Prediction of two-dimensional Dirac materials with intrinsic magnetism, quantum anomalous Hall effect and high Curie temperature

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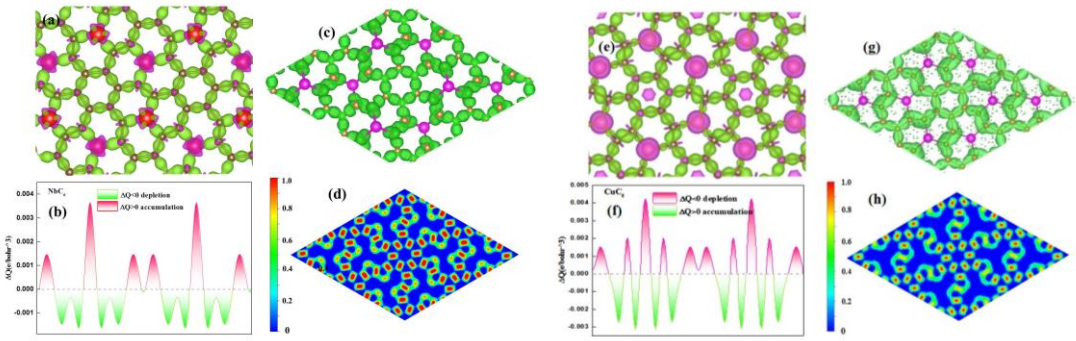


Fig. S1 Charge density difference of monolayer NbC_6 (a) and CuC_6 (e). The line projection (b,f), pink map ($\Delta Q > 0$) is shown in order to show the electron accumulation region and cyan map ($\Delta Q < 0$) represents the electron depletion region. The ELF (c,g) of NbC_6 and CuC_6 monolayers with an isovalue of 0.0135 and 0.25 e/bohr^3, respectively. ELF maps sliced perpendicular to the (001) direction (d,h). The red and blue colors refer to the highest (1.0) and lowest value (0) of ELF, respectively.

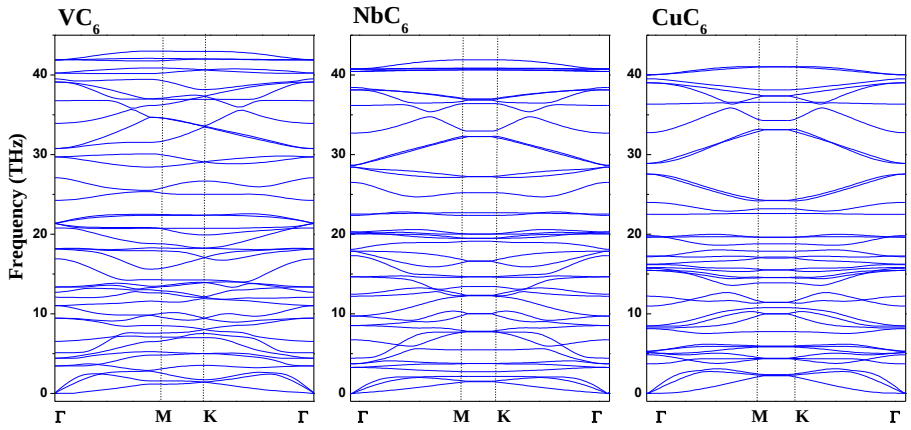


Fig. S2 The calculated phonon spectrum of the VC_6, NbC_6 and CuC_6 monolayers, respectively.

