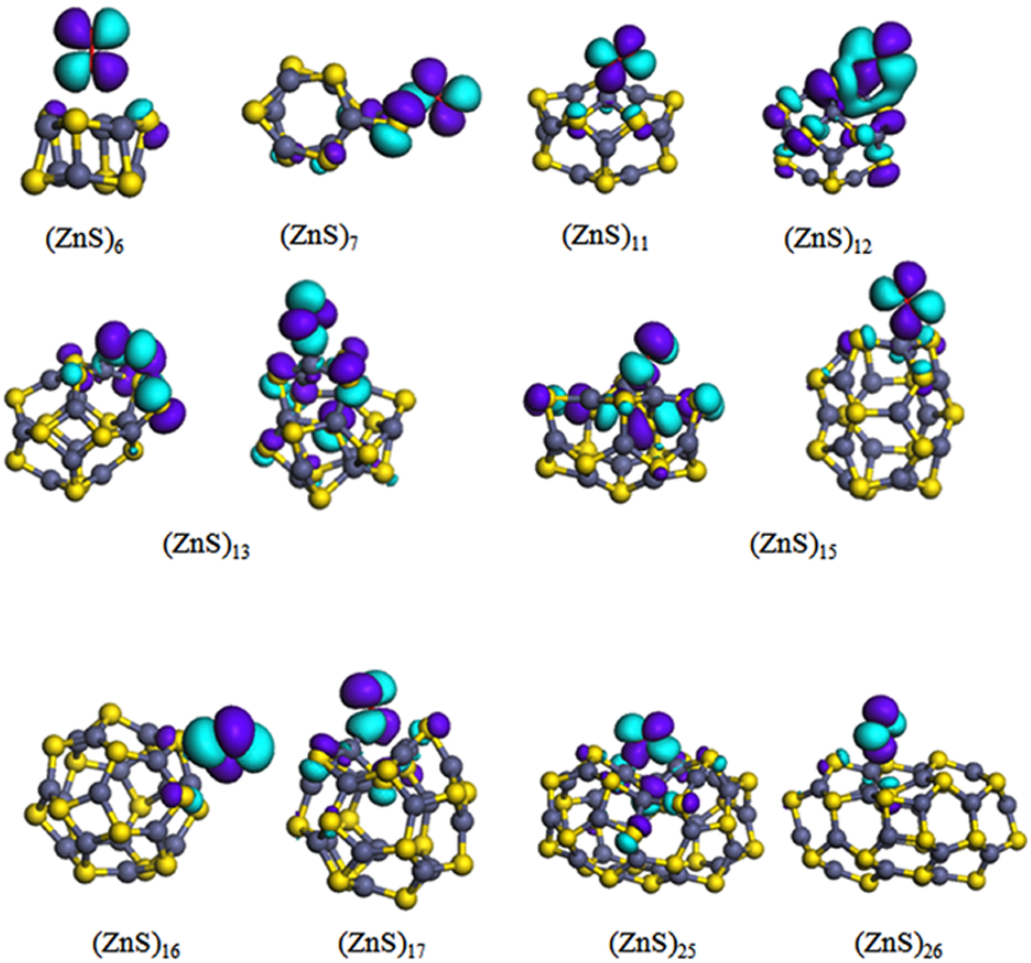

Figure S2 HOMO of $(ZnS)_n$ nanoclusters when oxygen molecule adsorbed on them.

