

Supplementary Information for

Study on the origin of the active sites of HDN catalysts using alumina-supported

MoS₃ nanoparticles as a precursor

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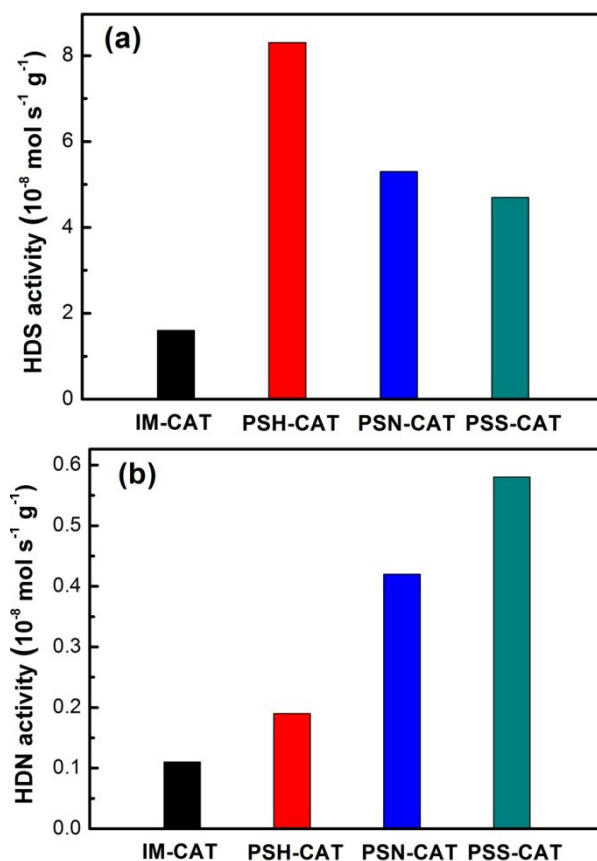


Fig. S1 HDS (a) and HDN (b) activity of the conventional catalyst IM-CAT and the MoS₃-derived catalysts PSH-CAT, PSN-CAT and PSS-CAT. It can be clearly seen that, compared with the conventional catalyst IM-CAT, the three MoS₃-derived catalysts all exhibit much higher DBT-HDS and Q-HDN activity. The different variation tendency between HDS and HDN activity with the change of the treatment atmosphere (H₂, N₂ or H₂S) indicates the two kind reactions may proceed on different active sites. The reaction conditions are that, 280 °C for HDS and 360 °C for HDN, liquid hourly space velocity (LHSV) 20 h⁻¹, total pressure 4.0 MPa, and H₂/hydrocarbon volumetric ratio 500.

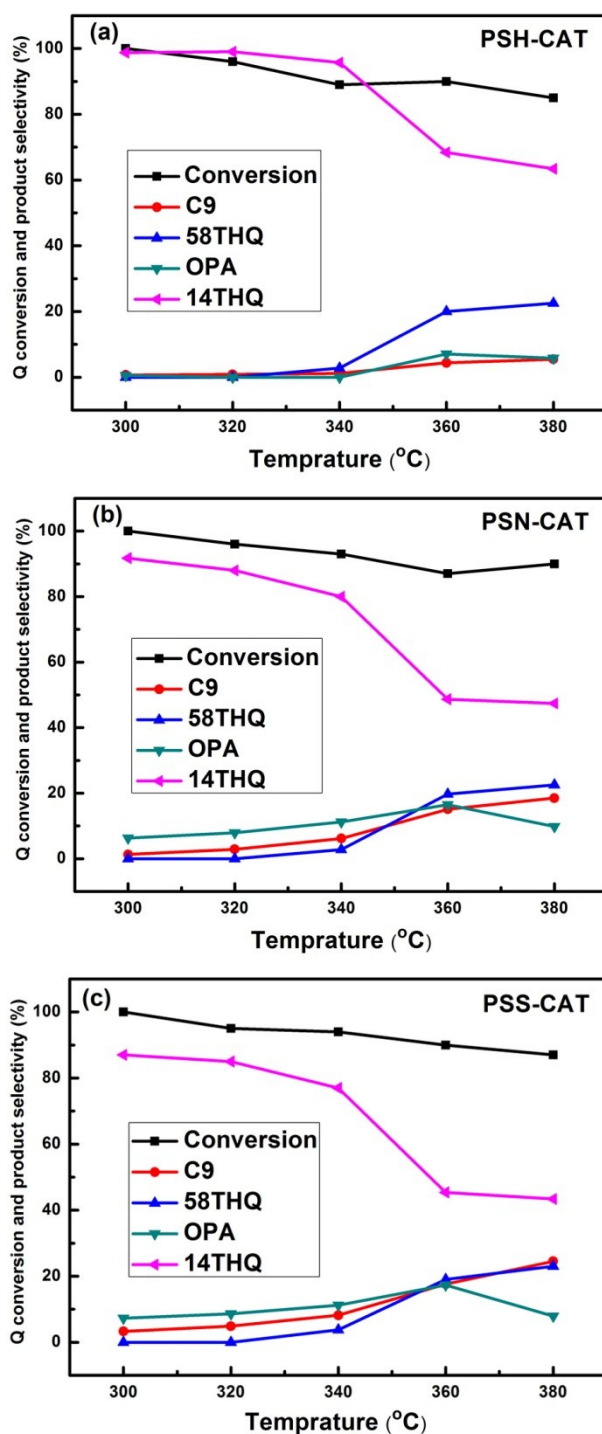


Fig. S2 The Q-HDN conversion and product selectivity over PSH-CAT (a), PSN-CAT (b) and PSS-CAT (c) as a function of reaction temperatures (C9 represent HDN product compounds PCHE, PCH and PB). It is noteworthy that, consistent with the most studies, no PCHA and DHQ in the products were detected, mainly due to their high reactivity. It is well known that, the HYD reactions are usually limited by the thermodynamic

equilibrium. For any of the three MoS₃-derived catalysts, the selectivity of 14THQ decreases with the increase of the reaction temperature, and when at above 340 °C the trend becomes very severe, whereas that of 58THQ increases remarkably, indicating the two HYD reactions Q→14THQ and Q→58THQ bear obviously different extent thermodynamic equilibrium limit. On the contrary, the selectivity of C-N bond hydrogenolysis (DN) products OPA and C9 increases, implying the DN reactions can proceed more easily at higher reaction temperatures. Overall, the conversion of Q presents a downtrend, demonstrating the thermodynamic equilibrium limit is the important impact factor of the HDN reactivity.