

Supplementary Materials for “Large valley polarization and valley-dependent Hall effect in TiTeBr monolayer”

Bingwen Su,^{1,*} Xiao Peng,¹ Zhibo Yan,¹ Lin Lin,^{1,2} Xiaokun Huang,³ and Jun-Ming Liu¹

¹*Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China*

²*Department of Applied Physics, College of Science, Nanjing Forestry University, Nanjing 210037, China*

³*School of Materials Science and Engineering, Jingdezhen Ceramic Institute, Jingdezhen 333001, China*

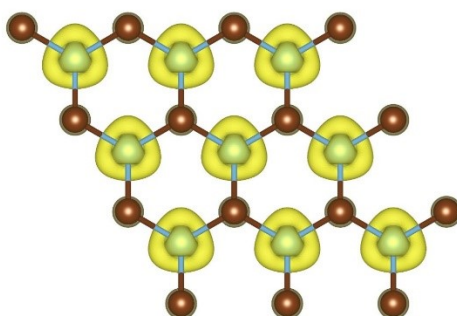


Fig. S1. Spin-polarized charge density of TiTeBr monolayer.

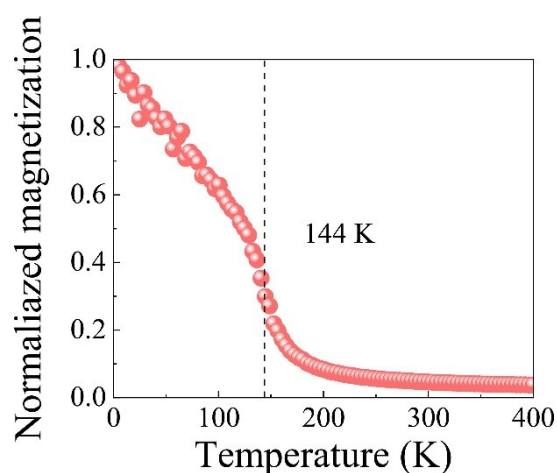


Fig. S2. Normalized magnetic moment as a function of temperature by Monte carlo

* Corresponding author: bwsu@smail.nju.edu.cn

simulations for TiTeBr monolayer at 5% tensile strain.

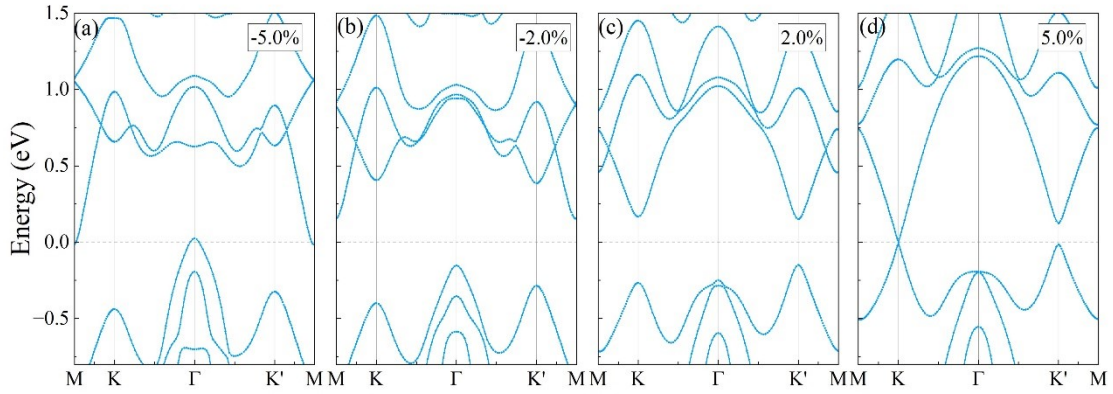


Fig. S3. Band structure of TiTeBr monolayer at (a) -5%, (b) -2%, (c) 2%, and (d) 5% strain. The magnetization is set along the +z direction.

