Abstract Submitted
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Moiré pattern of a single layer MoS_2 grown on Cu(111)[1] DUY LE, TALAT S. RAHMAN, University of Central Florida — We present results of first principles calculations of the geometric and electronic structures of a single layer of Molybdenum disulfide (MoS_2) on Cu(111) utilizing the van der Waals density functional [1]. The lowest energy Moiré structure consists of (4×4) MoS_2 on (5×5) Cu(111), in agreement with experimental observation [2]. Examination of the local density of electronic states and charge redistribution shows that the layer is not purely physisorbed on the surface, rather there exists a chemical interaction between it and the Cu surface atoms. Interestingly the MoS_2 film is found to be not appreciably buckled, while the atoms in the top Cu layer gets reorganized and vertically disordered. The sizes of Moiré patterns for a single layer of MoS_2 adsorbed on several other close packed metal surfaces are estimated by minimizing the lattice mismatch between the film and the substrate.

[1] M. Dion *et al*, Phys. Rev. Lett. **92**, 246401 (2004)
[2] D. Kim *et al*, Langmuir **27**, 11650 (2011)

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