Supporting Information for Two-dimensional stable Mn based half metal and antiferromagnets promising for spintronics

Bingwen Zhang,*,† Guang song,‡ Jie Sun,¶ Jiancai Leng,¶ Cheng Zhang,† and Jun Wang*,†

†*Fujian Provincial Key Laboratory of Functional Marine Sensing Materials, Minjiang University, Fuzhou 350108, P. R. China*

‡*Department of Physics, Huaiyin Institute of Technology, Huaian 223003, P. R. China*

¶*School of Electronic and Information Engineering (Department of Physics), Qilu University of Technology (Shandong Academy of Sciences), 250353 Jinan, Shandong, P. R. China*

E-mail: turney0524@163.com; wjnaf@163.com

Abstract

This supporting information includes bond-length revolution along with time steps of AIMD at 300 K of both $MnC_{0.5}Si_{0.5}$ monolayer and bilayer MnSi nanosheet; electronic projection band structures of Hubbard $U_{eff} = 4$ eV of both MnSi and $MnC_{0.5}Si_{0.5}$ monolayer; structure search of monolayer MnSi and $MnC_{0.5}Si_{0.5}$ as well as bilayer MnSi nanosheets; electronic band structures of Hubbard $U_{eff} = 3$ eV and $U_{eff} = 5$ eV of both MnSi and $MnC_{0.5}Si_{0.5}$ monolayer; phonon band structure of bilayer $MnC_{0.5}Si_{0.5}$ nanosheet; different magnetic states of bilayer MnSi nanosheet, electronic band structure of Hubbard $U_{eff} = 4$ eV and Monte Carlo simulation of bilayer MnSi nanosheet.

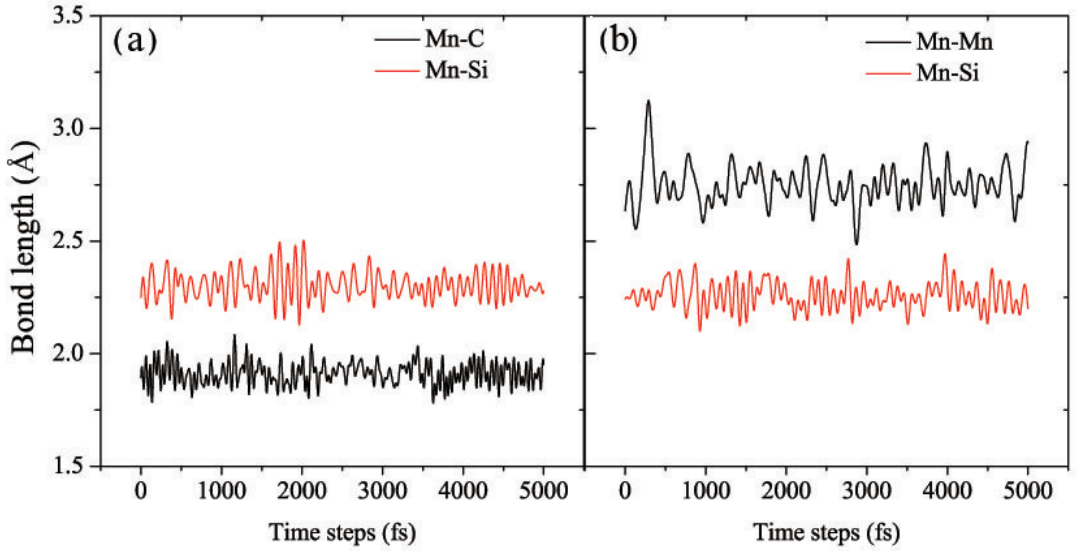

Figure S1: The bond-length revolution along with the 5000 fs time steps of AIMD at 300 K for (a) $MnC_{0.5}Si_{0.5}$ monolayer and (b) bilayer MnSi nanosheet.