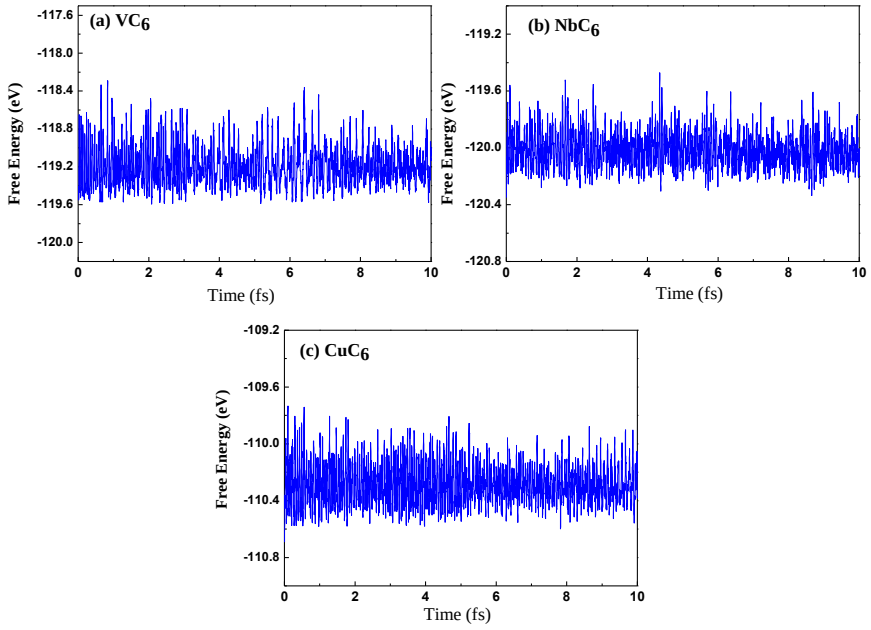


Fig. S3 Fluctuation of total potential energy of VC_6 (a), NbC_6 (b) and CuC_6 (c) monolayers during the AIMD simulations at 300 K.

