Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Controllable dual-polarization valley physics in strain engineered 2D monolayer of VC_2N_4

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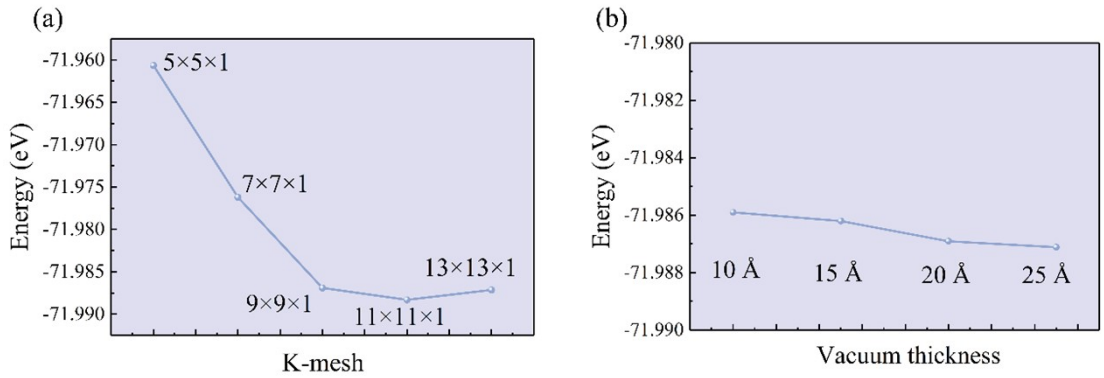

Fig. S1. The convergence tests of (a) K-mesh and (b) vacuum thickness.

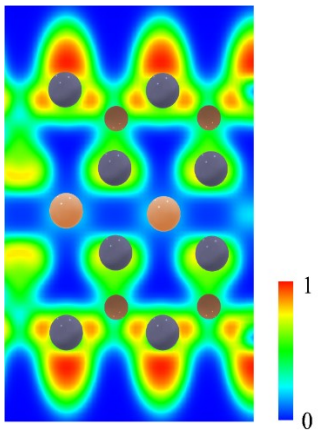

Fig. S2. Electron localization function of monolayer VC_2N_4.

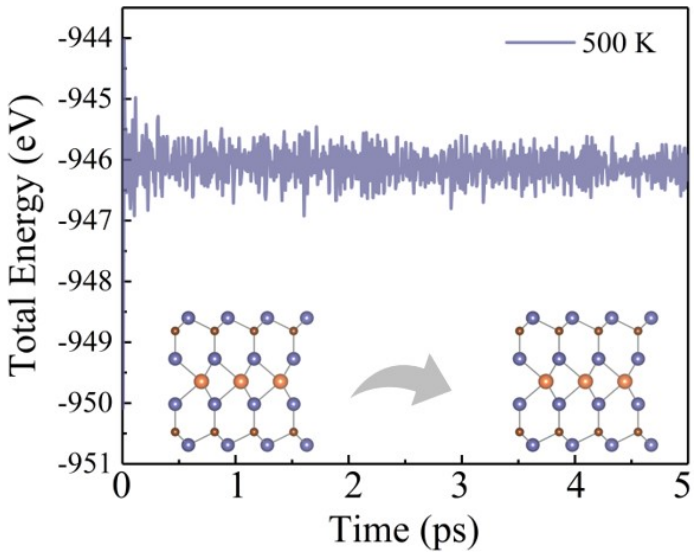

Fig. S3. Evolution of the total energy during 5 ps from AIMD simulation at 500 K; insets show the snapshots of initial and final structures of monolayer VC_2N_4.

