Electronic Supplementary Information for

First-principles study of bilayer hexagonal structure of SN_2 nanosheet: a

highly stable non-metal platform for the quantum anomalous Hall effect

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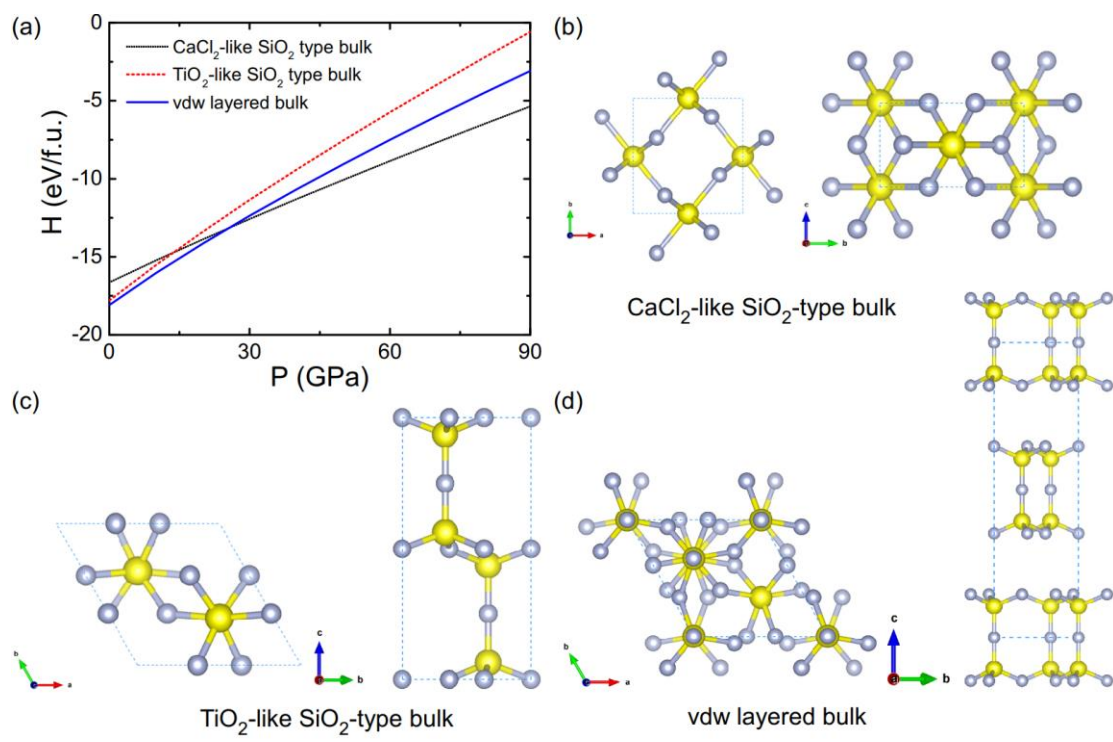
Contents:

Figure S1: The enthalpies of different SN_2 bulk structures as a function of pressures. The geometries of (b) $CaCl_2$-like SiO_2-type, (c) TiO_2-like SiO_2-type, and (d) vdw layered bulk structures for the SN_2 system.
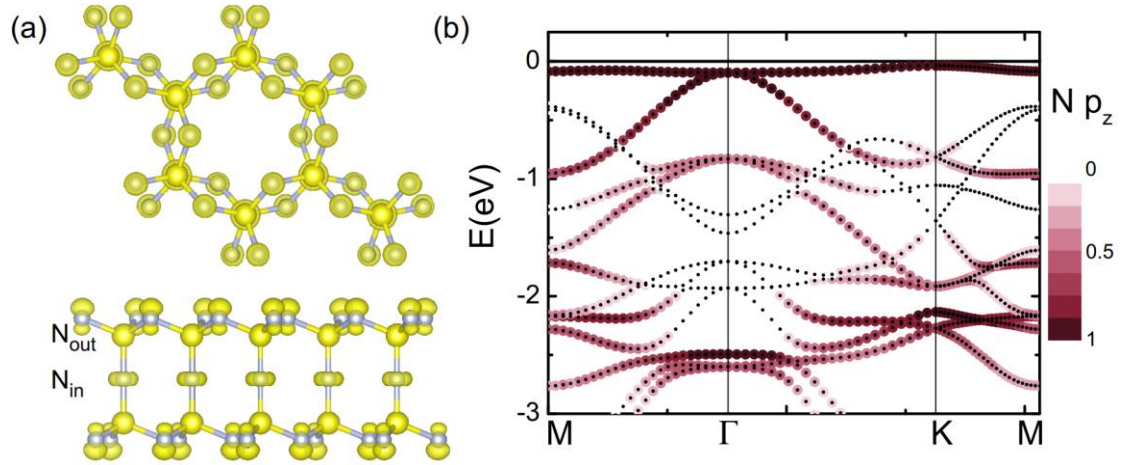
Figure S2: (a) The partial charge density of the flat band at Γ point. The isosurface is set to 0.003 $|e|/\mathring{A}^3$. (b) The fat-band analysis of the PBE bands of BHS-SN$_2$ nanosheet. The contribution of N$_{out}$ p$_z$ orbitals is labelled by colors, and the maximum value is normalized to 1.
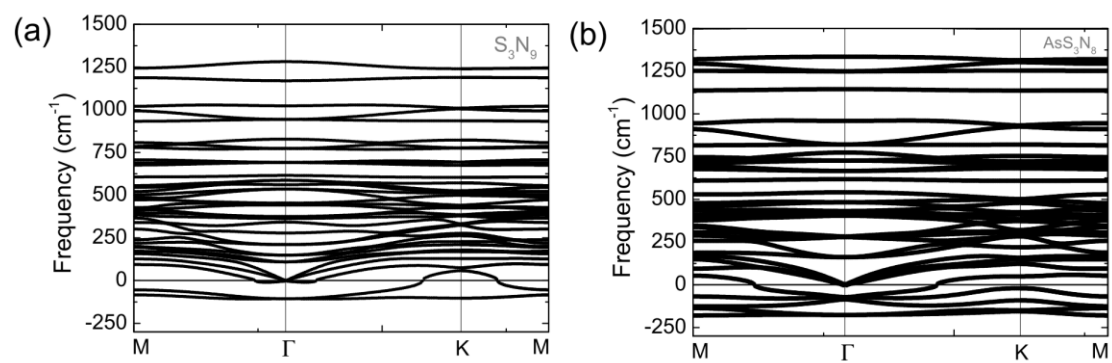
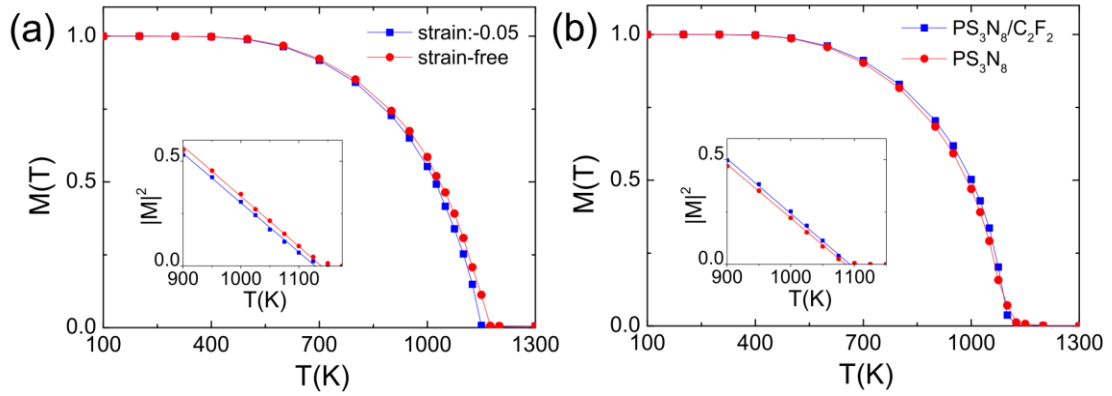Figure S3: The phonon bands of (a) S_3N_9 and (b) AsS_3N_8 nanosheets.

