Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Tuning Local Electronic Structure of Monolayer MoS_2 through Defect Engineering[1] SHENGXI HUANG, YAN CHEN, XIANG JI, KIRAN ADEPALLI, XI LING, MILDRED DRESSELHAUS, BILGE YILDIZ, JING KONG, Massachusetts Institute of Technology — Two-dimensional molybdenum disulfide (MoS_2) has shown promising applications in electronics, photonics, energy and electrochemistry, and defects have shown to play an essential role in altering the performance of MoS_2. However, the mechanism of defects in affecting the MoS_2 properties is unsettled. In this work, we perform a systematic study on the effect that MoS_2 defects play on the electronic structure and electrochemical reactivity. Using chemical-vapor deposited monolayer MoS_2 combined with thermal driving and ion irradiation, we fabricate monolayer MoS_2 with different defect densities on various substrates. We reveal that the electronic state of MoS_2 is sensitive to both substrates and defects, supported by our X-ray photoelectron spectroscopy, Raman and photoluminescence spectroscopies, and scanning tunneling microscopy/spectroscopy. We further found that the defect density in MoS_2 can effectively tune the hydrogen evolution reactivity. Our findings provide useful guidance for defect engineering in MoS_2 and show the potential application of such defect engineering in using MoS_2 for a clean and effective energy source.

[1]US Department of Energy grant DE-SC0001299

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Date submitted: 09 Nov 2016 Electronic form version 1.4