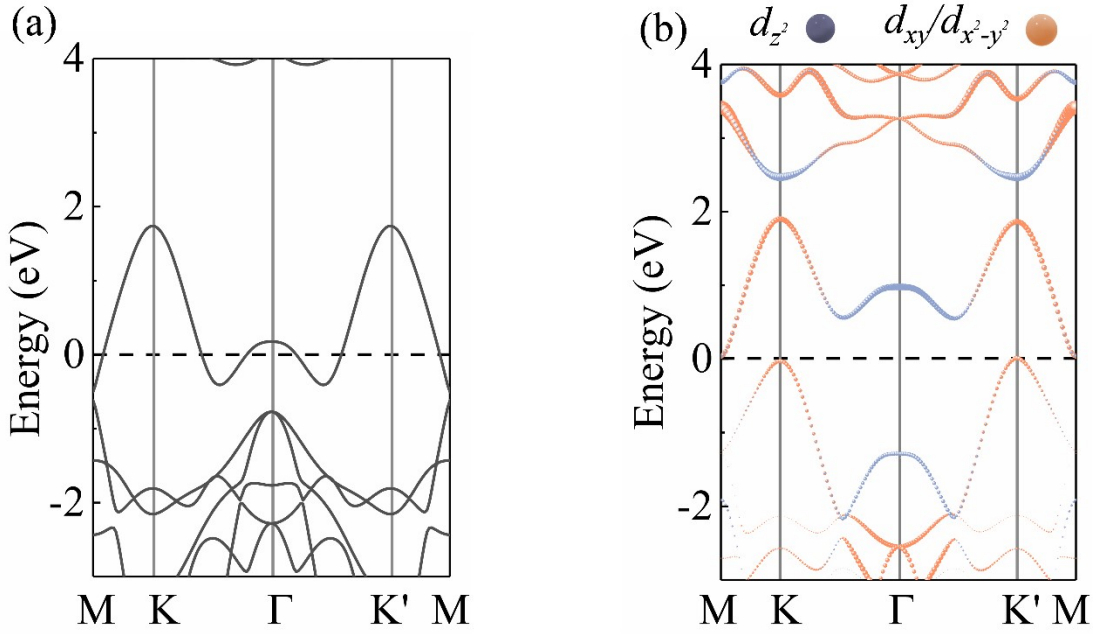

Fig. S4. (a) Band structure of monolayer VC_2N_4 without spin polarization and SOC. (b) Orbital-resolved band structures of monolayer VC_2N_4 with spin polarization and SOC.

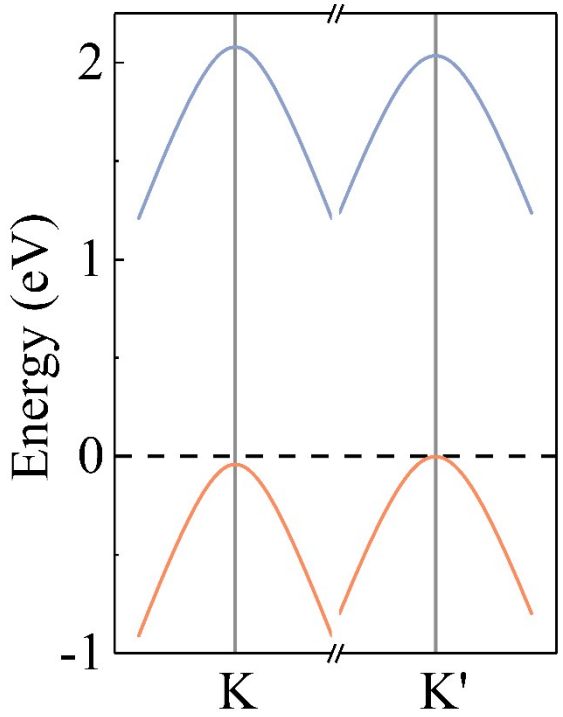

Fig. S5. Low-energy electronic bands around K and K' valleys based on the tight-binding models. The orange and blue lines are spin-up and spin-down states, respectively.

