**Supporting Information for:**

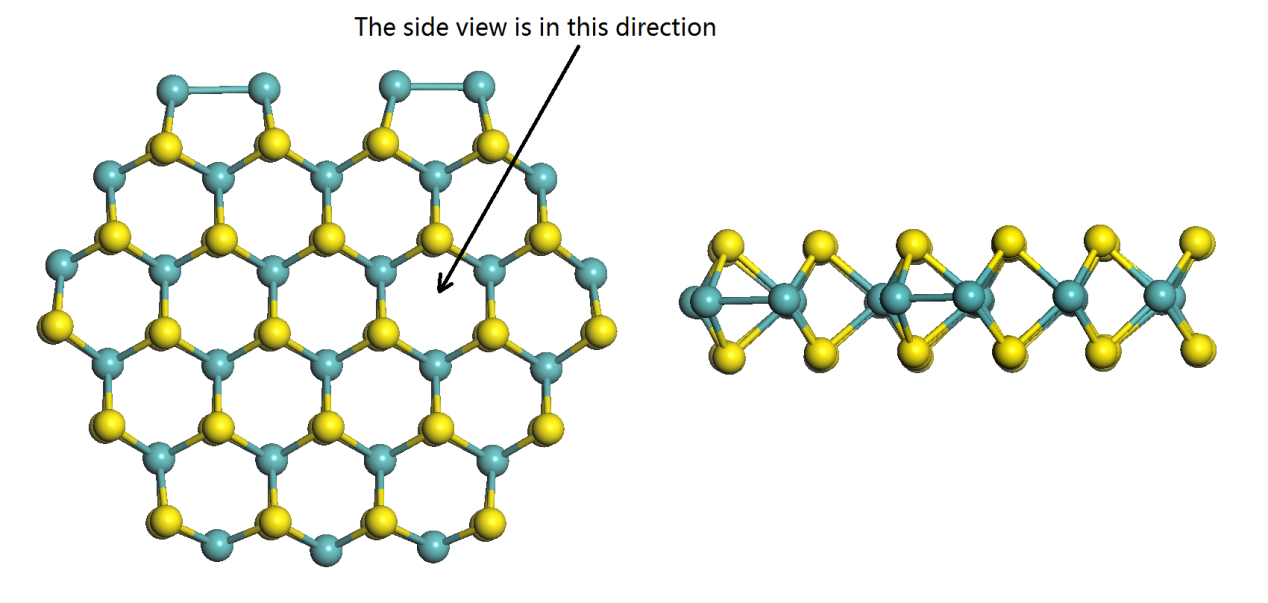
**A Combined Computational and Experimental Study of the Adsorption of Sulfur Containing Molecules on Molybdenum Disulfide Nanoparticles**

Tao Yang, Junpeng Feng, Xingchen Liu,, Yandan Wang, Hui Ge, Dongbo Cao,Hao Li, Qing Peng, Manuel Ramos, Xiao-Dong Wen, and Baojian Shen