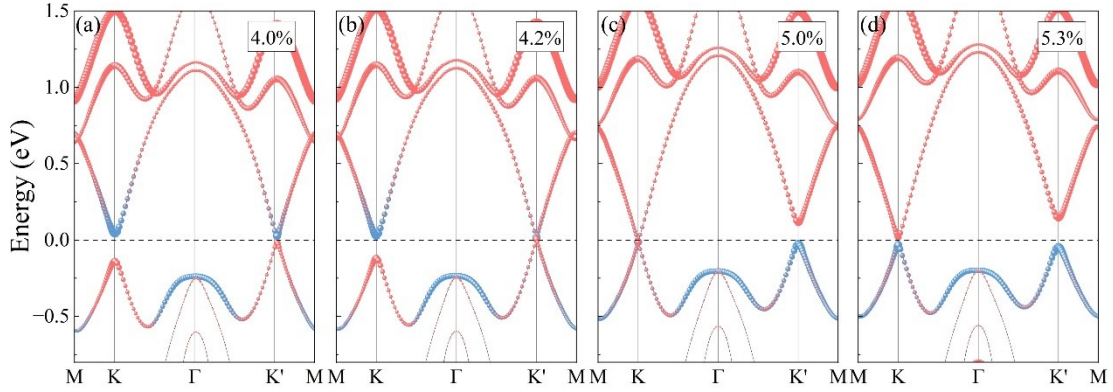


Fig. S4. Orbital-resolved band structure of TiTeBr monolayer at (a) 4.0%, (b) 4.2%, (c) 5.0% and (d) 5.3% tensile strain. The magnetization is set along the +z direction. Red and blue ball represent the $E(d_{xy}, d_{x^2-y^2})$ orbital and $A_1(d_z^2)$ orbital, respectively.

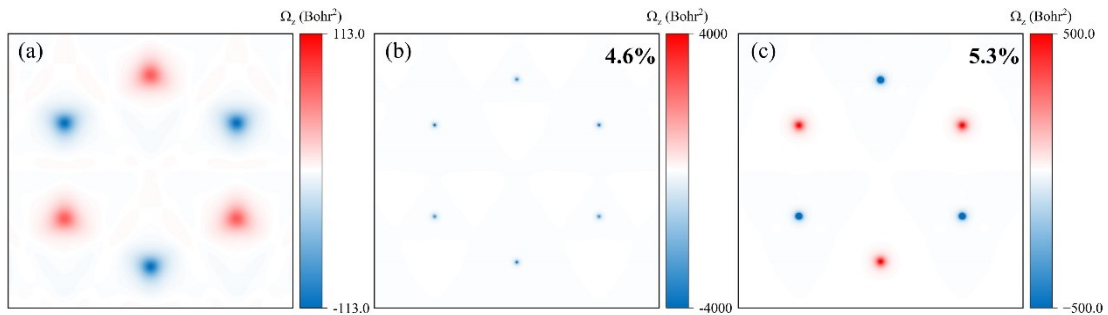


Fig. S5. Berry curvature of TiTeBr monolayer at different tensile strain. (a) is the no strain case. (b) and (c) correspond to 4.6% and 5.3% strain, respectively.

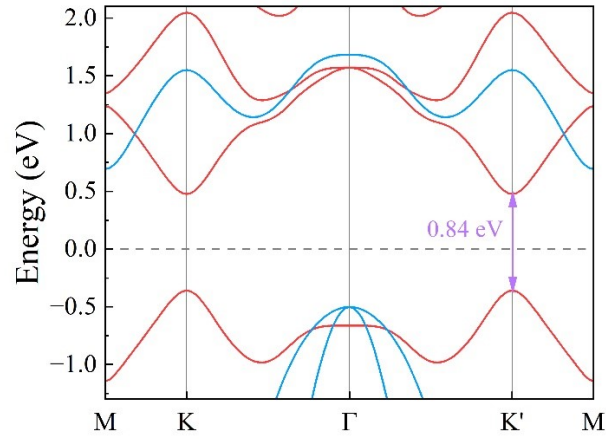


Fig. S6. Spin-resolved band structure of TiTeBr monolayer without SOC at the HSE06 level. Red and blue lines represent the spin-up and spin-down channel, respectively.

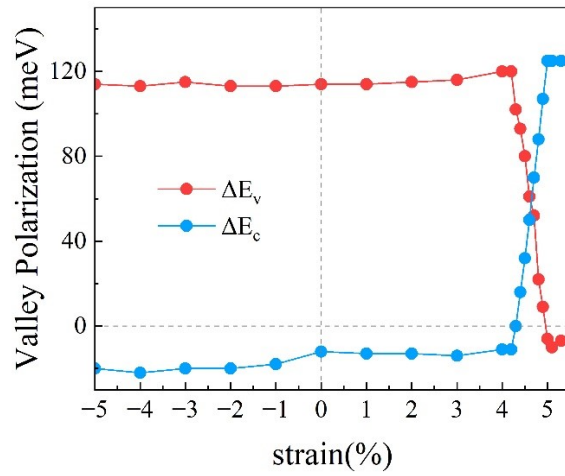


Fig. S7. Valley polarization of TiTeBr monolayer at different strain. Red and blue lines represent the valley polarization of the valence band and the conduction band, respectively.