

Abstract Submitted  
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**Electronic Structure of Defect-Single-Layer MoS<sub>2</sub>**<sup>1</sup> TAKAT RAWAL, DUY LE, TALAT S. RAHMAN, University of Central Florida — We present density functional theory based investigations of the electronic structural properties of a single-layer molybdenum disulfide (MoS<sub>2</sub>) with a sulfur vacancy row. We show that the vacancy row introduces a defect state in the band-gap of MoS<sub>2</sub>. This state is unoccupied and localized at the vacancy row. We also present detailed analysis of the density of states and charge density of the system. The defect state reduces the band gap of the system to 0.5 eV from 1.8 eV that we obtain for the clean single-layer. In particular, we find Kohn-Sham wave functions that are confined to the defective site are responsible for this particular energy band. We discuss the possible applications of this effect on other physical properties of the system. We also extend the calculations to the case of a MoS<sub>2</sub> on Cu(111) for which experimental observations [1] suggest the presence of structures of the type under discussion here. [1] D. Kim, D. Sun, W. Lu, Z. Cheng, Y. Zhu, D. Le, T. S. Rahman, and L. Bartels, *Langmuir* 27, 11650 (2011).

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