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Structural Properties of Finite MoS_2 Nanowires SHAYLYN CLARK, Department of Physics & Astronomy, The University of Texas at San Antonio, ANDRES SALGADO, University of Texas - Pan American, LUCAS FERNANDEZ-SEIVANE, Dept. of Physics. Universidad de Oviedo, XOCHITL LOPEZ-LOZANO, Department of Physics & Astronomy, The University of Texas at San Antonio — Molybdenum disulfide (MoS_2) has been one of the most important catalysts used in refineries worldwide for hydrodesulfurization over the past century. In the last decade, and with the advent of nanotechnology, there has been a special interest in MoS_2 nanostructures due to their high potential as novel nanocatalysts. The study of the properties of these systems is of fundamental interest for the experimental design of their catalytic activity and efficiency. In this work, we have performed ab initio density-functional calculations (DFT) to investigate the structural properties of finite MoS_2 nanostrutures. All the models here presented were based on newly experimentally observed morphologies in MoS_2 industrial catalysts using high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) images. We simulated STEM images of the theoretical models to compare it with the experimental ones. In contrast with infinite models, the finite models prefer a rippled/twisted structure morphology over the planar or helical ones. The rippled/twisted models appear to be structurally more stable.

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