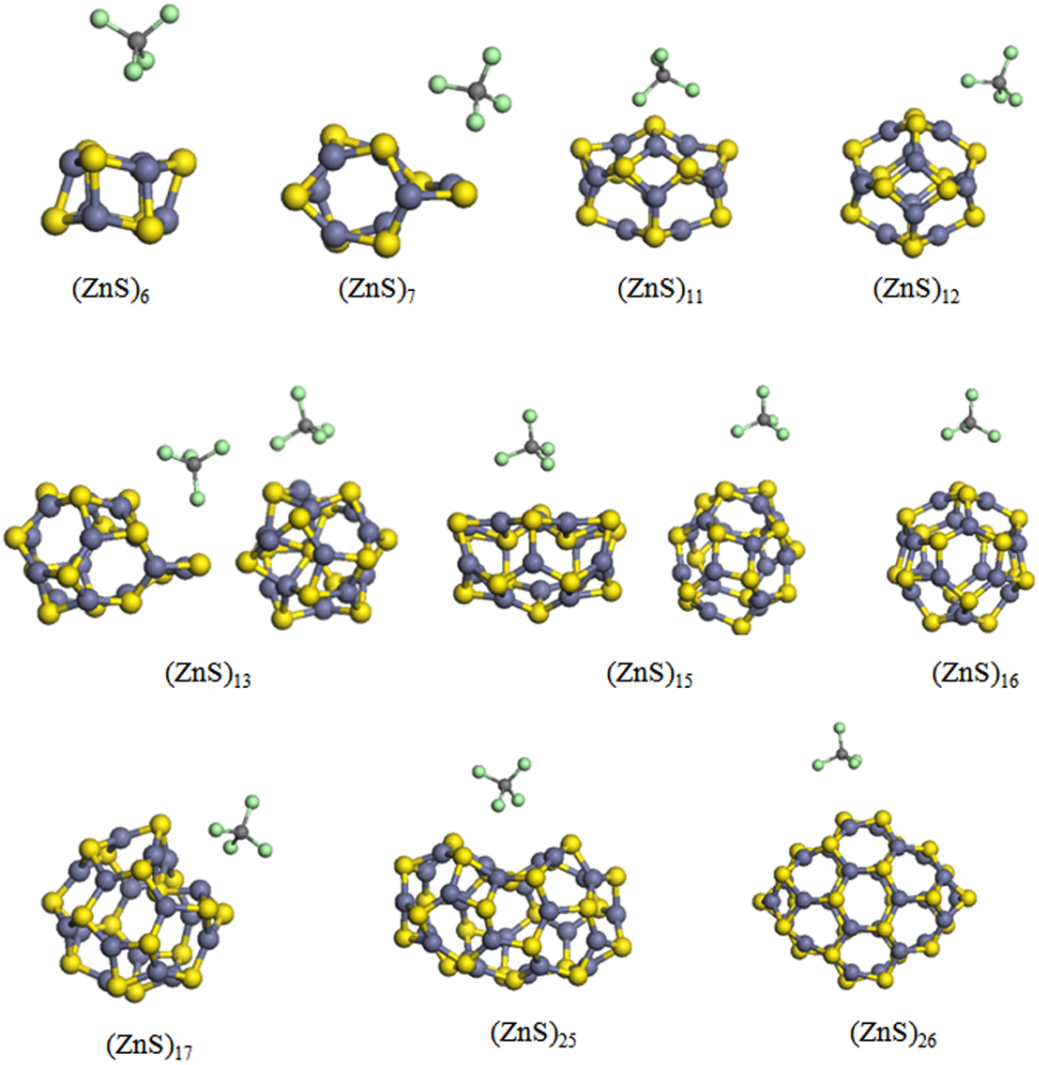

Figure S3 Structures of CCl_4 adsorbed on the $(ZnS)_n$ nanoclusters.