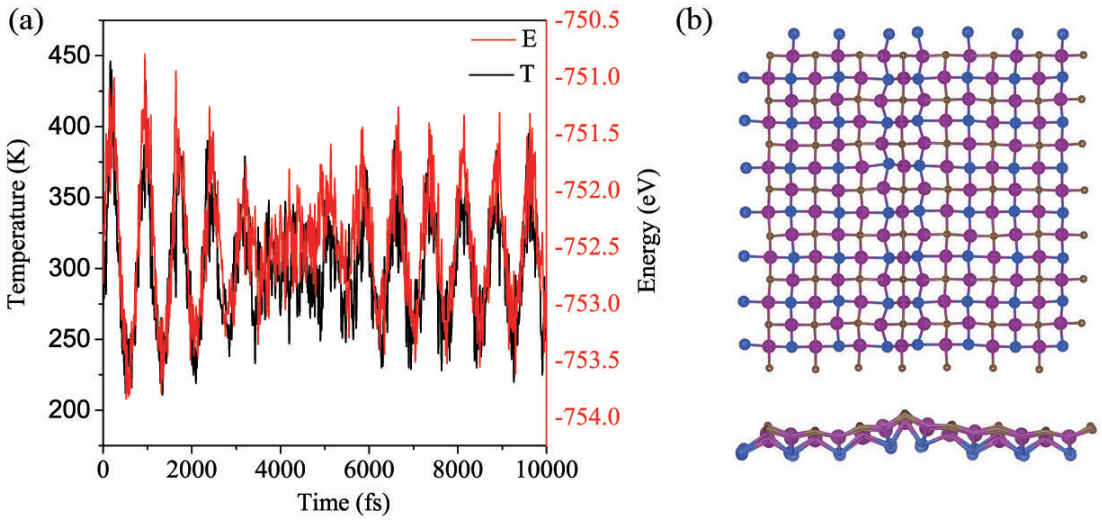

Figure S2: (a)The evolution of temperature (K) and the corresponding energy (eV) during the 300 K AIMD of 10000 fs time steps of $MnC_{0.5}Si_{0.5}$ monolayer; (b) the structure of $MnC_{0.5}Si_{0.5}$ monolayer at the end of the 300 K AIMD simulation.

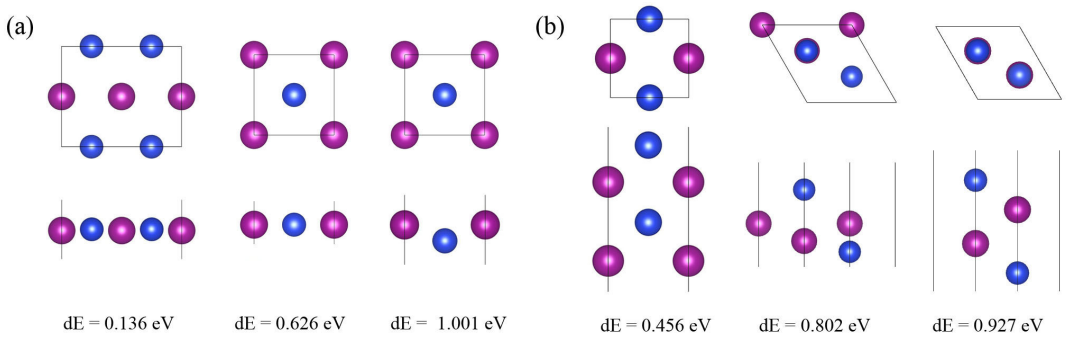

Figure S3: Three relatively low-energy MnSi monolayer (a) and bilayer (b) in the structure search, dE is the energy difference relative the lowest energy.

