

Supporting Information

Surface morphology and sulfur reduction pathways of MoS₂ Mo-edges of monolayer, (100) and (103) surfaces by molecular hydrogen: A DFT study

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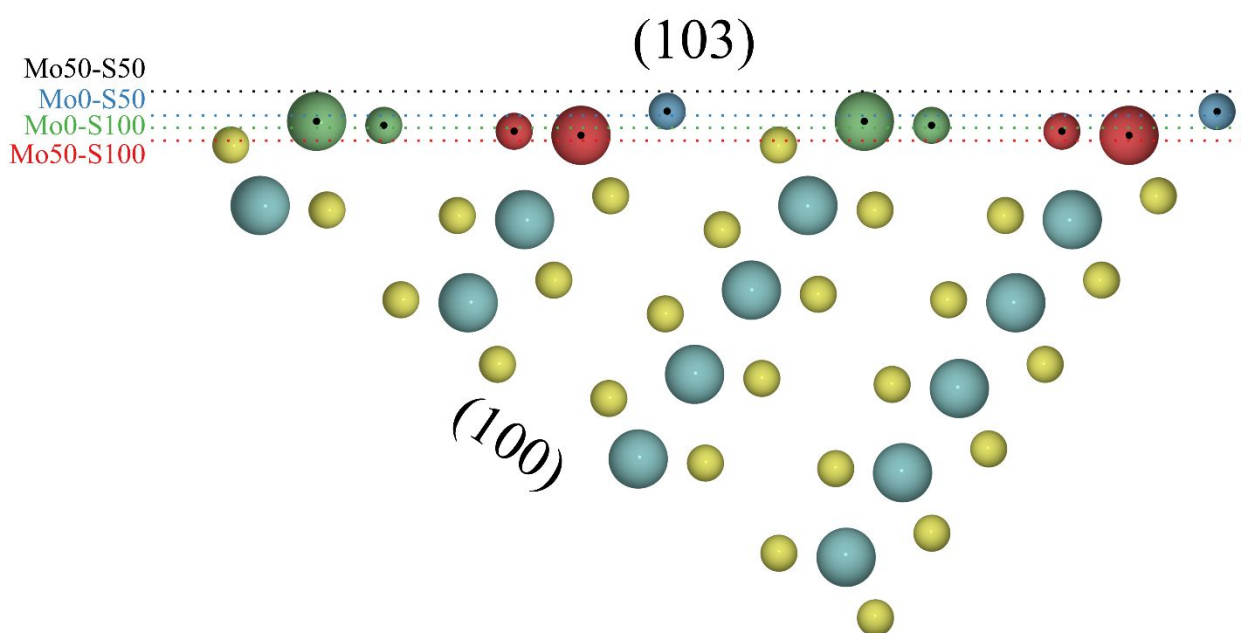


Figure S1. Planar terminations of the MoS_2 (103) surface. Black dots indicate the center of atoms. The Mo50-S50 termination includes all atoms. The Mo0-S50 termination is created by removing the sulfur atoms shown in blue. The Mo0-S100 termination is created by removing the molybdenum and sulfur atoms shown in green. The Mo50-S100 termination is created by removing the molybdenum and sulfur atoms shown in red.