Quantum Anomalous/Valley Hall Effect in silicene with 3d and 4d TM adatoms

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I. Introduction

The quantum hall states is very important in modern condensed matter physics, and has been observed in many 2D systems. Here, we provide a physical picture of how to realize quantum anomalous/valley hall (QAH and QVH) effect in 2D honeycomb silicene, and by using first-principle calculation methods we systematically searched the QAH and QVH states in silicene with 3d and 4d transition metal atoms. We find that the QAH states could be driven by electric field in some TM@silicene systems and QVH states arise in the Ni@silicene. Most importantly, the Nb@silicene opened a sizable nontrivialed bulk band gap and it's Fermi level is just located in the bandgap, so this system would be a very suitable candidate for observing the QAH effect in experiment.

II. Methods

a. Tight-binding model

$$H = -t\sum_{\langle i,j\rangle\alpha} c_{i\alpha}^{\dagger}c_{j\alpha} + i\frac{\lambda_{SO}}{3\sqrt{3}}\sum_{\langle\langle i,j\rangle\rangle_{\alpha,\beta}} v_{ij}c_{i\alpha}^{\dagger}\sigma_{\alpha\beta}^{z}c_{j\beta}$$
$$+i\lambda_{R1}(E_z)\sum_{\langle i,j\rangle\alpha\beta} c_{i\alpha}^{\dagger}\left(\boldsymbol{\sigma}\times\hat{\mathbf{d}}_{ij}\right)_{\alpha\beta}^{z}c_{j\beta}$$
$$-i\frac{2}{3}\lambda_{R2}\sum_{\langle\langle i,j\rangle\rangle_{\alpha,\beta}} u_i c_{i\alpha}^{\dagger}\left(\boldsymbol{\sigma}\times\hat{\mathbf{d}}_{ij}\right)_{\alpha\beta}^{z}c_{j\beta}$$
$$-\ell\sum_{i\alpha}u_iE_zc_{i\alpha}^{\dagger}c_{i\alpha} + M\sum_{i\alpha}c_{i\alpha}^{\dagger}\sigma_z c_{i\alpha}$$

b. First principle calculation

Berry curvature

$$\Omega_n(\mathbf{k}) = -2\,\mathrm{Im}\sum_{m\neq n}\frac{\hbar^2\langle\psi_{n\mathbf{k}}|v_x|\psi_{m\mathbf{k}}\rangle\langle\psi_{m\mathbf{k}}|v_y|\psi_{n\mathbf{k}}\rangle}{(\mathrm{E}_m-\mathrm{E}_n)^2}$$

$$\Omega(\mathbf{k}) = \sum_n f_n\Omega_n(\mathbf{k}),\quad C = \frac{1}{2\pi}\sum_n\int_{BZ}d^2k\,\Omega_n$$

Band evolution form TB simulation

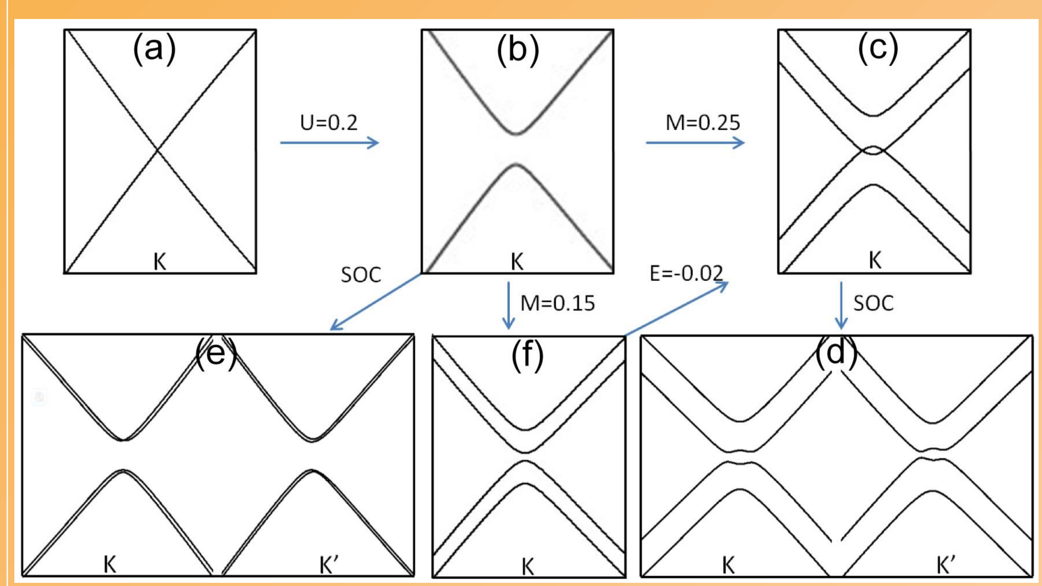


FIG.1.Evolution of the TB band structure of 4x4 supercell silicene with the TM datoms, where the staggered sublattice potential, exchange field and extrinsic Rashba spin-orbital coupling are only considered around the Hollow-site adatoms.