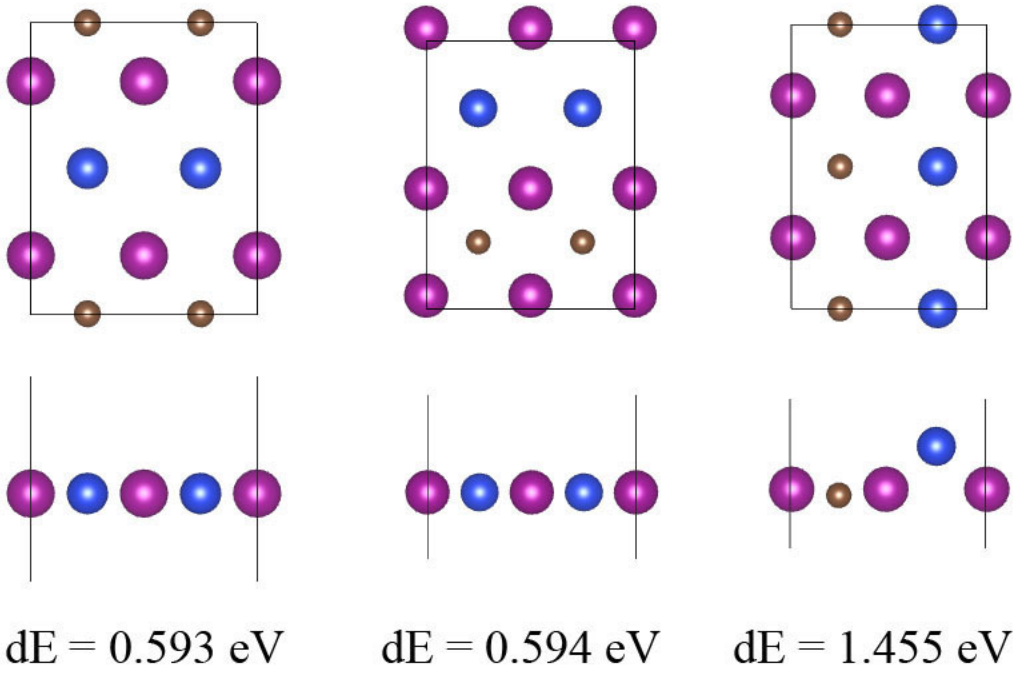

Figure S4: Three relatively low-energy $MnC_{0.5}Si_{0.5}$ monolayer in the structure search, dE is the energy difference relative the lowest energy.

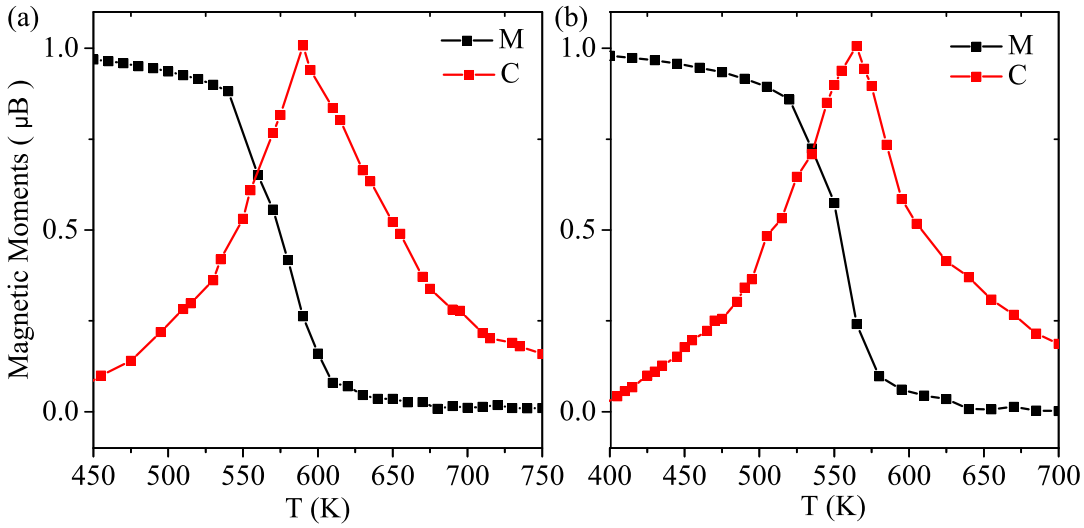

Figure S5: Variation of the average normalized magnetic moment (M) and specific heat (C) of MnSi (a) and $MnC_{0.5}Si_{0.5}$ (b) monolayer with the NN and NNN interactions.