Figure S4: The mean-field theory results for the Curie temperature. (a) The temperature-dependent magnetic moment of hole-doped BHS-SN$_2$ nanosheet with a compressive strain of -0.05 and without strain. (b) The temperature-dependent magnetic moment of the isolated and fluorographene-supported PS$_3$N$_8$ nanosheets. The insets depict the magnetic moment squared near the transition temperature, where a linear fitting is performed to evaluate the T$_c$ values.
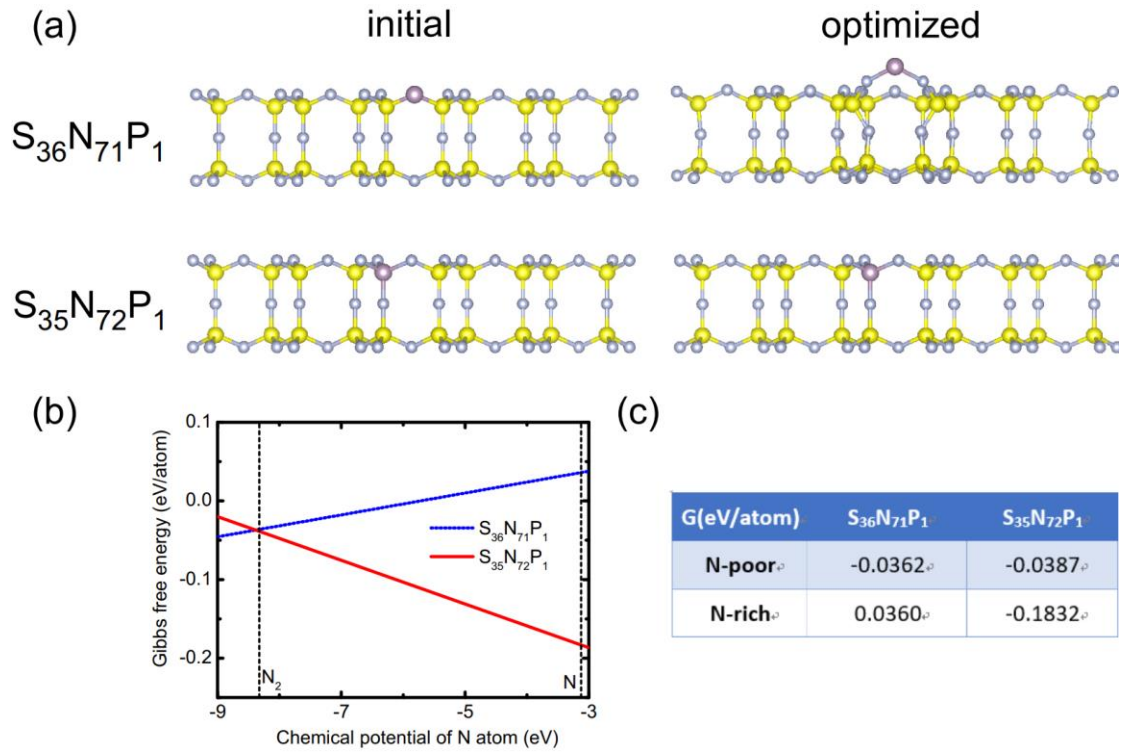
Figure S5: (a) The initial and optimized geometries of $S_{36}N_{71}P_1$ and $S_{35}N_{72}P_1$ nanosheets. (b) The variations of Gibbs free energies versus the chemical potential of N element for the $S_{36}N_{71}P_1$ and $S_{35}N_{72}P_1$ nanosheets. (d) The Gibbs free energy values of $S_{36}N_{71}P_1$ and $S_{35}N_{72}P_1$ nanosheets under the N-poor and N-rich conditions. Here, the N-poor and N-rich conditions correspond to $\mu_N = E_{N2}/2$ and $\mu_N = E_{Natom}$, respectively.