DFT investigation of MoS_2 nanoclusters used as desulfurization catalysts

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Supported single layer MoS_2 is a well established catalyst used by the oil industry to remove sulfur from fossil fuels. It is believed that the catalytic activity occurs at the edge of the MoS_2 nanoparticles. Recently atomic-scale images of MoS_2 nanoclusters under catalytic working conditions have been obtained with scanning tunneling microscopy (STM). The images show that certain triangular shaped "magic clusters" are formed, where the triangular shape is attributed to stabilization from excess sulfur at the cluster edges. We will present the results from density functional theory (DFT) calculations on $Mo_{10}S_x$ clusters with x = 24, 30 and 36 and compare their predicted STM images with image attributed to $Mo_{10}S_{24}$ in the STM experiments. The cluster DFT total energies and the computed STM images suggest the experimental STM image is most likely due to a 100% S coverage at the $Mo_{10}S_x$ cluster edge corresponding to either $Mo_{10}S_{30}$ (S edge) or $Mo_{10}S_{36}$ (Mo edge).