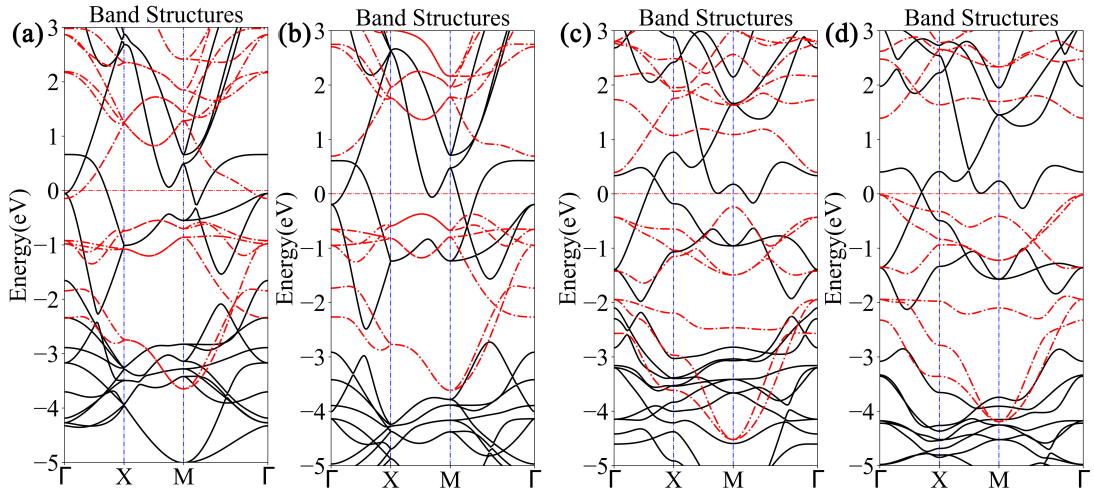

Figure S6: The electronic band structures of MnSi monolayer (a) U_{eff} = 3 eV, (b) U_{eff} = 5 eV, and $MnC_{0.5}Si_{0.5}$ monolayer (c) U_{eff} = 3 eV, (d) U_{eff} = 5 eV.

