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Quantum Molecular Dynamics Study on Sufidation Process of Molybdenum Oxide CHUNYANG SHENG, AIICHIRO NAKANO, RAJIV KALIA, PRIYA VASHISHTA, University of Southern California — Molybdenum disulfide (MoS_2) monolayer, a direct bandgap semiconductor, is a promising candidate for future electronics applications due to its unique mechanical and electronic properties, for which fundamental understanding of growth processes is indispensable. *In situ* transmission electron microscopy (TEM) study has shown that MoS_2 nanocrystals are formed from a submonolayer molybdenum oxide dispersed on an oxide support by sulfidation in an H_2S/H_2 atmosphere. Time-resolved TEM images revealed that single-layer MoS_2 nanocrystals form preferentially and that multi-layer nanocrystals form later in the sulfidation process. Here, we use quantum molecular dynamics simulation to investigate the sulfidation process of molybdenum oxide monolayer in H_2S/H_2 atmosphere. Simulation results identify key reaction pathways and intermediate products for MoS_2 formation. We also quantify the interplay between H_2 and those intermediate products. These atomistic mechanisms not only explain experimental results but also shed light on controlled growth of MoS_2 monolayers.

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