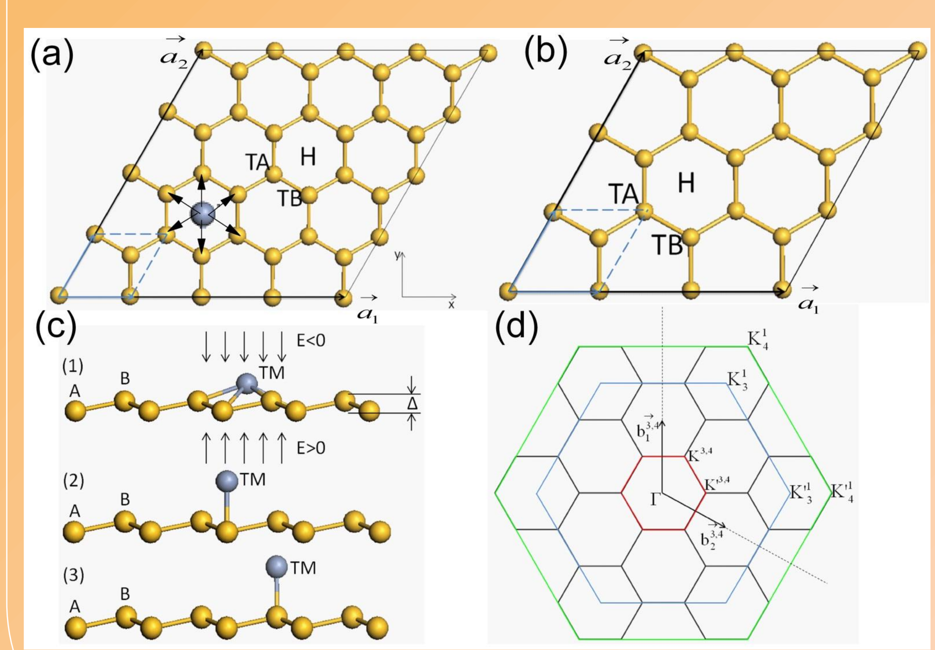


FIG.2. (a)and(b): top view of 4x4 and 3x3 silicene.(c)side view of the buckled silicene. A, B and TM labeled as the sublattice A, sublattice B and adatom; (1) show the direction of external vertical electric field E and small buck Δ. (d):The reciprocal momentum space structures