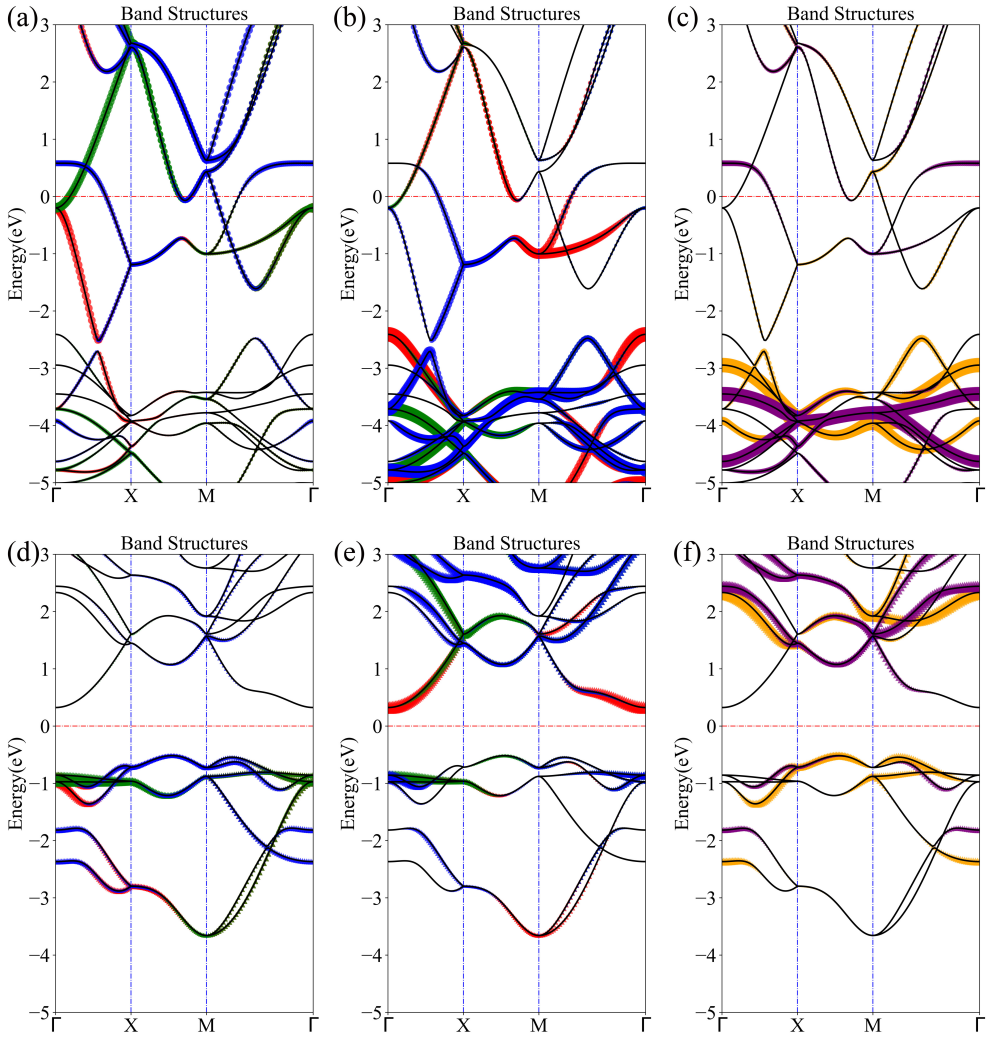

Figure S7: The electronic projection band structure spin up (a+b+c) and spin down (d+e+f) of MnSi monolayer: (a+d) p_x (red line), p_y (green line) and p_z (blue line) orbitals; (b+e) d_{xy} (red line), d_{yz} (green line) and d_{xz} (blue line) orbitals; (c+f) d_{x^2} (orange line), d_{z^2} (purple line) orbitals.