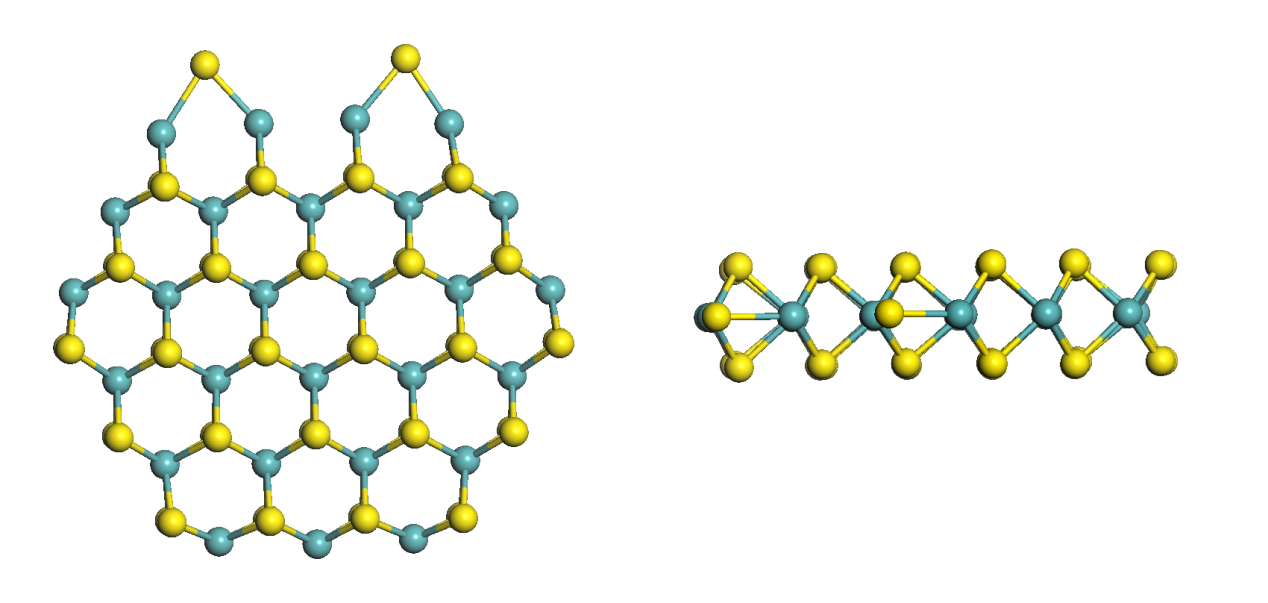
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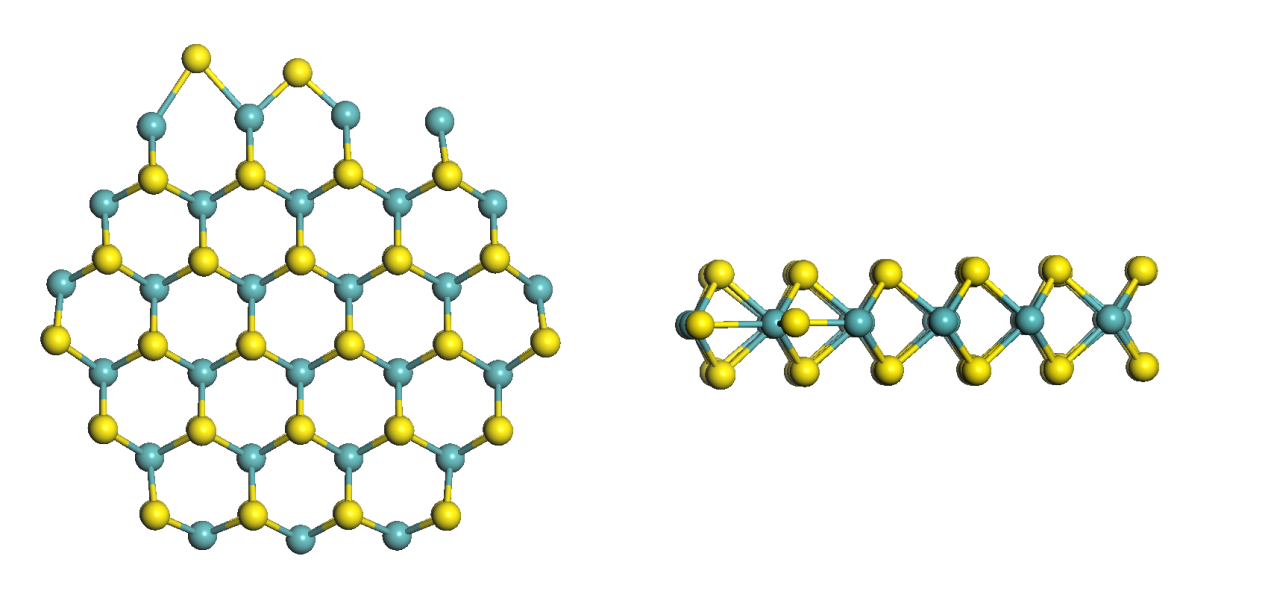
**1. The top and side view of the Mo27Sx nanoparticles used for the adsorption studies**



