Structure and Energy of $\text{Mo}_{27}\text{S}_x\text{C}_y$ Clusters: A Density Functional Theory Study

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Table S1. The computed total electronic energies (E_{tot} , au)

Model	E_{tot}	Model	E_{tot}
I ($\text{Mo}_{27}\text{S}_{54}$)	−23353.86943	20	−21836.93907
II ($\text{Mo}_{27}\text{S}_{51}$)	−22159.17979	21	−21836.96679
III ($\text{Mo}_{27}\text{S}_{52}$)	−22557.43663	22	−21836.98740
IV ($\text{Mo}_{27}\text{S}_{56}$)	−24150.50329	23	−21116.52280
V ($\text{Mo}_{27}\text{S}_{60}$)	−25743.77317	24	−21798.92963
VI ($\text{Mo}_{27}\text{S}_{51}$)	−22159.52381	25	−21798.93906
S	−398.07726	26	−21438.68777
C	−37.78216	27	−21438.70114
1	−23790.23646	28	−21078.47015
2	−23429.96700	29	−19260.01746
3	−22993.65811	30	−23582.29590
4	−22993.65771	31	−17098.47284
5	−22633.43951	32	−18917.54360
6	−22633.44966	33	−19998.05129
7	−22633.44306	34	−16755.94336
8	−22633.45639	35	−22993.66196
9	−22273.22895	35	−22993.64486
10	−22273.23439	37	−22993.63762
11	−22273.24107	38	−22993.63047
12	−22273.23462	39	−22633.44058
13	−21913.02577	40	−22633.46231
14	−21913.02410	41	−22273.24052
15	−21913.02668	42	−21913.00981
16	−21913.02400	43	−19031.28304
17	−21192.60870	44	−16870.07119
18	−22197.17255	45	−12547.43091
19	−22197.21043		

Figure S1. The bond lengths for different Mo_{27}S_x cluster model

Figure S2. The bond lengths for carbonization structures on 33% sulfur coverage Mo edge

Figure S3. The bond lengths for carbonization structures on 100% sulfur coverage S edge

Figure S4. The bond lengths for carbonization structures on 67% sulfur coverage S edge

Figure S5. The bond lengths for carbonization structures on 50% sulfur coverage S edge

Figure S6. The bond lengths for carbonization structures on 100% sulfur coverage S edge and 33% sulfur coverage Mo edge

Figure S7. The bond lengths for carbonization structures on 50% sulfur coverage S edge and 33% sulfur coverage Mo edge

Figure S8. The bond lengths for carbonization structures with replacement bulk S atoms

Figure S9. The bond lengths for carbonization structures with replacement two, three and four S_1 atoms

Figure S10. The bond lengths for carbonization structures with replacement bulk S atoms and 100% sulfur S edge on the $\text{Mo}_{27}\text{S}_{54}$ cluster