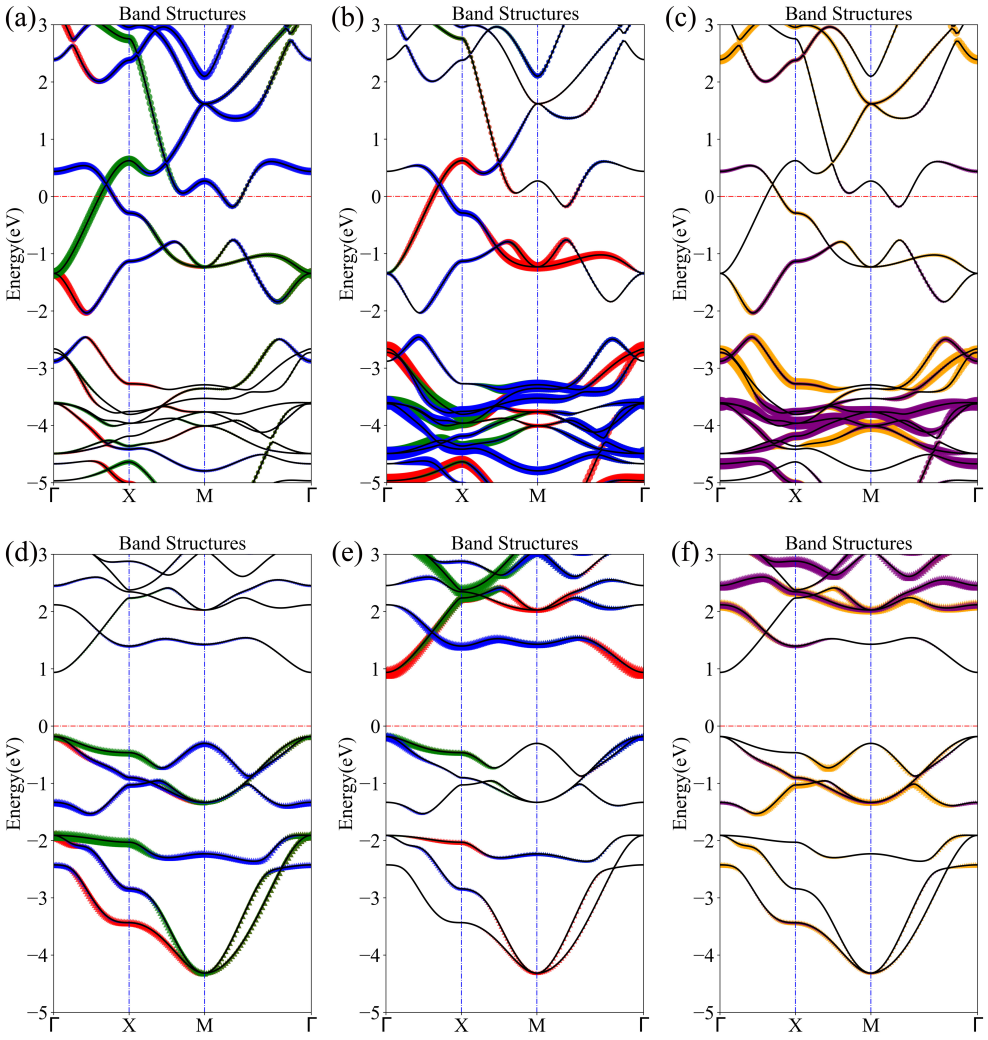

Figure S8: The electronic projection band structure spin up (a+b+c) and spin down (d+e+f) of $MnC_{0.5}Si_{0.5}$ monolayer : (a+d) p_x (red line), p_y (green line) and p_z (blue line) orbitals; (b+e) d_{xy} (red line), d_{yz} (green line) and d_{xz} (blue line) orbitals; (c+f) d_{x^2} (orange line), d_{z^2} (purple line) orbitals.

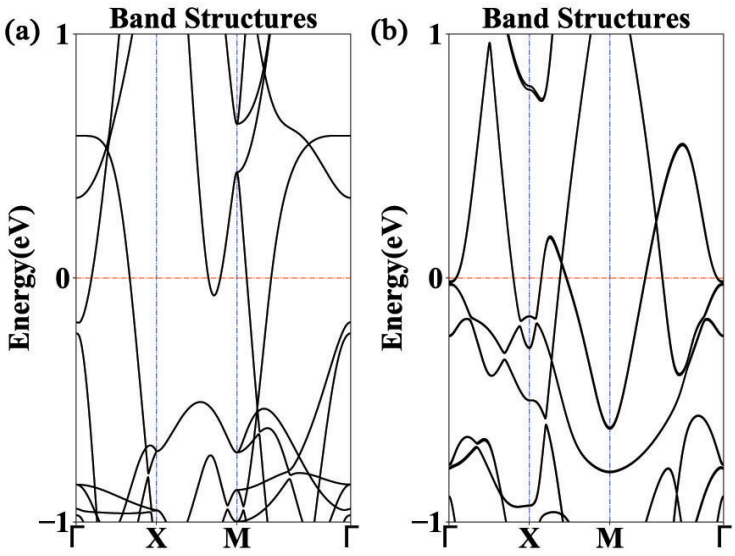

Figure S9: The band structures of MnSi nanosheet with SOC: (a) monolayer, (b) bilayer.

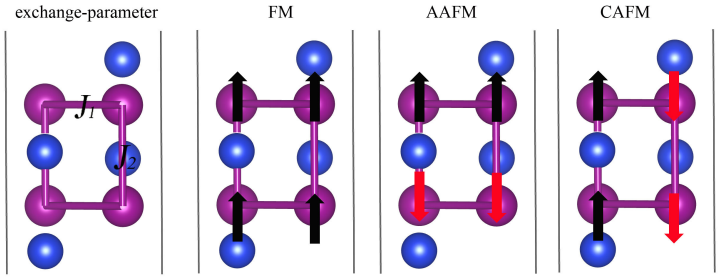

Figure S10: The different magnetic states of bilayer MnSi nanosheet.

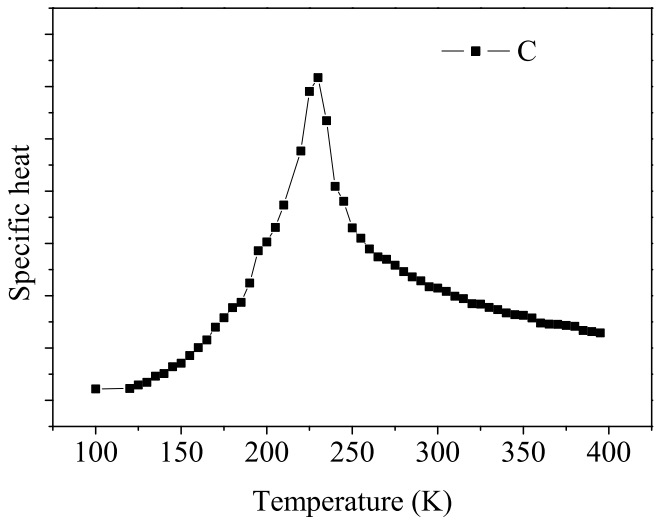

Figure S11: The specific heat versus temperature during the Monte Carlo simulation of bilayer MnSi nanosheet.