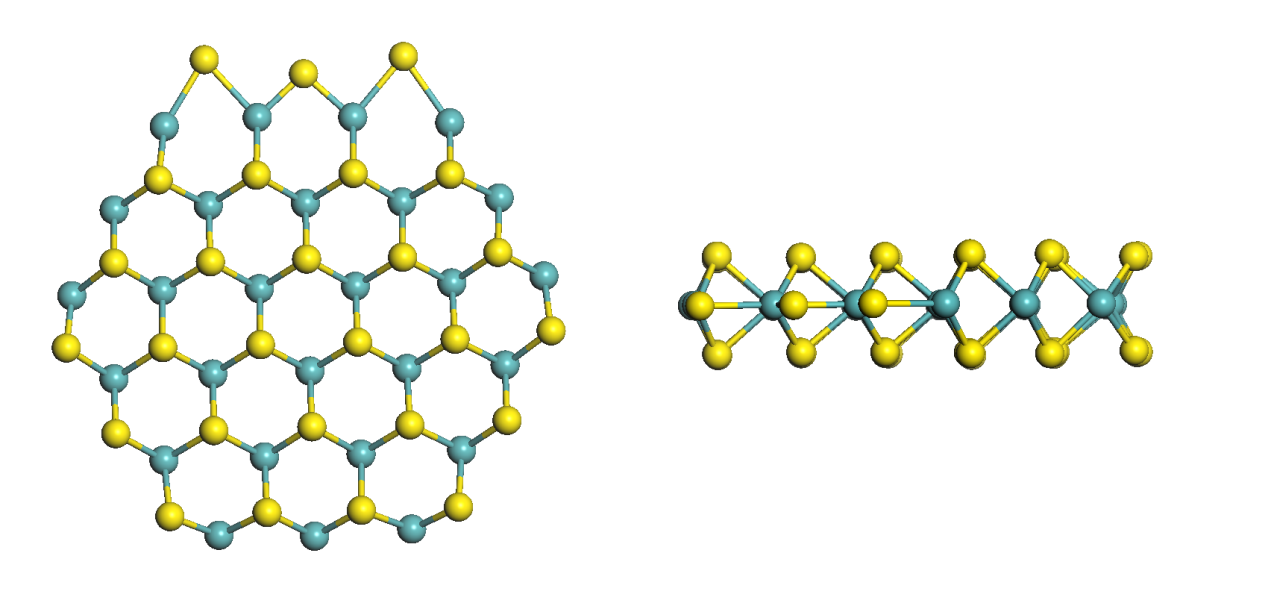
**Figure S-1**. The top (left) and side (right) of the Mo27S48 cluster used to accommodate site-5 and site-6.