III. Results

(a) Quantum Anomalous Hall Effect

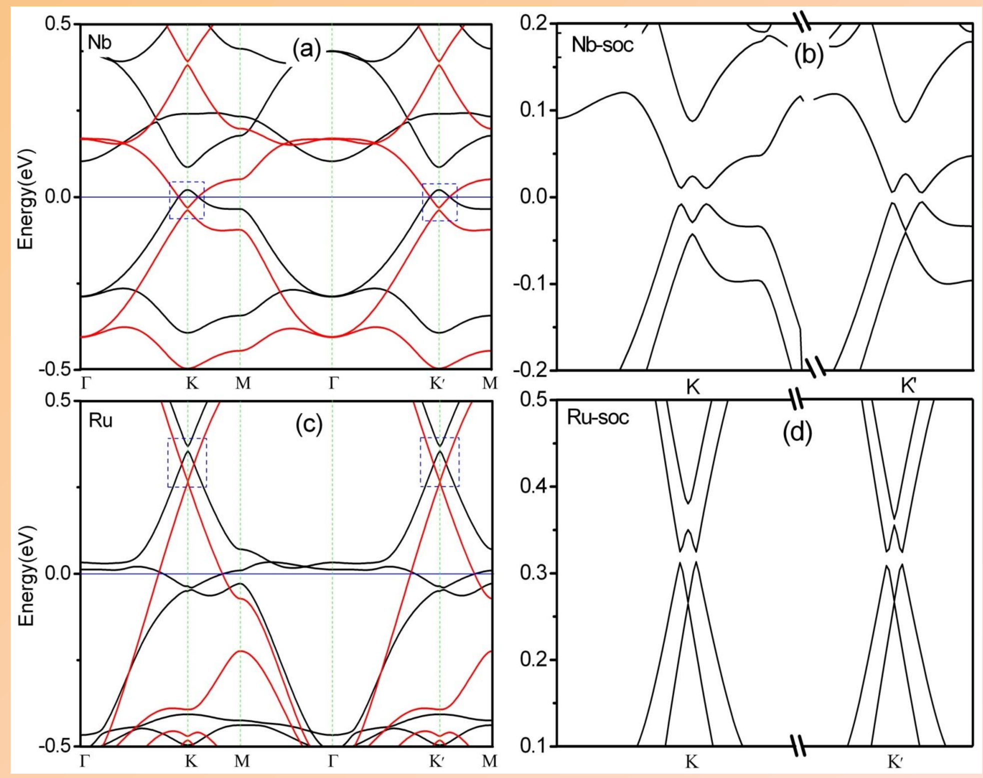


FIG.3.(a),(c): The band structures of 4x4 supercell of silicene dopped by Nb(a) and Ru(b) on the hollow site with spin-polarized. Spin-up and spin-down bands are denoted by red and black. (b),(d): band structures with spin-orbit coupling and the magnification of bands around the SOC induced band gaps of K and K' Dirac points.

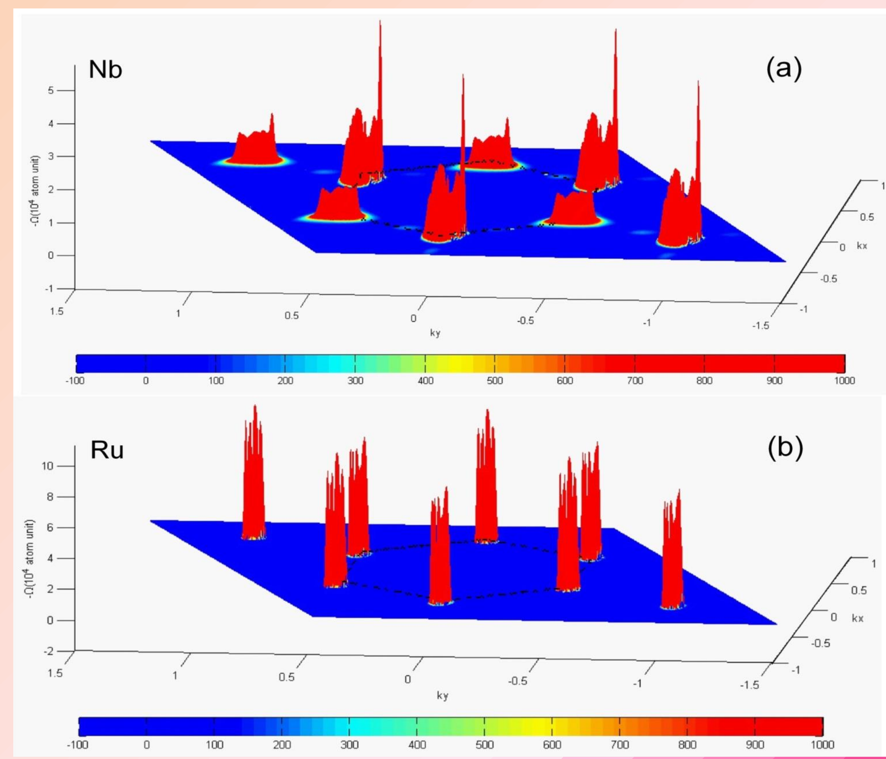


FIG.4.(a)and(b):The 2D distribution of Berry curvature Ω(k) in the momentum space for the system of Nb(a) and Ru(b) adsorbed at the hollow site on 4x4 supercell of silicene. The first BZ is denoted by the black hexagon.

