Electronic Supplementary Material (ESI) for Catalysis Science & Technology

HRTEM and Molecular Modeling of the MoS_2-Co_9S_8 Interface: Understanding the Promotion Effect in Bulk HDS Catalysts

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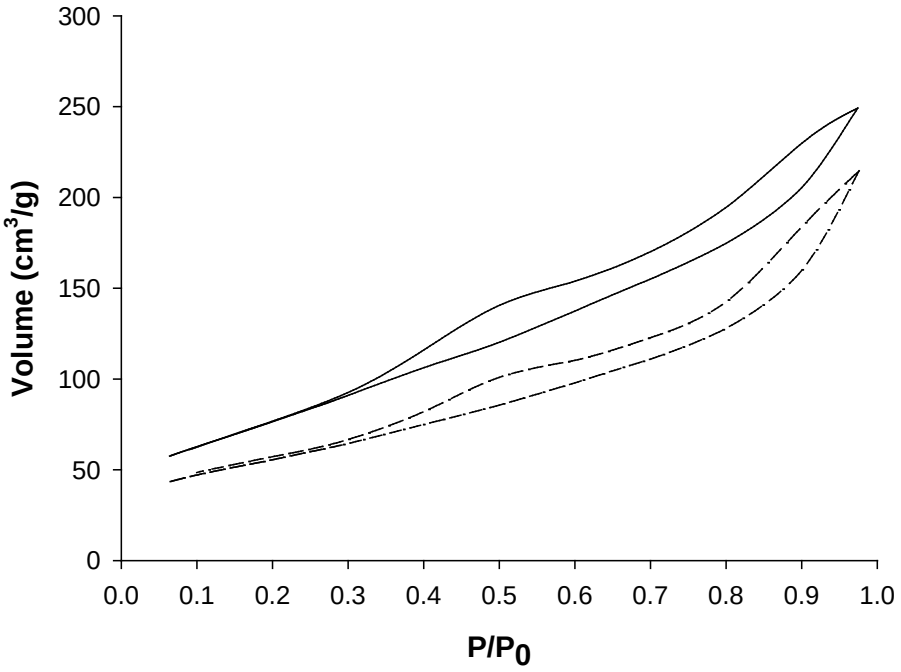


Fig. S1 N_2 adsorption-desorption isotherms of the Co/MoS_2 catalyst before and after the hydrodesulfurization (HDS) of dibenzothiophene (DBT).

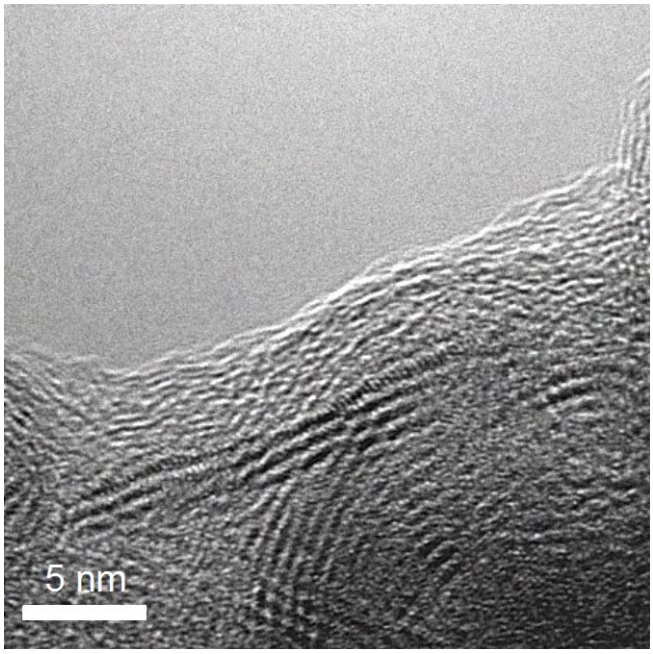
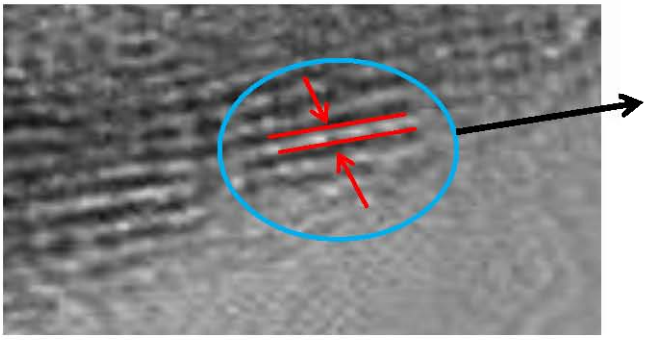
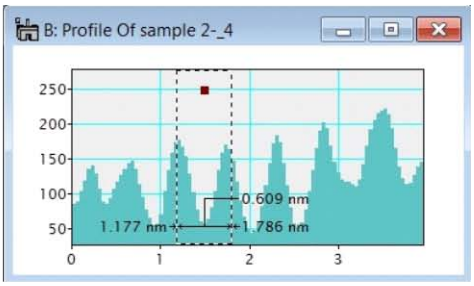


