Electronic Supplementary Material (ESI) for Nanoscale Horizons.


# A novel two-dimensional Superconducting Ti layer: density functional theory and electron beam irradiation

Xiao-Min Zhang [a//], Jiawei Tang[b//], Jing Zhang[b], Jin Yu[c], Litao Sun[b], Zhiqing Yang [d,e*], Ke Xia[a*], Weiwei Sun[b,c//,*]

[a] *School of Physics, Southeast University, Nanjing 211189, China*

[b] *SEU-FEI Nano-Pico Center, Key Laboratory of MEMS of Ministry of Education, Southeast University, Nanjing 210096, China*

[c] *Jiangsu Province Key Laboratory of Advanced Metallic Materials, Southeast University, Nanjing, 219210, China*

[d] *Ji Hua Laboratory, Foshan 528251, China*

[e] *Foshan University, Foshan 528231, China*

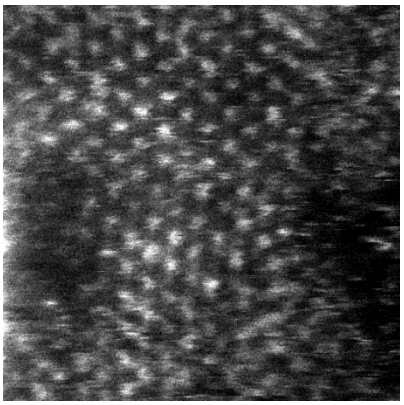

**Fig. S1.** A magnified STEM image recorded after tilting the sample for several degrees

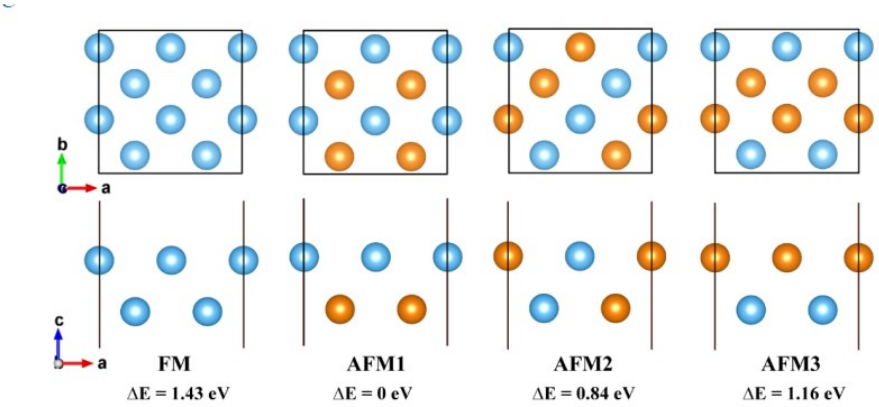


**Fig. S2.** The magnetic orders considered in this work, including FM and three AFM orders. The blue and yellow spheres represent atoms with opposite spin directions, respectively.

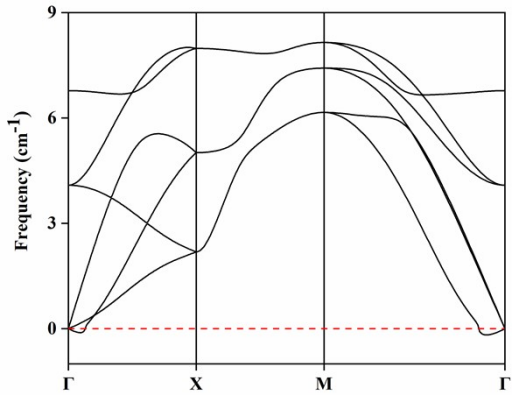


**Fig. S3.** Phonon dispersion curves obtained with DFT+U calculation (U=2eV).

**Fig. S4.** The free energy (eV) along with the step of Ti layer calculated with (red) and without Hubbard U correction (black) at 300K. The averaged structures in each case are also provided on top of the free energy curves.

