

Supplementary Mastherial for

Structure, Stability, and Superconductivity of Two-Dimensional

Janus NbSH Monolayers: A First-Principle Investigation

Yan Li ¹, Chunying Pu^{2*}, and Dawei Zhou^{2*}

¹ Institute for Computational Materials Science, School of Physics and Electronics, International Joint Research Laboratory of New Energy Materials and Devices of Henan Province, Henan University, Kaifeng 475004, China

² Henan International Joint Laboratory of MXene Materials Microstructure, College of Physics and Electronic Engineering, Nanyang Normal University, Nanyang 473061, China;

* Correspondence: puchunying126.com(C.P.); zhoudawei@nynu.edu.cn(D.Z.)

Figure S1 The phonon dispersion relations (a) 2H-NbSH (b) 1T-NbSH.

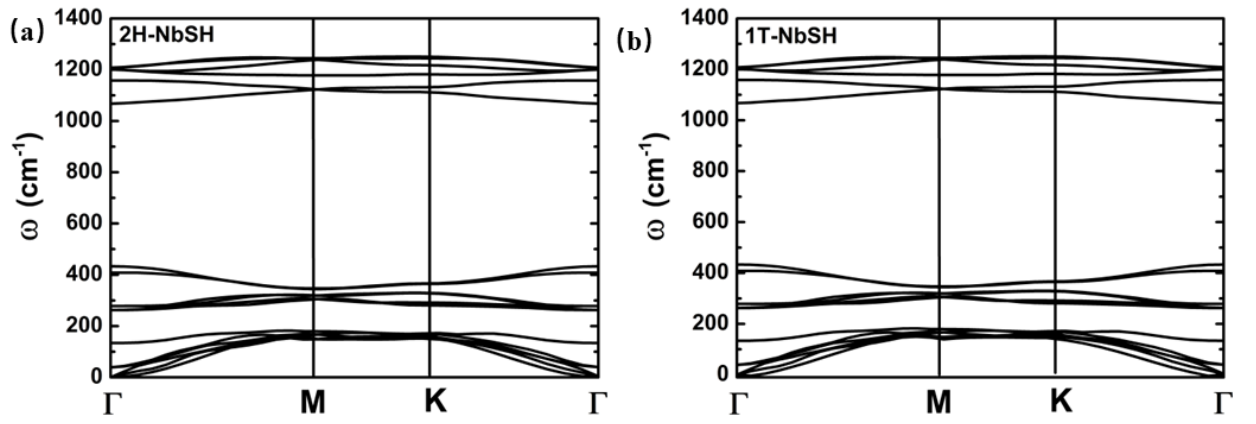


Figure S2 The calculated total density of states (TDOS) of the three NbSH phases with spin-polarized effect considered (a) 1T-NbSH, (b) 2H-NbSH and (c) Predicted-NbSH

