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MoS_2 grain-boundary: First-principles investigations[1] DUY LE, TALAT S. RAHMAN, Department of physics, University of Central Florida, Orlando, FL 32816, USA — We present results of our first-principles electronic structure investigations, using the spin-polarized density-functional-theory, of the electronic and geometric structures of various models of grain-boundaries formed between different MoS_2 domains when grown as a single layer. From analysis of electronic band structures, we find, in all considered models, that the grain-boundaries exhibit metallic behavior. More interestingly, we find signatures of magnetism in the grain-boundary formed between two sulfur edges with 0% sulfur coverage. Details analysis of the geometric structures lead us to the conclusion that certain grain-boundaries undergo (2×1) reconstructions. We provide full details of the electronic and spin density states and change redistribution at the domain boundaries. We make contact with recent experimental observations and discuess the modifications in the characteristics for MoS_2 grown on Cu(111) [1].

[1] D. Kim *et al*, Langmuir **27**, 11650 (2011) and unpublished results.

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