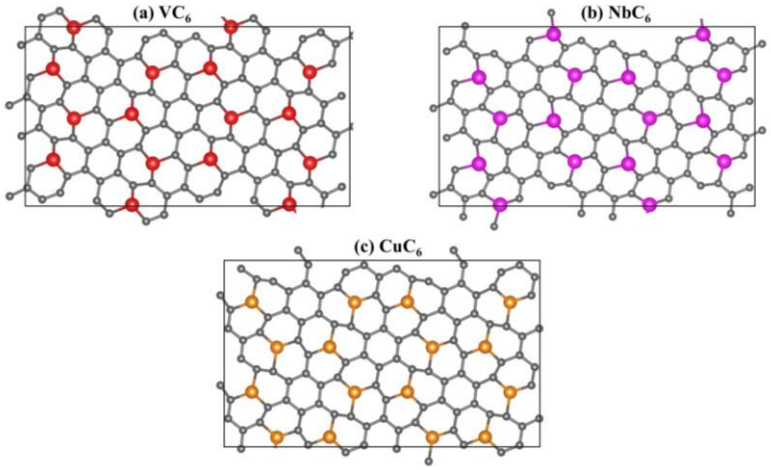
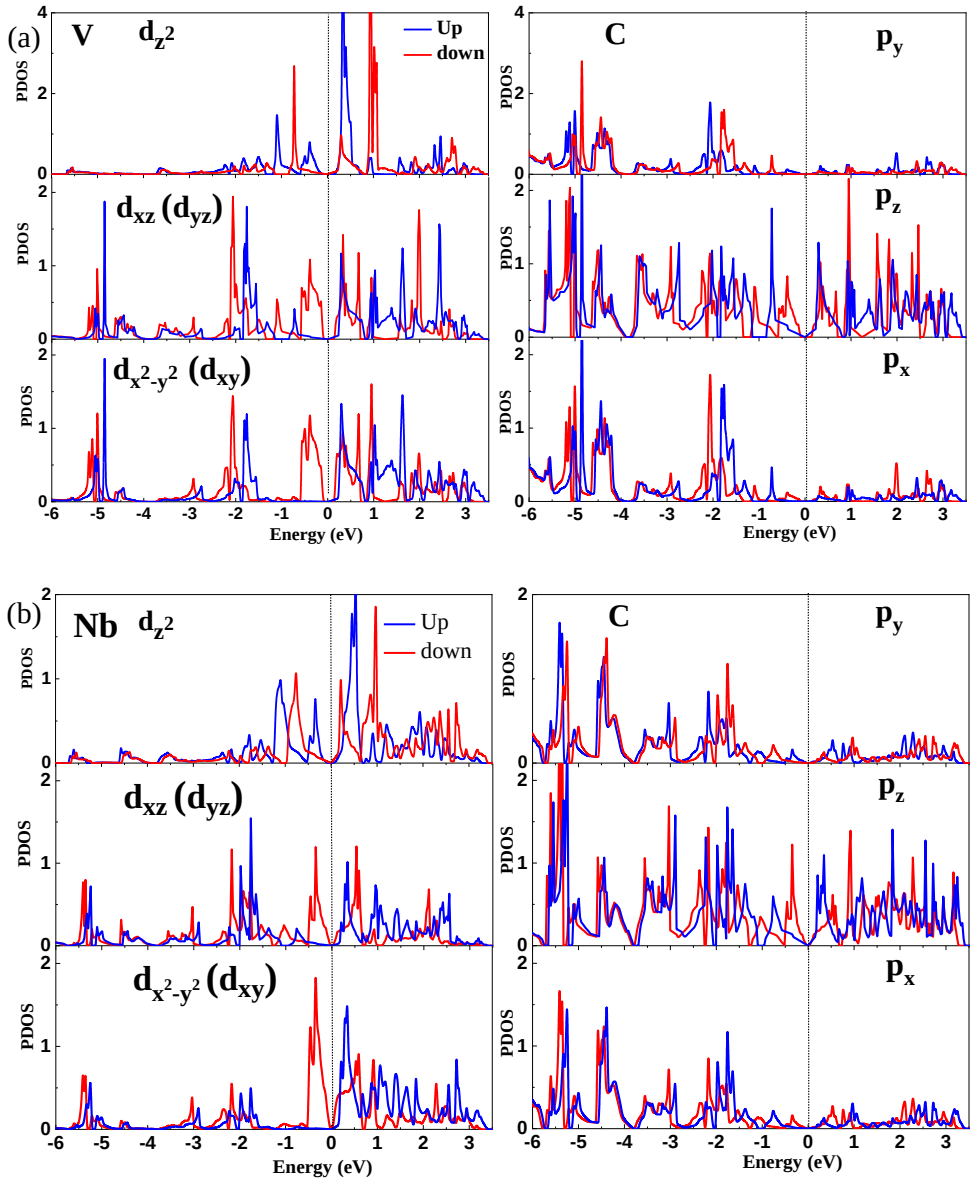


Fig. S4 the structures of VC_6, NbC_6 and CuC_6 monolayers after the simulations for 10 ps at 300 K.