Fig. S2 Another example of a TEM image showing interaction between edge planes of molybdenum sulfide with Co_9S_8.

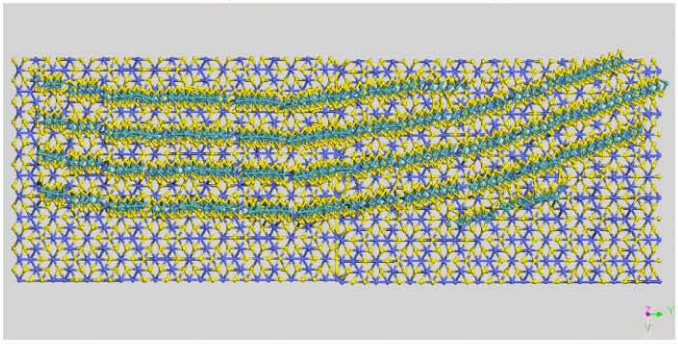
1a) Digitalization of a selected experimental HRTEM image



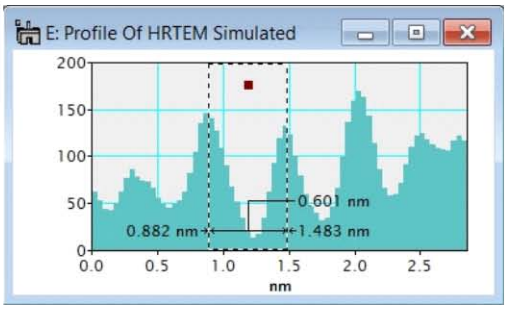
1b) Line profile analysis of the experimental TEM image



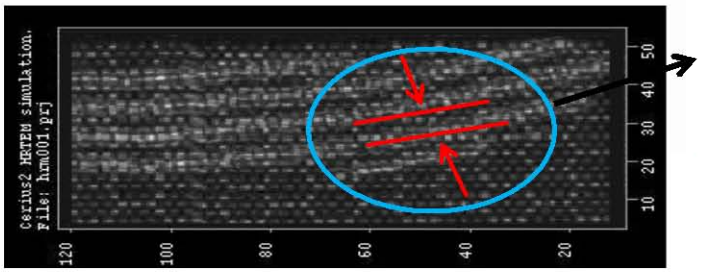
2) Molecular representation of the experimental TEM image



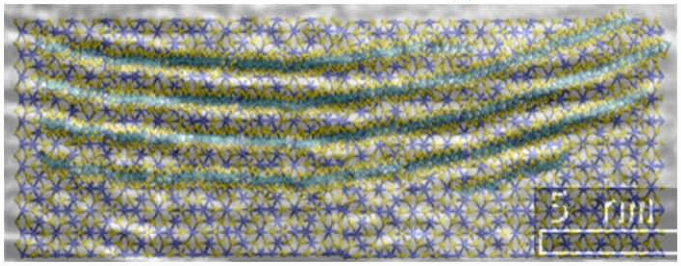
3b) Line profile analysis of the simulated TEM picture



3a) The resulting simulated TEM picture



4) Digital fitting between experimental and simulated TEM images



5) Using a portion of the interface, further analysis of Band Structure, Density of States and Mulliken was performed using this "seed" model interface

