

Mechanistic Study on Adsorption Desulfurization Using Modified Graphene

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Experiments:

1. Synthesis of Graphite Oxide

First, concentrated H_2SO_4 was loaded into a 1 L beaker, and the beaker was placed in an ice bath. Then graphite powder of 5 g and NaNO_3 of 2.5 g were slowly added to concentrated H_2SO_4 . KMnO_4 of 15 g was slowly added to the above mixture in batches under stirring. The reaction was carried out for 2 h under ice bath conditions. The temperature was then raised to 308K and lasted for 4 h under stirring. 230 mL deionized water was slowly added. Meanwhile, the temperature was raised to 371 K, and the reaction mixture was stirred for 15 min. The suspension was then diluted to 700 mL and stirred for another 30 min. Finally, 12 mL H_2O_2 was added to terminate the reaction. The mixture was then rinsed several times with dilute HCl and deionized water until the pH reached 7. The dried graphite oxide was obtained by lyophilization.

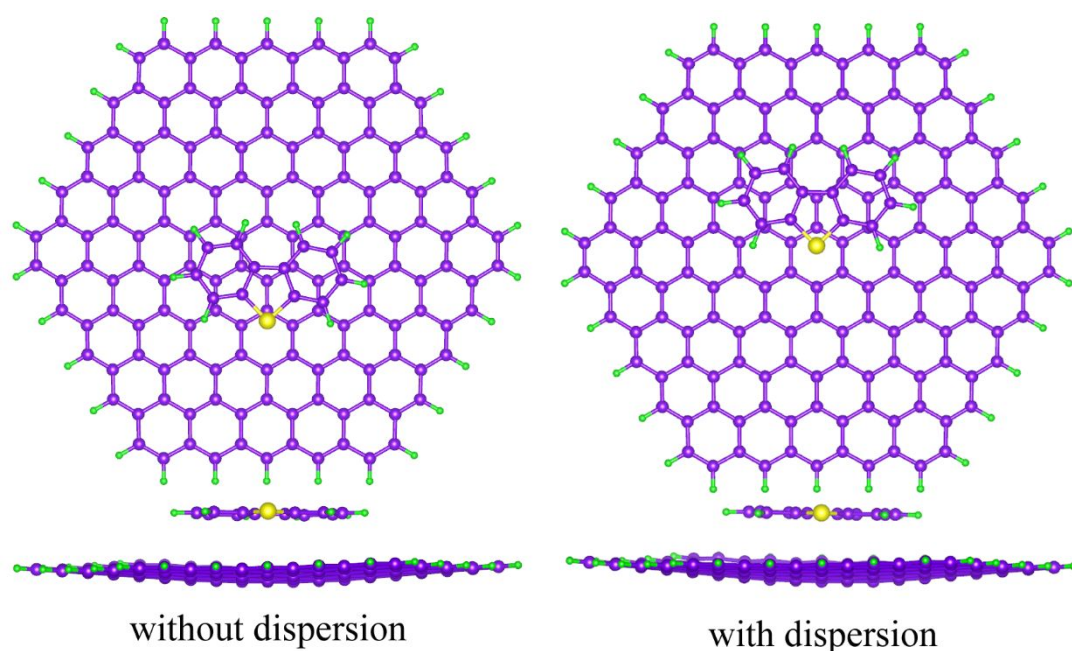


Fig.S1 Adsorption configuration of DBT on graphene obtained DFT calculation without and with dispersion corrections.

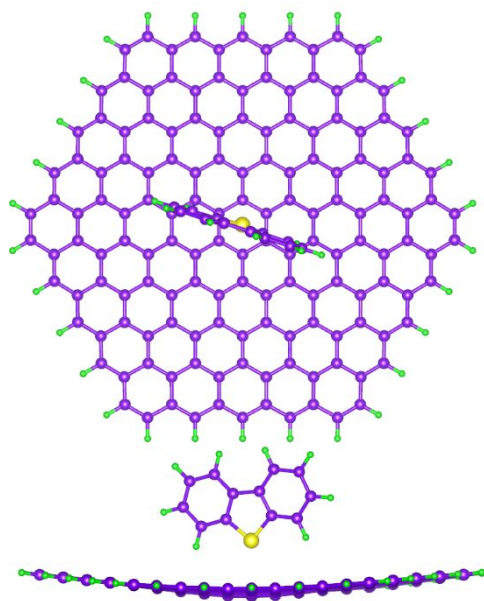


Fig.S2 DBT adsorbed on graphene with thiophenic ring perpendicular to graphene surface.