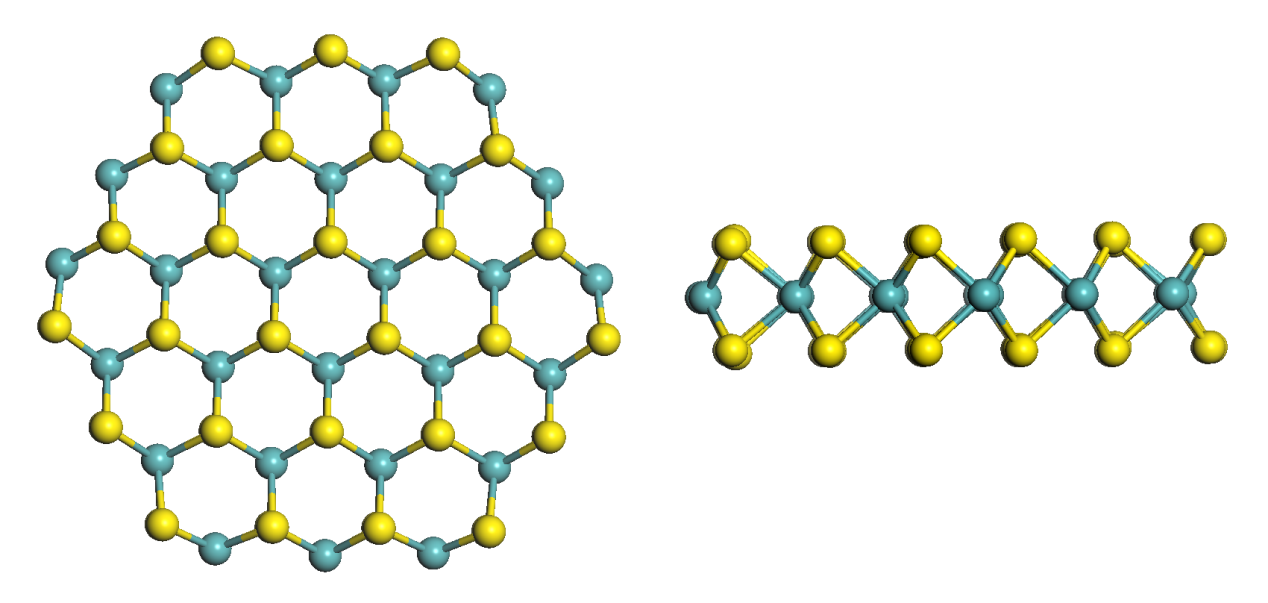
**Figure S-2**. The top (left) and side (right) of the Mo27S50 cluster used to accommodate site-3