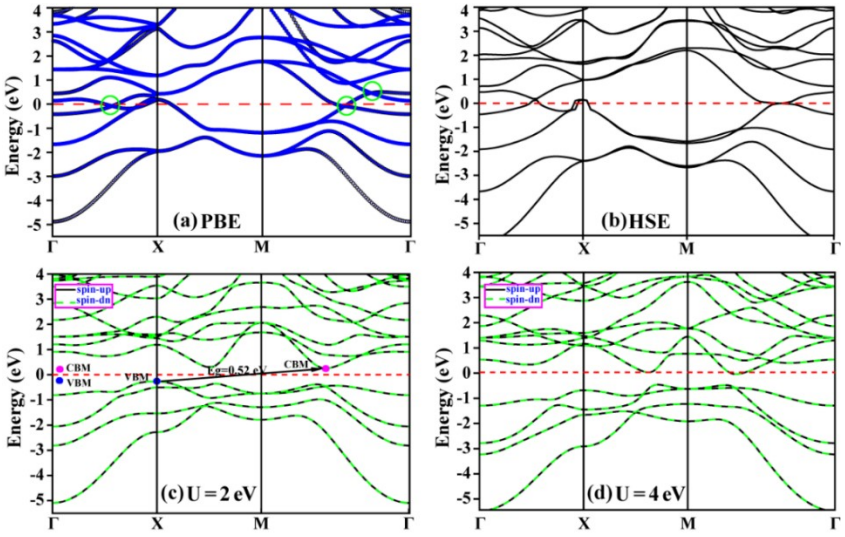


**Fig. S5.** The band structures of Ti layer calculated in (a) PBE, (b) HSE, (c) DFT+U: U=2eV and (d) U=4eV.

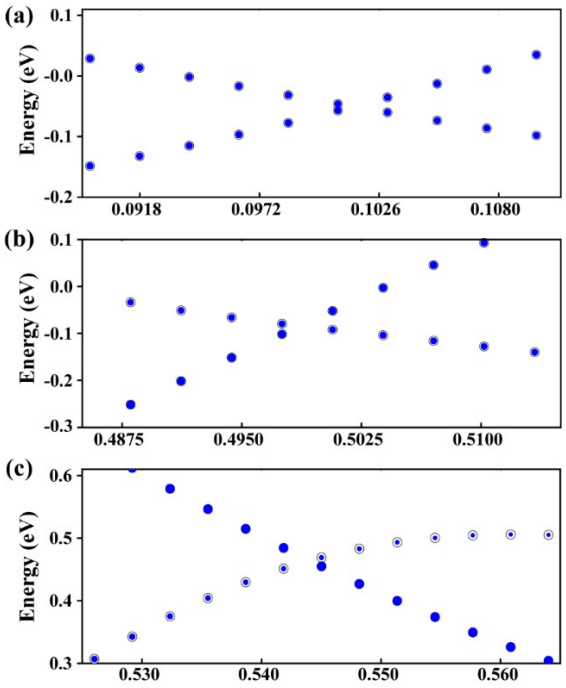


**Fig. S6.** (a-c) The bands of the Dirac points corresponding to the three points from left to the right of the band structure in Fig. 5(a).

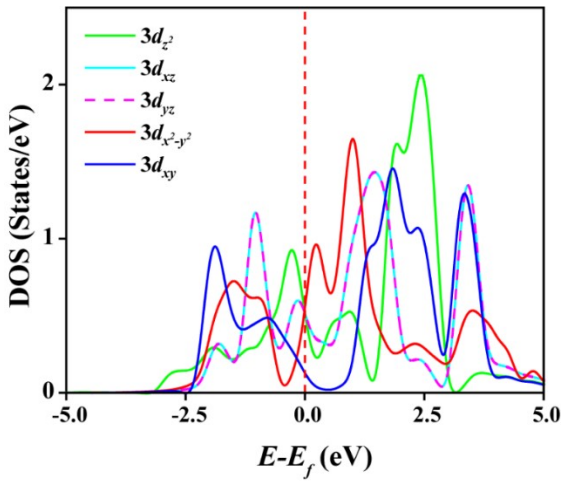


**Fig. S7.** The Ti-3*d* orbital-resolved DOS of the Ti monolayer obtained in the plain-DFT method.