

# Formation of Coherent Phase Domain Heterojunctions in Single Layer MoS<sub>2</sub> on Au(111)

F. Wu,<sup>1,2</sup> Z. Liu,<sup>1</sup> N. Hawthorne,<sup>1</sup> M. Chandross,<sup>3</sup> Q. Moore,<sup>1</sup> N. Argibay,<sup>3</sup>  
J.F. Curry<sup>3</sup> and J.D. Batteas<sup>1</sup>

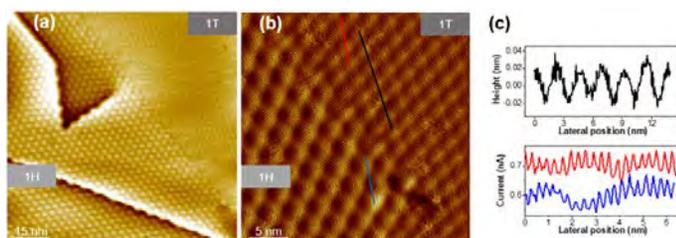
<sup>1</sup> Department of Chemistry, Texas A&M University, College Station, TX 77843

<sup>2</sup> Department of Materials Science and Engineering, Texas A&M University,  
College Station, TX 77843

<sup>3</sup> Material, Physical, and Chemical Sciences Center, Sandia National Laboratories,  
Albuquerque, NM 87123

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted tremendous attention over the past decade due to their exciting mechanical, electronic and frictional properties [1-5]. Heterojunctions of semiconductors and metals are the fundamental building blocks of modern electronics. Coherent heterostructures between dissimilar materials can be achieved by composition, doping or heteroepitaxy of chemically different elements. Here we report, the formation of coherent single-layer MoS<sub>2</sub> heterostructures

(Figure 1), which are chemically homogenous with matched lattices, but show electronically distinct semiconducting (1H phase) and metallic (1T phase) character, when deposited by mechanical exfoliation on Au(111). The facile exfoliation technique here eliminates tape residues usually found in many exfoliation methods, and yields single-layer MoS<sub>2</sub> with millimeter (mm) size. Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have collectively been employed to elucidate the structural and electronic properties of MoS<sub>2</sub> monolayers on Au substrates. Our work provides a basis to produce macroscale two-dimensional heterostructures, which represent unique candidates for future electronic devices and applications.



**Figure 1.** STM of the coherent heterostructures of MoS<sub>2</sub> monolayers. (a) Large-scale STM image of single-layer MoS<sub>2</sub> with two different Moiré patterns from the 1H and 1T phases. (b) Corresponding high resolution STM current image of single-layer MoS<sub>2</sub> on Au(111). (c) Line profile (black) showing the periodicity and the corrugation of the 1T-MoS<sub>2</sub> Moiré pattern in (b) and line profiles (blue and red) presenting the atomic distances for the two different phases.

[1] K. Novoselov, D. Jiang, F. Schedin, T. Booth, V. Khotkevich, S. Morozov and A. Geim, *Proc. Natl. Acad. Sci. U.S.A.* **2005**, *102*, 10451-10453.

[2] R. Ma and T. Sasaki, *Adv Mater* **2010**, *22*, 5082-5104.

[3] C. Lee, Q. Li, W. Kalb, X.-Z. Liu, H. Berger, R.W. Carpick and J. Hone, *Science* **2010**, *328*, 76-80.

[4] I. Song, C. Park and H.C. Choi, *RSC Adv.* **2015**, *5*, 7495-7514.

[5] X. Huang, Z. Zeng and H. Zhang, *Chem Soc Rev* **2013**, *42*, 1934-1946.