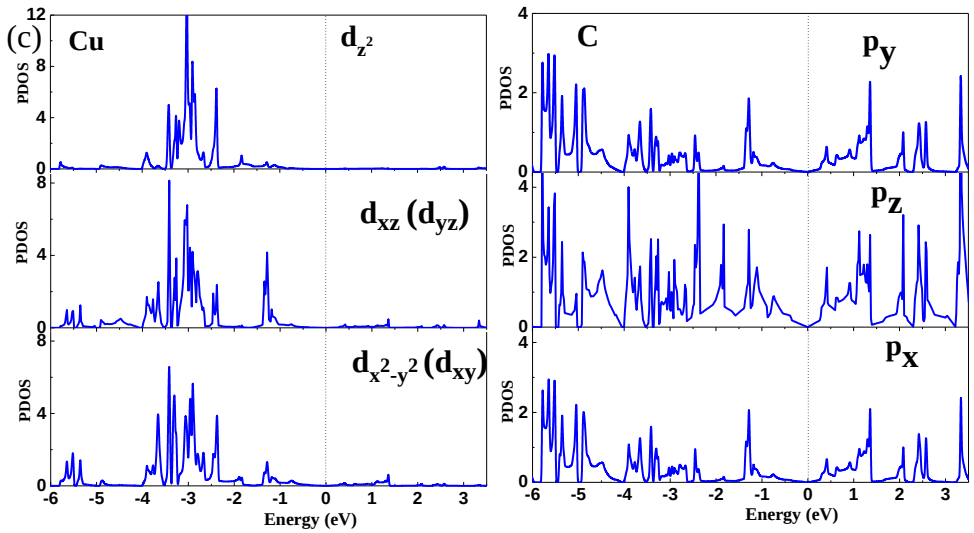


Fig. S5 The orbit-resolved partial densities of states of V, Nb, Cu and C atoms in monolayer VC_6, NbC_6 and CuC_6, respectively. The red (green) line represents the spin-up (spin-down) channel of the VC_6 and NbC_6 monolayers. The Fermi level is set at zero.

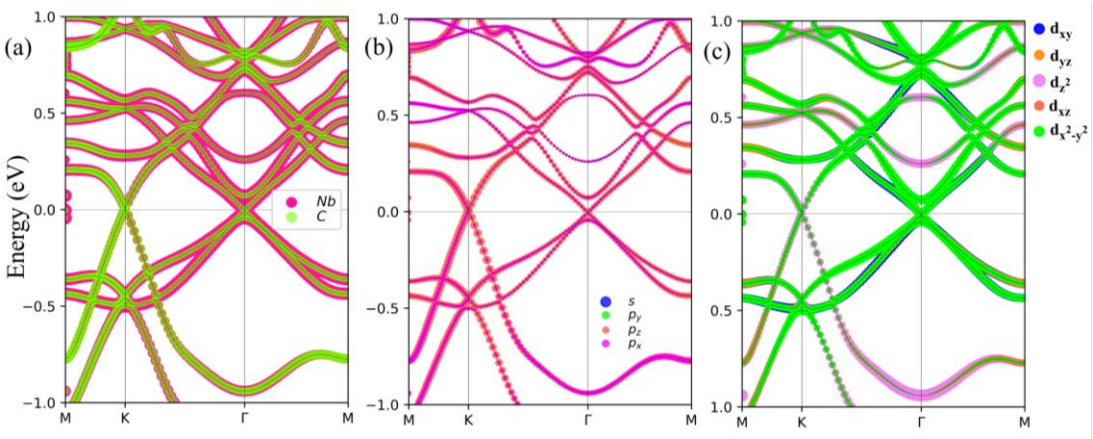


Fig. S6 Energy and *k* contribution of atom-resolved (a), C-*s*/*p* resolved (b), and Nb-*d* resolved (c) for NbC_6 monolayer with PBE+SOC. The color intensity denotes the amplitude of the atom and orbital-resolved character.

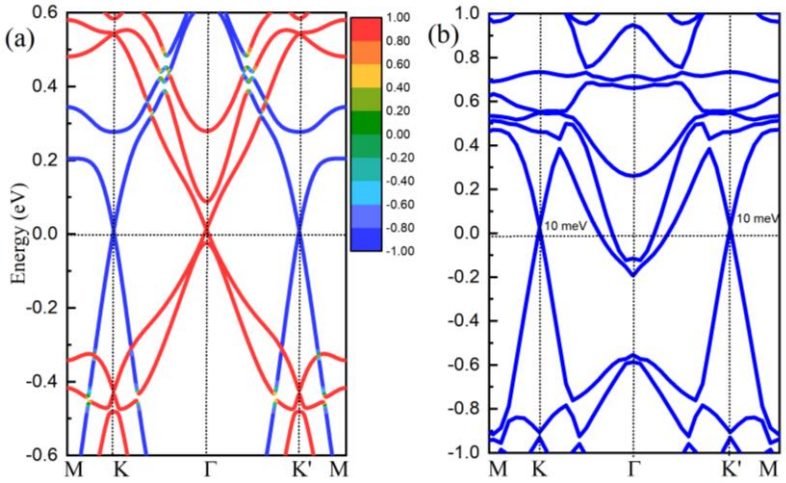


Fig. S7 The spin-resolved band structure at the GGA+SOC level (a) and the band structure at the HSE+SOC level for the NbC_6 monolayer (b).

