Supplementary Materials

Quantum Anomalous Hall Effect in Two-dimensional Ferromagnetic NpF Monolayer with High Curie Temperature

Yuqing Mao, Jie Li, Xiaokang Xu, Xinghao Chang, Yuxuan Liu, Xiuyun Zhang,[*] Ailei He[*]

College of Physics Science and Technology, Yangzhou University, Yangzhou 225002, China.
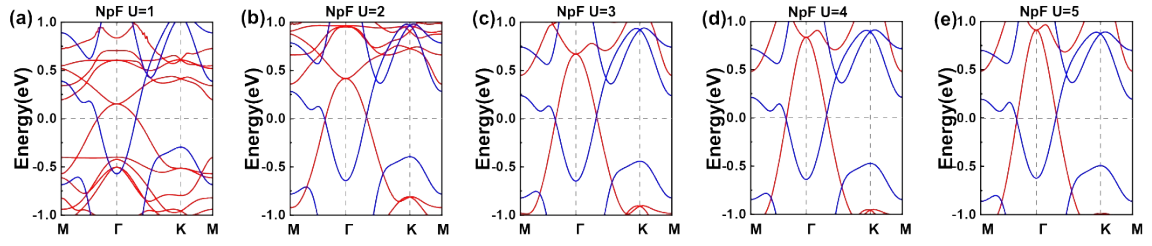
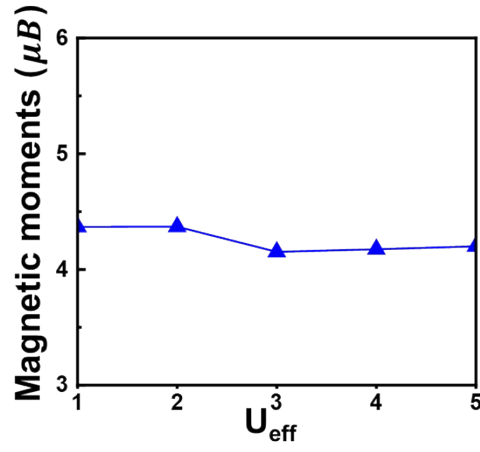Fig. S1. (a) - (e) Band structures of the NpF monolayer with different U_{eff}.

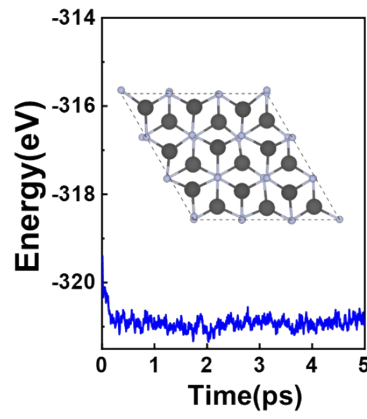Fig. S2. Magnetic moments of the NpF monolayer with different U_{eff}.

Fig. S3. The snapshots of 3×3×1 supercell of NpF monolayer after AIMD simulations of 5 ps at 300K.
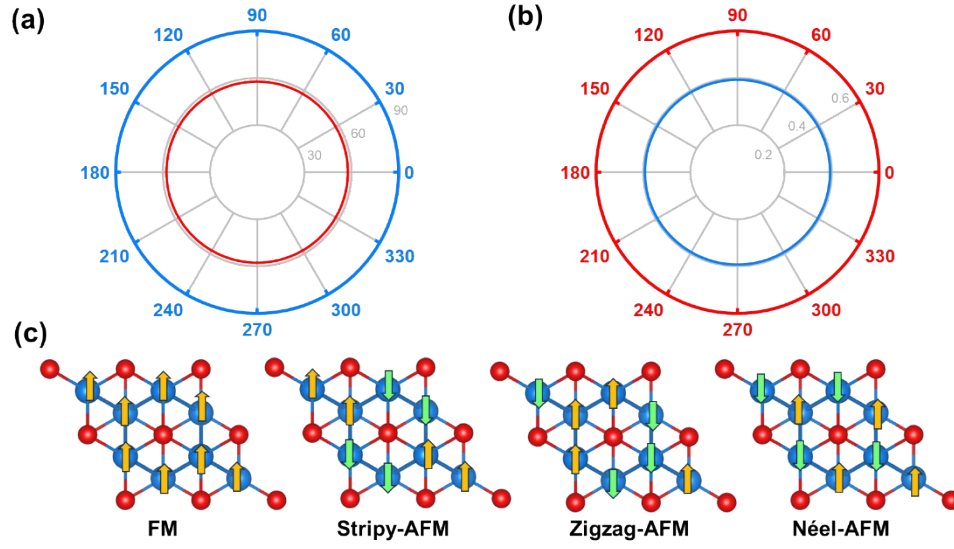
Fig. S4. (a) The polar diagrams of (b) Young's modulus E (φ) (N/m) and (c) Poisson ratio v (φ) as a function of the azimuthal angle φ. (c) The four different magnetic configurations of NpF monolayer.
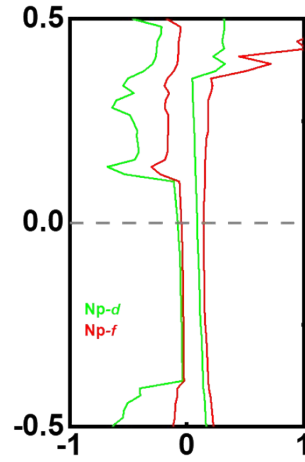

