

### Supporting Information (SI)

#### **Achieving Ultra-Low Contact Barriers in $\text{MX}_2/\text{SiH}$ ( $\text{M} = \text{Nb, Ta}$ ; $\text{X} = \text{S, Se}$ ) Metal-Semiconductor Heterostructures: First-Principles Prediction**

S. T. Nguyen<sup>1</sup>, Chuong V. Nguyen<sup>2,†</sup>, Huynh V. Phuc<sup>3,†</sup>, Nguyen N. Hieu<sup>4,5</sup>, Cuong Q. Nguyen<sup>4,5,†</sup>

<sup>1</sup>Faculty of Electrical Engineering, Hanoi University of Industry, Hanoi 100000, Vietnam.

Email: [nguyensontung@hau.edu.vn](mailto:nguyensontung@hau.edu.vn)

<sup>2</sup>Department of Materials Science and Engineering, Le Quy Don Technical University, Hanoi 100000, Vietnam.

Email: [chuong.vnguyen@lqdtu.edu.vn](mailto:chuong.vnguyen@lqdtu.edu.vn)

<sup>3</sup>Division of Theoretical Physics, Dong Thap University, Cao Lanh 870000, Vietnam.

E-mail: [hvphuc@dthu.edu.vn](mailto:hvphuc@dthu.edu.vn)

<sup>4</sup>Institute of Research and Development, Duy Tan University, Da Nang 550000, Vietnam.

E-mail: [nguyenquangcuong3@duytan.edu.vn](mailto:nguyenquangcuong3@duytan.edu.vn)

<sup>5</sup>Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Vietnam

† To whom correspondence should be addressed.

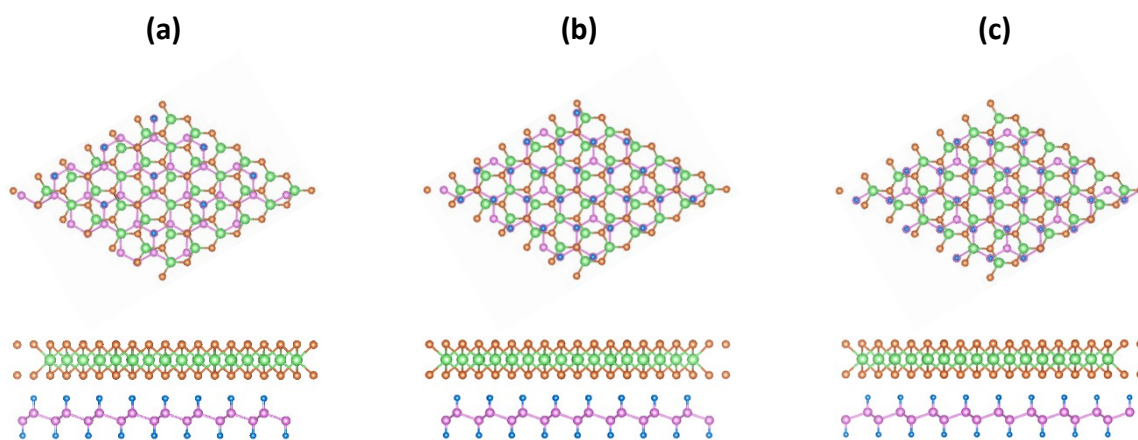


Figure S1. Atomic structures of the MX<sub>2</sub>/SiH heterostructures for three different stacking configurations of (a) SP-II, (b) SP-III and (c) SP-IV.

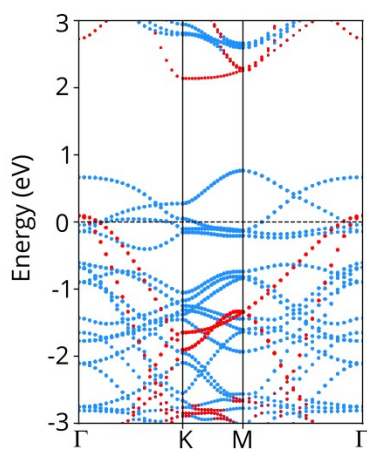


Fig. S2. Projected band structure of NbS<sub>2</sub>/SiH MHS under the compressive strain of  $\varepsilon_b = -3\%$ .