

applying an external electric field to a 2D NI material such that it transforms electronically into a TI. Such an integration of electric fi

fold rotation axis. In addition, the band dispersion along the k_x and k_y direction shows strong anisotropy (see the 2D rectangular Brillouin zone in Figure 1c). The effective mass along Γ -X is much lower than that along Γ -Y because of the preference of bonding direction along x direction,³² as shown in Figure 1a. The topological invariant at zero \tilde{f}

method that evaluates the band parity¹ does not apply. Here,

provides the possibility to construct a “field effect topological transistor (FETT)” by applying different gate voltages. Here, we propose a dual-gated FETT model composed of few-layer phosphorene as the channel, as shown in Figure 4a. Compared

with single gate, a dual-gated device can tune not only the perpendicular electric field working on the channel but also the Fermi level.⁴⁴ Figure 4b–d explains the phase transition and the corresponding spin and charge current on the channel. When $F < F_c$

system becomes intrinsically metallic. The topological band inversion originates entirely from the field-induced Stark effect, whereas the effect of SOC is to open an energy gap at the Dirac-like band crossing, rendering the system a 2D TI. This topological nontrivial feature persists after the system becomes metallic at higher fields. Such tunable phase transition could lead to spin-separated gapless edge states, that is, quantum spin Hall effect, which is easy to detect as well as normal insulating and conducting states based on the current FET technology. This finding opens the possibility of making a multifunctional “field effect topological transistor” that could manipulate simultaneously both spins and charge carrier.

Method. The calculations were performed with the Vienna ab initio package (VASP).⁴⁶ The geometrical and electronic structures are calculated by the projector-augmented wave (PAW) pseudopotential⁴⁷ and the generalized gradient approximation of Perdew, Burke, and Ernzerhof (PBE)⁴⁸ to the exchange-correlation functional unless specified. Electronic structures calculated by hybrid functional (HSE06)⁴⁹ is also provided for comparison. Spin-orbit coupling is calculated by a perturbation $\sum_{i,l,m} V_i^{SO} \vec{L}_i \cdot \vec{S}_i |l,m\rangle_i \langle l,m|$ to the pseudopotential, where $|l,m\rangle_i$ is the angular momentum eigenstate of i th atomic site.⁵⁰ The plane wave energy cutoff is set to 550 eV, and the electronic energy minimization was performed with a tolerance of 10^{-4} eV. All the lattice parameters and atomic positions were fully relaxed with a tolerance of 10^{-3} eV/Å. The van der Waals interaction is considered by a dispersion-corrected PBE-D2 method.⁵¹ The vacuum separation in the slab supercell is 20 Å to avoid the interaction between periodic images.

The electric field can be featured as an additional sawtooth potential along the z direction with discontinuity at the mid plane of the vacuum region of the supercell. The automatic symmetry constraint in VASP is switched off to avoid the incorrect rendering of the electric field.⁴⁴ To test the general correctness of the critical field, we also use Quantum Espresso⁵² as comparison and find that the dependence of the band gap on the electric field agrees well with the results of VASP.

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Notes

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- (41) Yao, Y.; Ye, F.; Qi, X.-L.; Zhang, S.-C.; Fang, Z. *Phys. Rev. B* **00**, 75, 041401.
- (42) Abdelouahed, S.; Ernst, A.; Henk, J.; Maznichenko, I. V.; Mertig, I. *Phys. Rev. B* **010**, 82, 125424.