Supplementary material

Density functional study on the resistance to sulfur poisoning of Pt_x (x=0, 1, 4 and 8) modified α-Mo_2C (0001) surface

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S.1 The possible configurations of S adsorption on the surface of Pt_1-Mo_2C surface

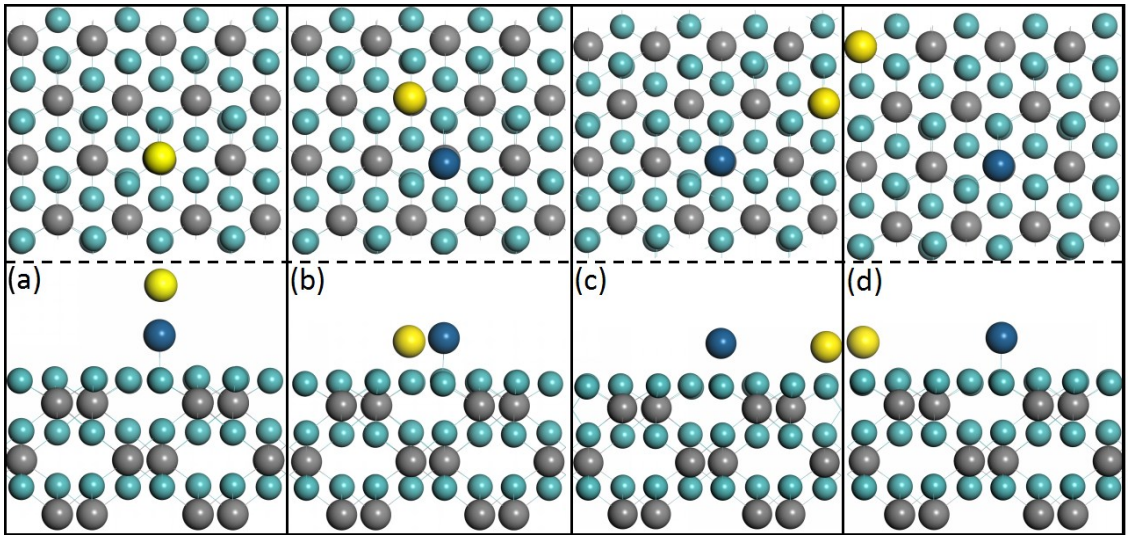

Figure S.1 The top-views (top panel) and the corresponding side-views (bottom panel) of single S adsorbed on Pt_1/Mo_2C(0001) surface.

Table S.1 The relative energies E(eV) and distances of the adsorbed S from the surface Pt atom D(Å) for different structures.

Structure	a	b	c	d
D(Å)	2.158	3.261	5.428	7.985
E(eV)	3.47	6.20	6.43	6.46

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S.2 The Coulomb attraction of SH on the surfaces of Pt_4-Mo_2C and Pt_1-Mo_2C

According to the calculation, we can draw the conclusion that the adsorbed HS on Pt_4-Mo_2C is larger than that on Pt_1-Mo_2C. The reasons for the different adsorption energies of SH on the four surfaces were roughly investigated according to Coulomb's law. The Mulliken charges of the involved species were calculated and listed in **Table S2**. According to Coulomb's law, the force (F) between two point charges can be described as:

$$F = \kappa \frac{Q_1 Q_2}{r_{12}^2} \tag{1}$$

where κ, Q_1, Q_2 and r_{12} represents Coulomb constant, the average charge of SH (SH-chg(e)), the average charge of 3 Mo atoms in the nearest neighbor of HS (Mo-chg(e)) and the average distance between 3 Mo atoms and SH, respectively. By Coulomb's law we know that F is proportional to Q_1Q_2 and inversely proportional to r_{12}^2. Moreover, the Coulomb attraction of the substrate to the SH is mainly provided by the nearest 3 Mo atoms on both the Pt_4-Mo_2C and Pt_1-Mo_2C surfaces, where SH adsorbed at the three-fold hollow sites perpendicularly with the S moiety down. So the impacts of κ and r_{12}^2 on F are roughly the same. Therefore, the attraction of SH on the Pt_4-Mo_2C surface is bigger than that on the Pt_1-Mo_2C surface due to the bigger product value of SH-chg(e) and Mo-chg(e) on the former.

Table S.2 The Mulliken charges of the preferable adsorption configurations (Conf.). The negative and positive numbers represent the gain and loss of electrons, respectively. Therein SH-chg(e) stands for the average charge of SH on the different surfaces and Mo-chg(e) represents the average charge of the 3Mo atoms in the nearest neighbor of the adsorbed HS .

	E_{ads}(eV)	SH-chg(e)	Mo-chg(e)
Mo_2C	4.15	-0.228	0.194
Pt_1-Mo_2C	4.15	-0.227	0.186
Pt_4-Mo_2C	4.50	-0.138	0.369
Pt_8-Mo_2C	3.28	0.007	0.355