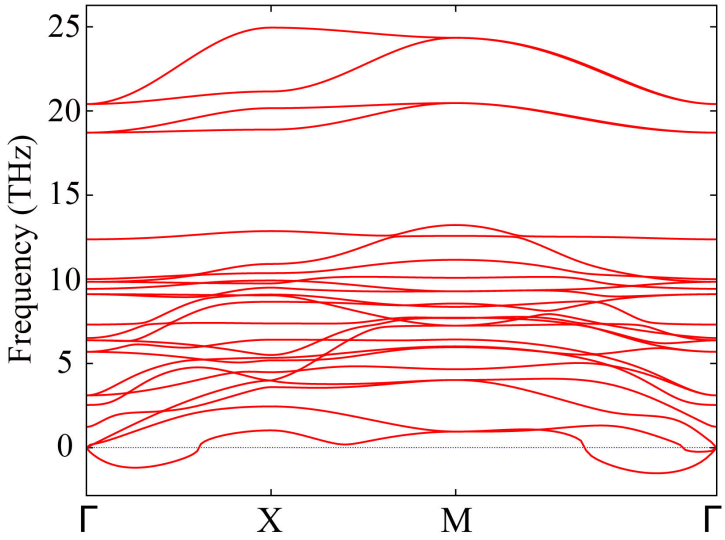

Figure S12: The phonon band structure of bilayer $MnC_{0.5}Si_{0.5}$.

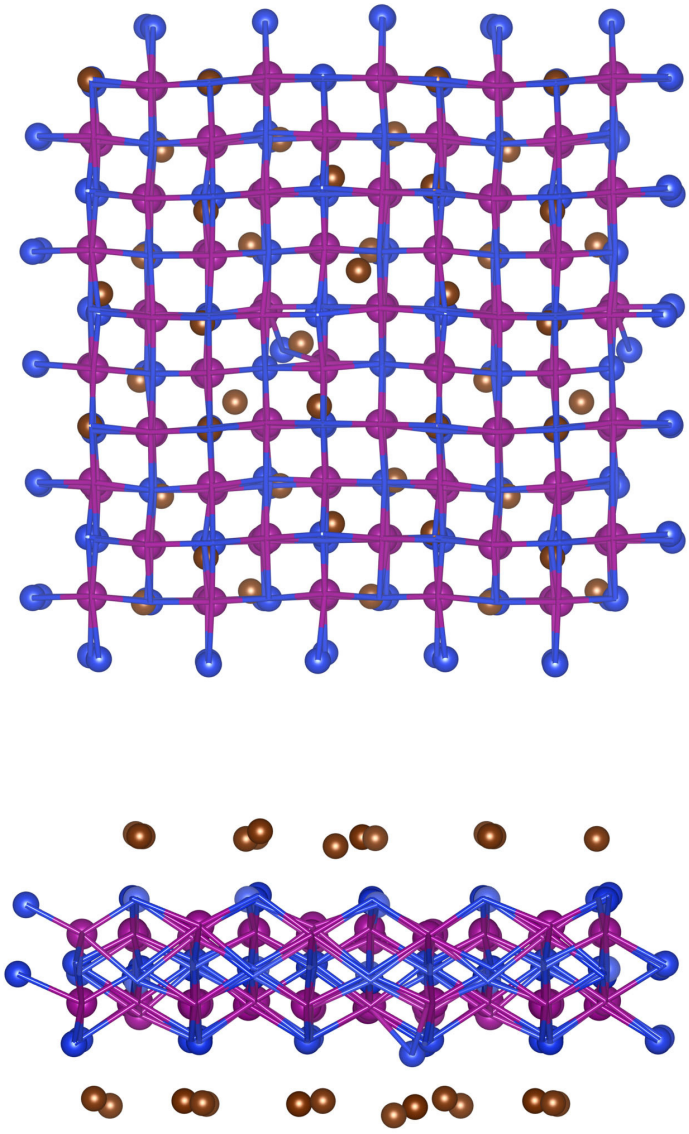

Figure S13: The AIMD simulation of surface functionalized bilayer MnSi nanosheet by Br atoms.