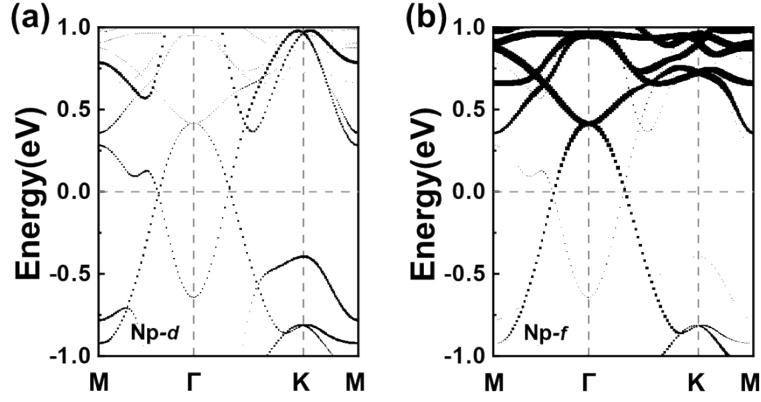Fig. S5. The orbital-projected density of state of NpF monolayer.

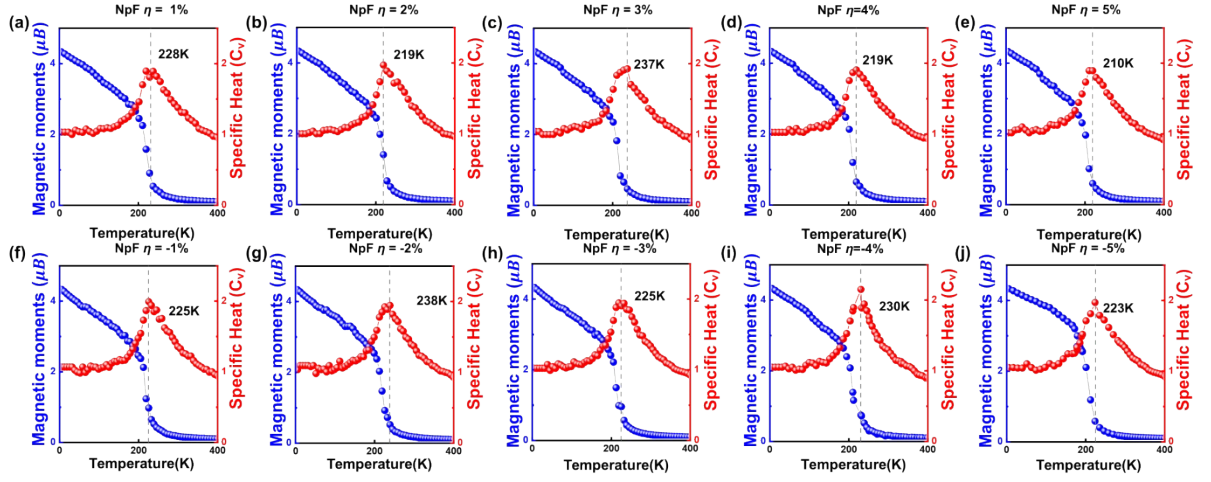Fig. S6. The orbitals projection band structures for NpF monolayer.

Fig. S7. Magnetic moment (μ_B) and heat capacity as a function of temperature from Monte Carlo simulation for NpF monolayer under biaxial strains.
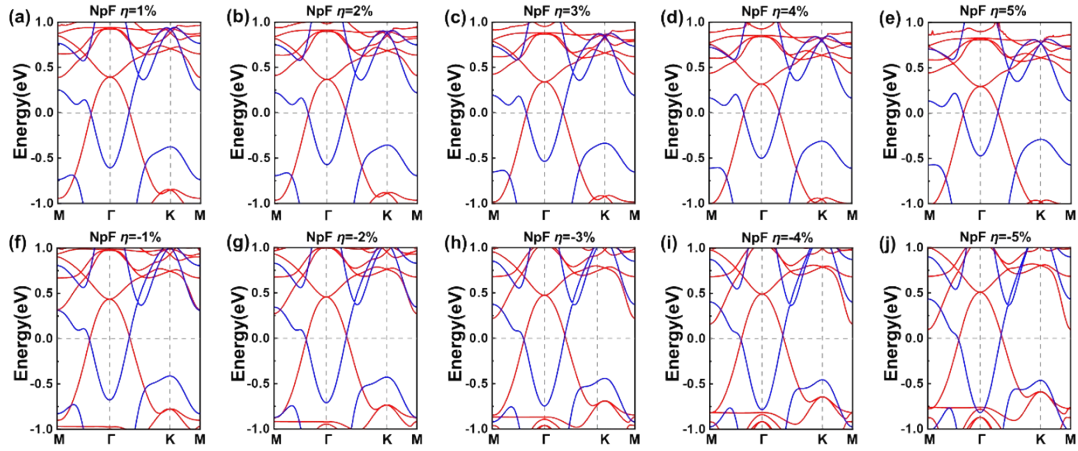

Fig. S8. (a) - (j) Band structures of the NpF monolayer at biaxial strain (-5% $\leq \eta \leq$ 5.0%) without SOC.