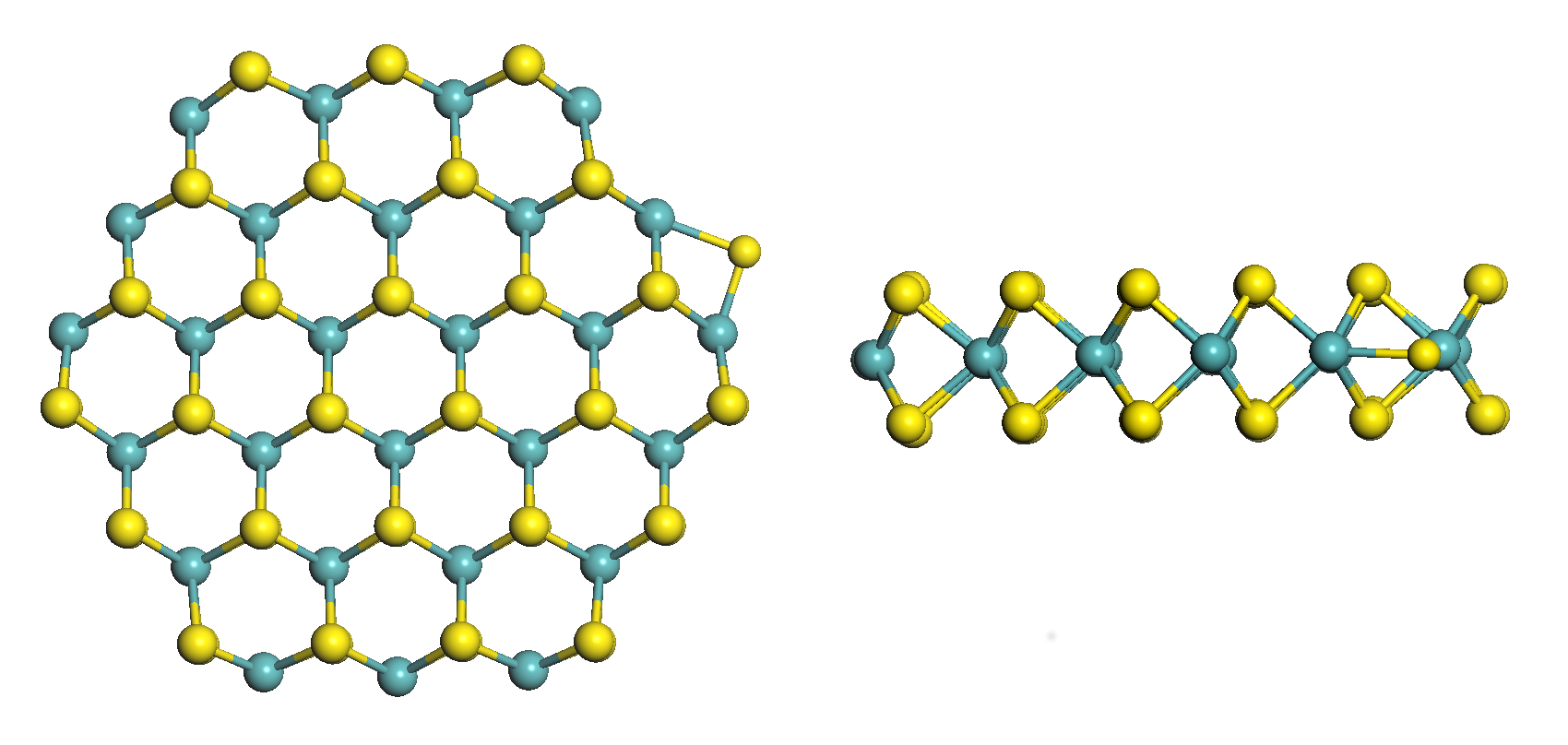
**Figure S-3**. The top (left) and side (right) of the Mo27S50 cluster used to accommodate site-4



