HRTEM and Molecular Modeling of the MoS$_2$-Co$_9$S$_8$ 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$_9$S$_8$. 
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

3a) The resulting simulated TEM picture

3b) Line profile analysis of the 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$_9$S$_8$ 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.