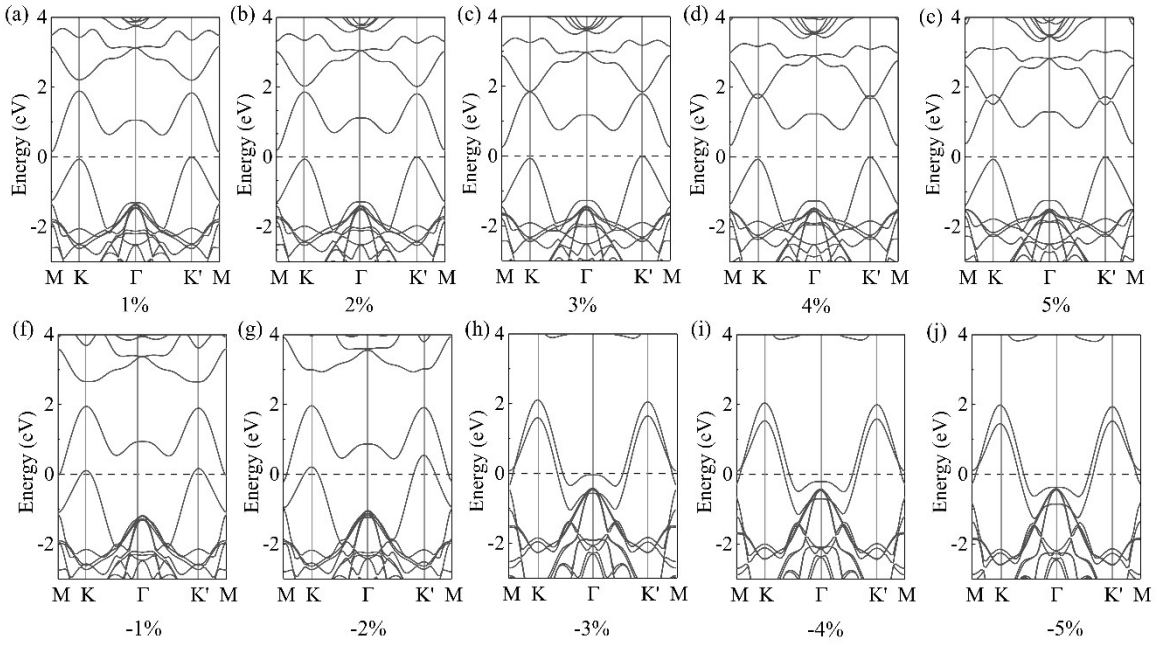

Fig. S6. Band structures of monolayer VC_2N_4 with SOC under different strains.

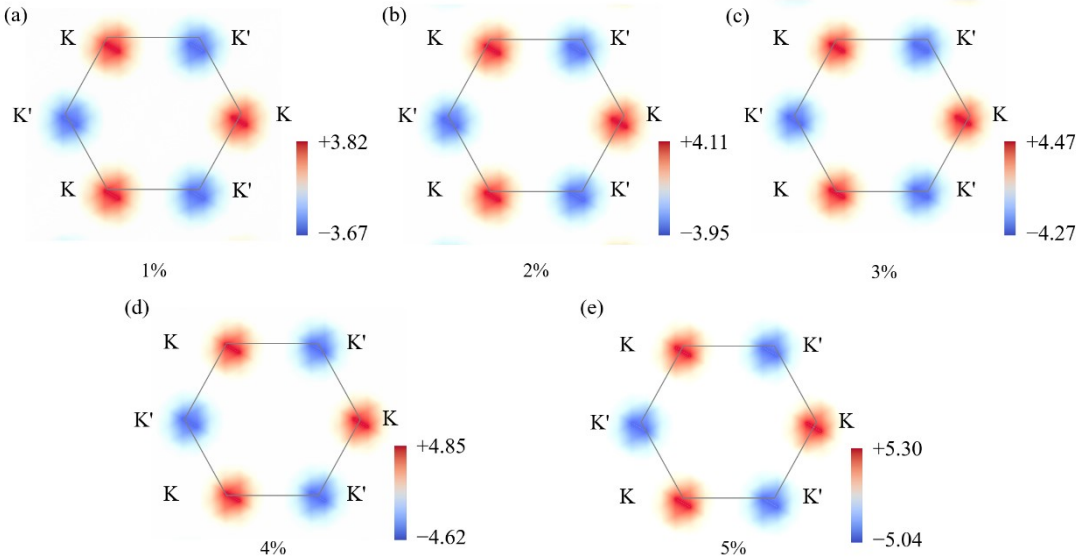

Fig. S7. Berry curvature of VB as a contour map over the 2D BZ for monolayer VC_2N_4 under different strains.