**Figure S-4**. The top (left) and side (right) of the Mo27S51 cluster



**Figure S-5**. The top (left) and side (right) of the Mo27S54 cluster used to accommodate site-1



**Figure S-6**. The top (left) and side (right) of the Mo27S55 cluster used to accommodate site-2

**2. Cartesian coordinates of the Mo27S54 nanoparticle**

Mo 5.6809452310 0.0300310040 -0.0658687350

Mo 5.5584153990 3.1611163320 -0.0060518810

Mo 5.6705660120 6.2933622300 0.0410838770

Mo 8.1891029620 -1.7084881460 -0.1007020830

Mo 8.1964319070 1.5789930820 -0.0163172540

Mo 8.1923814400 4.7491229610 0.0152482760

Mo 8.1714482510 8.0469821850 0.0459215250

Mo 10.9220871100 -3.2743797230 0.1239870550

Mo 10.9602576530 -0.0172168120 -0.0301791680

Mo 10.9664400980 3.1711091090 -0.0127847640

Mo 10.9504793770 6.3604733310 0.0222605750

Mo 10.8884838380 9.6093752990 0.0546598630

Mo 13.7166500030 -4.5163551690 0.1093736170

Mo 13.7471491660 -1.5826999480 -0.0382459070

Mo 13.7045189230 1.5989581350 -0.0409864290

Mo 13.7038466600 4.7575717120 -0.0058988490

Mo 13.7282340240 7.9428980450 0.0255242460

Mo 13.6610815730 10.9117670330 0.0473860650

Mo 16.4227212740 -3.0081342290 -0.0162572500

Mo 16.4432217770 -0.0097861890 -0.0694786260

Mo 16.4689908740 3.1685141930 -0.0176424340

Mo 16.4690352630 6.3559608280 -0.0022638150

Mo 16.4215674820 9.4305680180 0.0056940620

Mo 18.9396851400 -1.4608549390 0.1564007160

Mo 19.2647683860 1.5599410790 0.0904447530

Mo 19.3065606580 4.7118281600 -0.0999073110

Mo 19.0763321860 7.7620079320 -0.0655876800

S 6.3439391220 -1.5331346980 -1.6715901140

S 6.3239535440 -1.6121184730 1.4578980640

S 6.3781270680 1.6543827290 -1.6620972620

S 6.3542874760 1.5923187060 1.6068196010

S 6.3610981290 4.7270717270 -1.6180971020

S 6.3637404360 4.6773688710 1.6508283480

S 6.3118540390 7.9149282160 -1.5106627090

S 6.3234534930 7.8789260160 1.6202523820

S 9.0742399690 -3.3170455180 -1.5104190460

S 9.1136663350 -3.2793334370 1.5642095270

S 9.1131211720 -0.0213813170 -1.5874742400

S 9.0964533480 -0.0869427510 1.5080542000

S 9.1333804530 3.1834737080 -1.5748075820

S 9.1409476030 3.1492908120 1.5653297420

S 9.0885275320 6.4022609210 -1.5166207710

S 9.0978532690 6.3718627390 1.5744829340

S 9.0754441120 9.6154925090 -1.4992009010

S 9.0902139850 9.5897358930 1.6165305690

S 11.9682549630 -4.8611450370 -1.3893652940

S 12.0402847480 -4.7102538300 1.7316116840

S 11.8374535050 -1.7003863820 -1.5354771590

S 11.9128356730 -1.5807981240 1.5454392840

S 11.8629065880 1.5814324510 -1.6145135900

S 11.8787400450 1.5689863090 1.5538091720

S 11.8626465820 4.7880548310 -1.5819083630

S 11.8733116700 4.7564812570 1.5837190610

S 11.8519972600 7.9956631210 -1.5115861130

S 11.8685799180 7.9659485040 1.5802617960

S 11.9377063380 11.1449839270 -1.5075372890

S 11.9515564200 11.1271068410 1.6209515470

S 14.7132252550 -3.2222269150 -1.6393002750

S 14.7505634530 -3.0328164620 1.6711750500

S 14.6164006270 0.0216757220 -1.6359227330

S 14.6338819120 0.0287806110 1.5277153290

S 14.6361879550 3.1927780010 -1.6063420050

S 14.6321880870 3.1667188120 1.5599866680

S 14.6166280230 6.3498449040 -1.5656471700

S 14.6358409410 6.3232280980 1.5779813430

S 14.6651795690 9.5210616510 -1.6050608940

S 14.6982034290 9.4969439450 1.6582262670

S 17.3987802800 -1.6211479860 -1.6932659480

S 17.1924265570 -1.5079193480 1.1373503910

S 17.4663737280 1.5969996530 -1.5678198820

S 17.3381942170 1.5453332570 1.5534525190

S 17.3873055770 4.7676939100 -1.5797299330

S 17.4604513990 4.7444280480 1.5244004320

S 17.3167680050 7.9662636720 -1.6501571700

S 17.3879286620 7.9569760180 1.6139805810

S 20.1692289770 -0.1559164860 -1.3614432080

S 19.8781325260 -0.1693076280 1.7861692340

S 20.2345355890 3.1438839660 -1.5349619830

S 20.2101994990 3.0955720800 1.5372088310

S 20.0699388600 6.3977602190 -1.6791495160

S 20.1853474890 6.3676508510 1.4413316390

**Table S-1.** Bond lengths (Å) for free sulfur molecules and adsorption sulfur molecules on different adsorption sites. (μ2 coordination on site-2, site-3 and site-4 and π-Face coordination on Mo edge).

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Bond | S-C(DBT) | | S-C(4,6-DMDBT) | | S-C(3,7-DMDBT) | | S-C(2,8-DMDBT) | |
| Free | 1.762 | 1.762 | 1.763 | 1.763 | 1.763 | 1.763 | 1.762 | 1.762 |
| Site-2 | 1.792 | 1.794 | 1.819 | 1.819 | 1.791 | 1.791 | 1.787 | 1.799 |
| Site-3 | 1.798 | 1.78 | 1.808 | 1.809 | 1.800 | 1.799 | 1.794 | 1.794 |
| Site-4 | 1.796 | 1.796 | 1.807 | 1.808 | 1.797 | 1.795 | 1.791 | 1.791 |
| Mo edge | 1.778 | 1.820 | 1.795 | 1.794 | 1.790 | 1.790 | 1.787 | 1.788 |