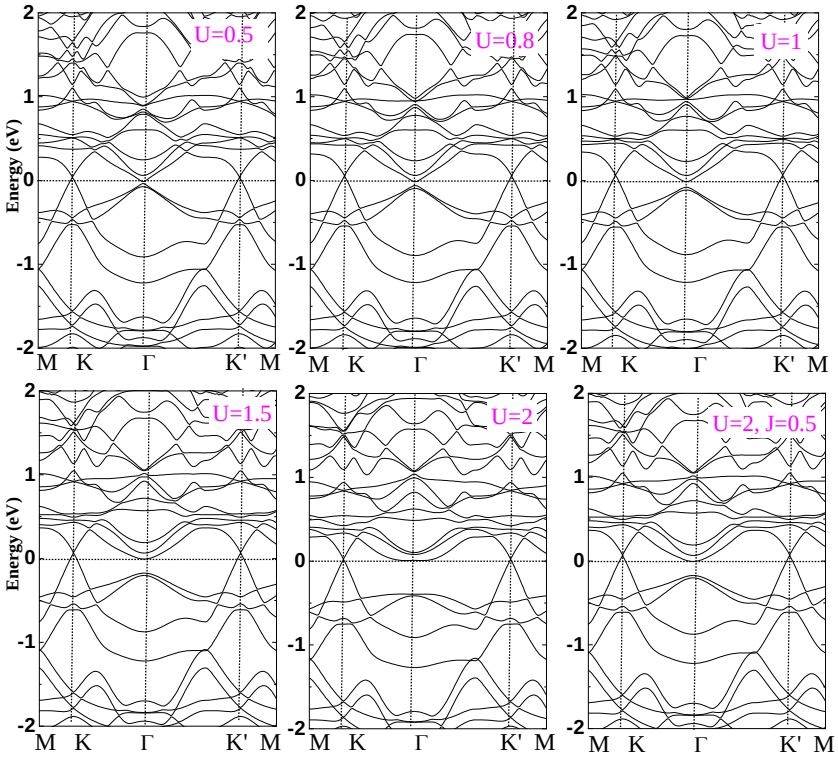


Fig. S8 Electronic band structure of NbC_6 monolayer calculated by PBE+SOC+U with different U values.

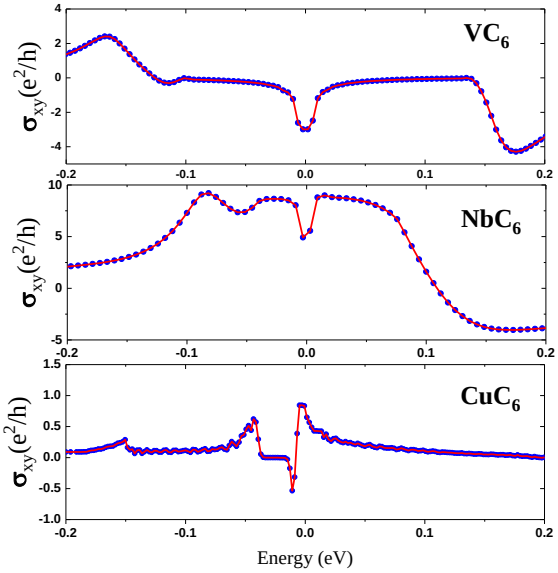


Fig. S9 The anomalous Hall conductance of VC_6, NbC_6 and VC_6 monolayers.