

## Supporting Information for

### First principles studies on electronic and contact properties of Single layer 2H-MoS<sub>2</sub>/1T'-MX<sub>2</sub> heterojunctions

Jiao Yu,<sup>a</sup> Cai-Juan Xia,<sup>a,\*</sup> Zhen-Yang Hu,<sup>a</sup> Jian-Ping Sun,<sup>b</sup> Xiao-Peng Hao,<sup>b</sup> Lu-Xia Wang,<sup>c</sup>

Qing-Long Fang,<sup>a,\*</sup>

*<sup>a</sup>School of Science, Xi'an Polytechnic University, Xi'an, 710048, China*

*<sup>b</sup>Division of Thermophysics and Process Measurements, National Institute of Metrology,*

*Beijing, 100013, China*

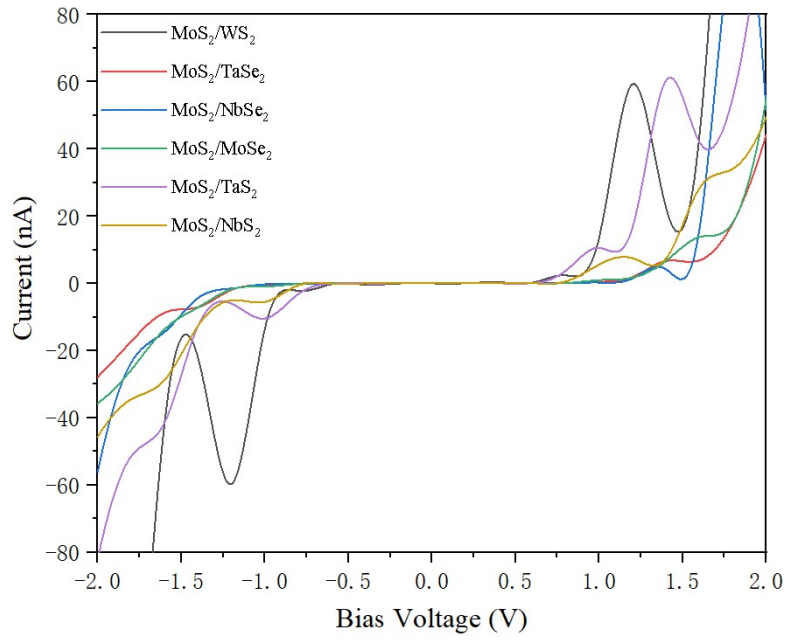
*<sup>c</sup>Department of Physics, University of Science and Technology Beijing, Beijing, 100083,*

*China*

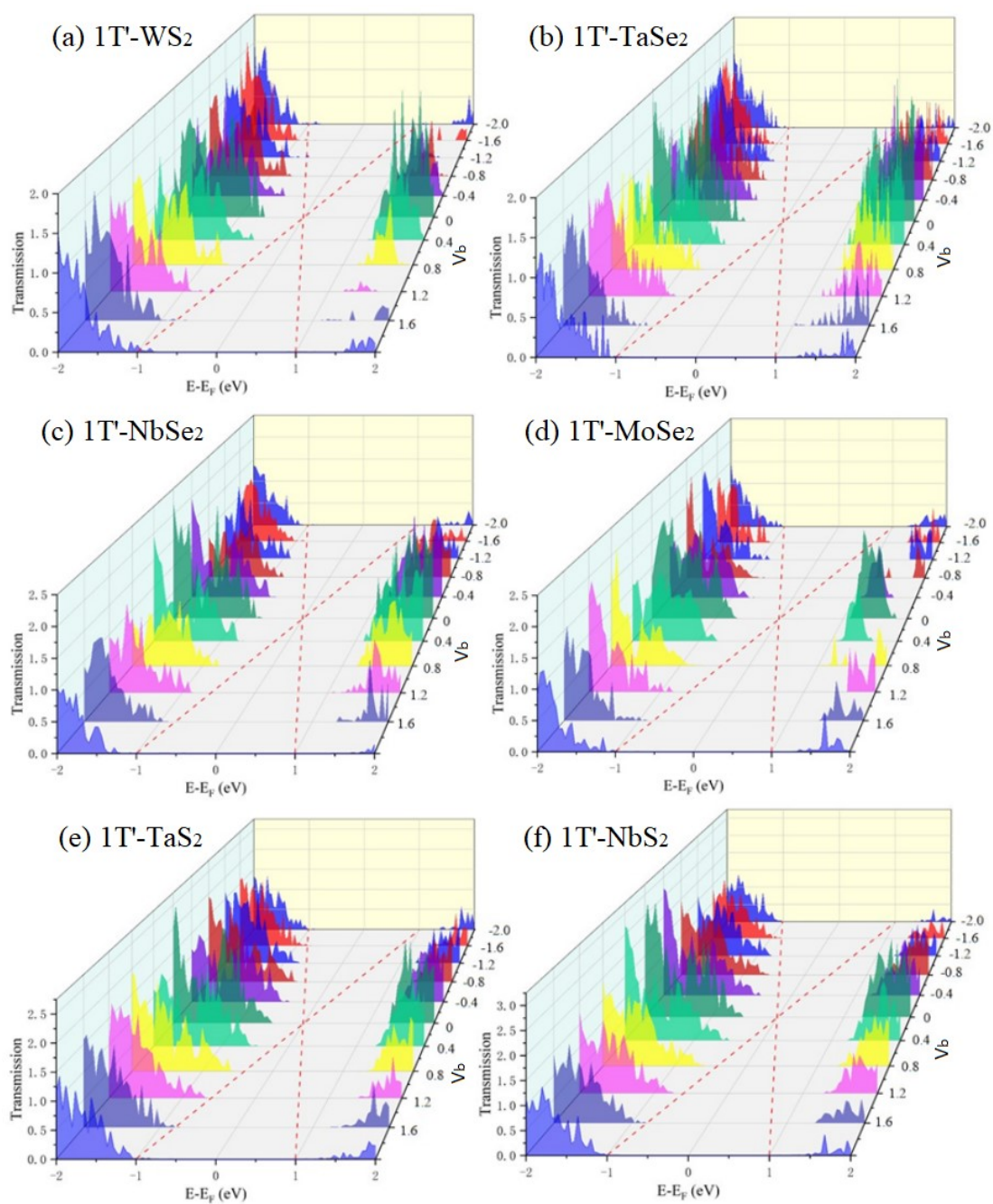
\* Corresponding authors.

E-mail addresses: [caijunxia@xpu.edu.cn](mailto:caijunxia@xpu.edu.cn) (Cai-Juan Xia);

[20190605@xpu.edu.cn](mailto:20190605@xpu.edu.cn) (Qing-Long Fang).



**Fig. S1.** *I-V* curve of the 2H-MoS<sub>2</sub>/1T'-MX<sub>2</sub> lateral contact transistor.



**Fig. S2.** Transmission spectrum of the 2H-MoS<sub>2</sub>/1T'-MX<sub>2</sub> lateral contact device at bias voltage [-2V, +2V].