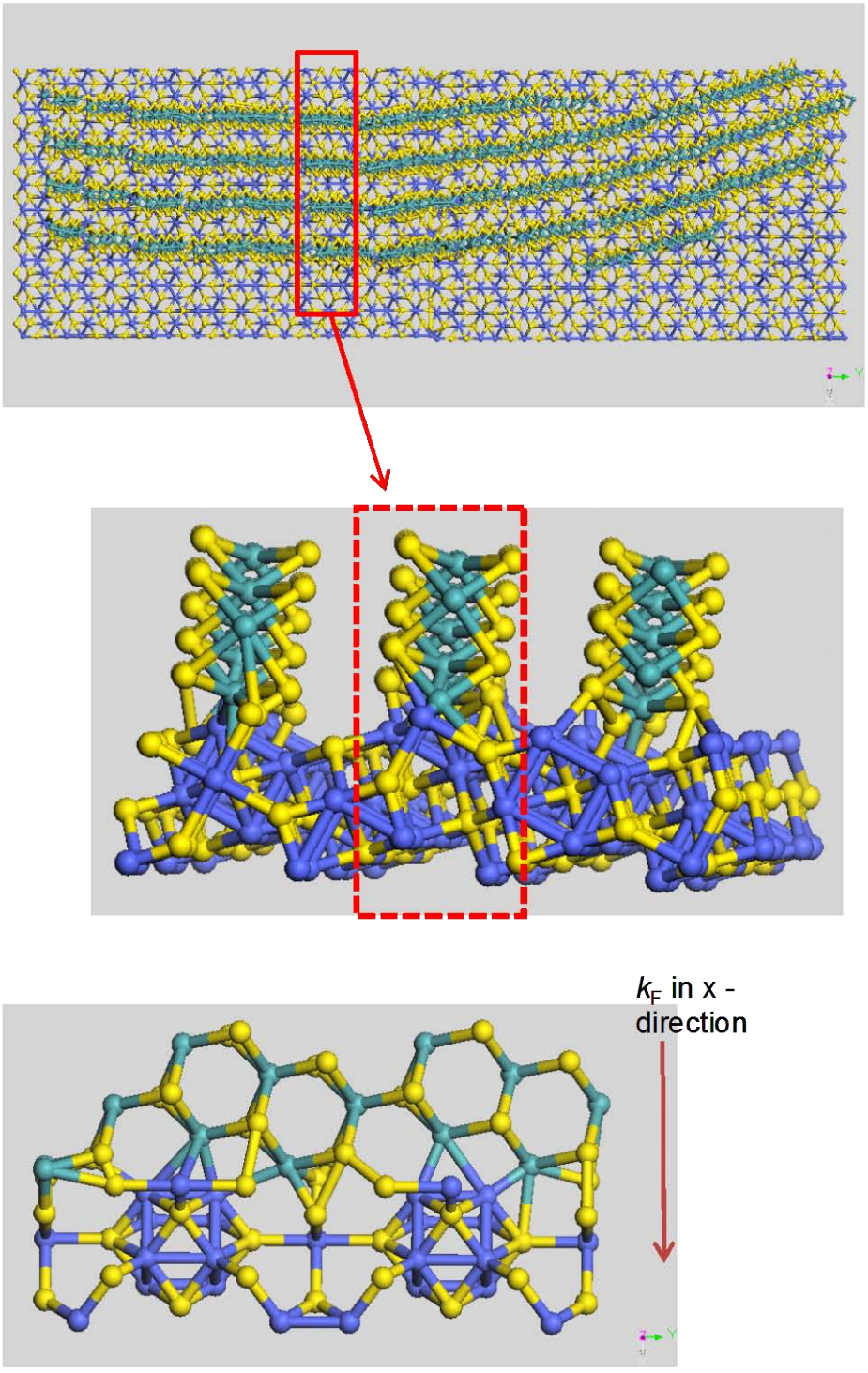


Fig. S3. Schematic of the procedure used to simulate HRTEM image starting from a selected experimental picture showing the interface between MoS_2 and Co_9S_8 and selection of a "seed" interface model used for further calculations.

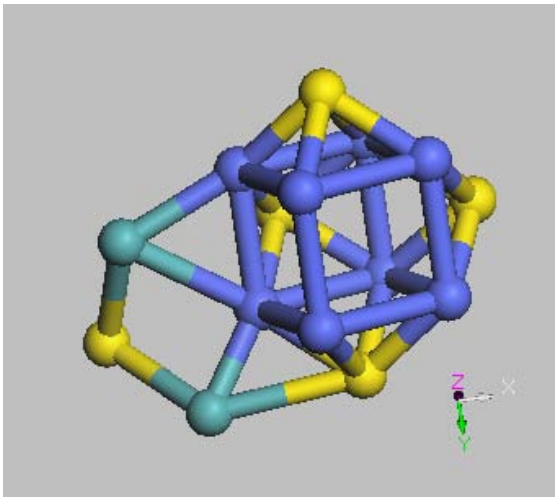


Fig. S4 Fragment of the “seed” from the interface model showing the connection between the fivefold coordinated Mo atoms and the Co cubic cluster arrangement.