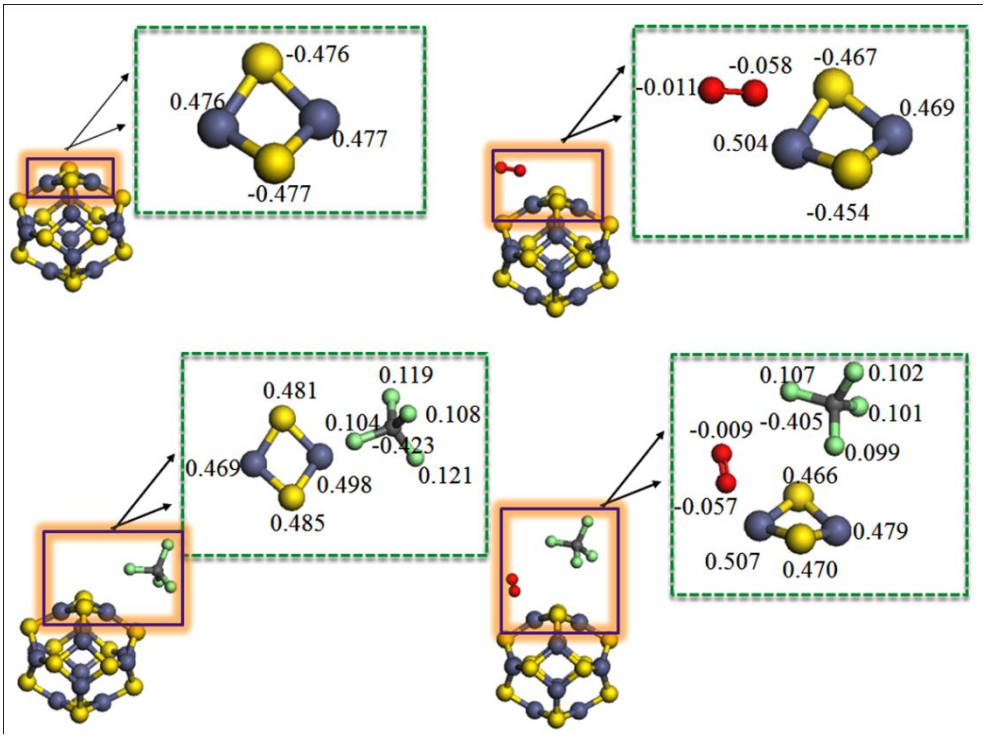

Figure S4 Mulliken atomic charges of $(ZnS)_{12}$, the separated adsorption and the co-adsorption of O_2, CCl_4.

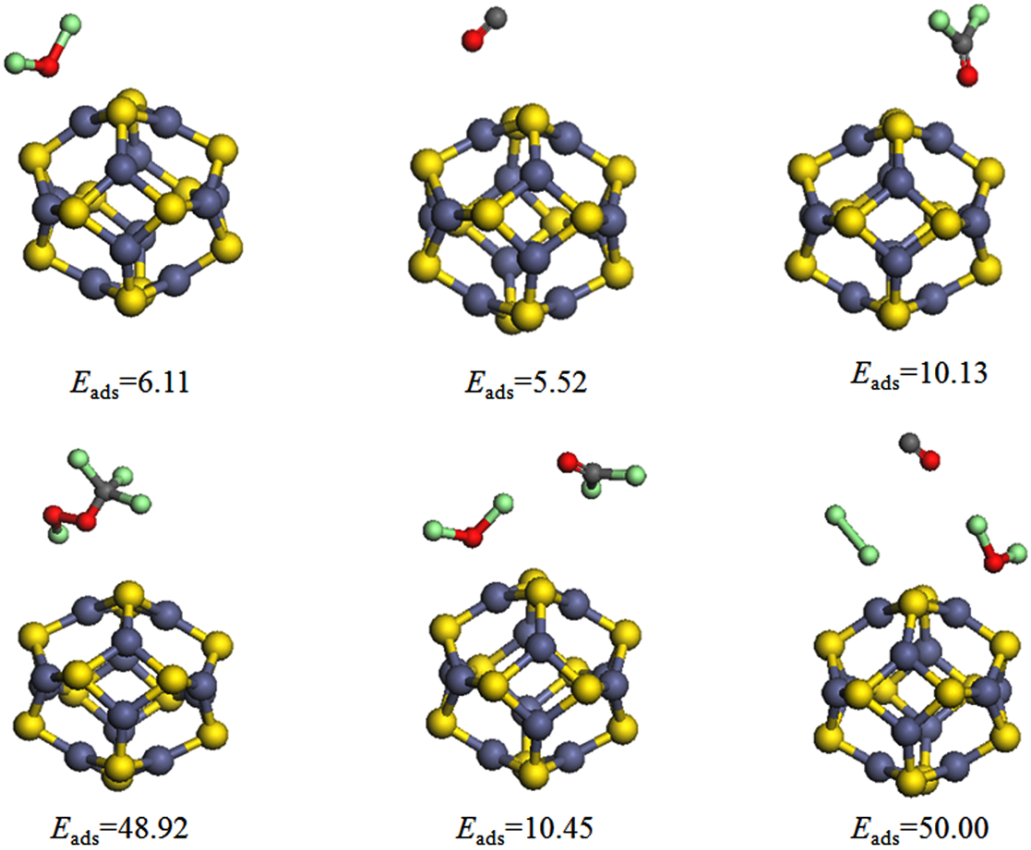

Figure S5 Adsorption energies (kcal/mol) and structures for Cl_2O, CO, $COCl_2$, and $ClOOCCl_3$.

Co-adsorption energies (kcal/mol) for $COCl_2$, Cl_2O and CO, Cl_2, Cl_2O