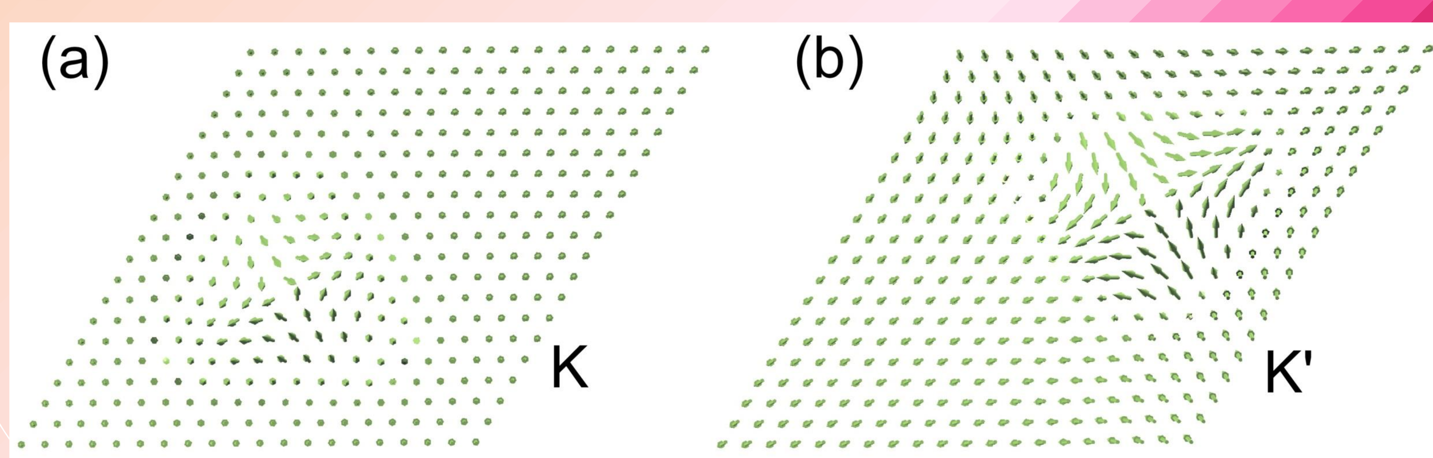


FIG.5(a) and (b): Top view of the spin configurations of the highest valence band below the bulk bandgap around K and K' Dirac points for the Nb-(4x4)silicene system with SOC.

(c) Electric field induce topological

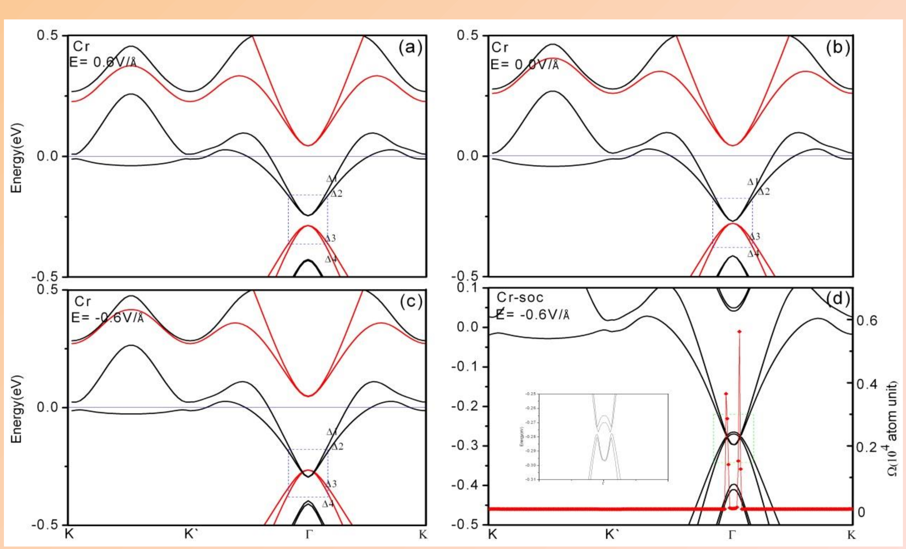
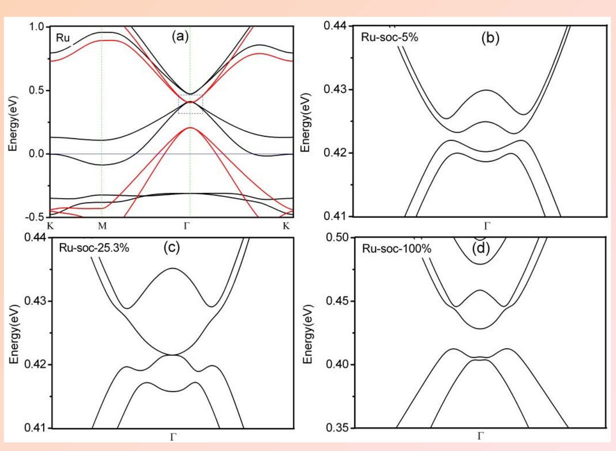


FIG.7.the band structures of 3x3 supercell of silicene dopped by Cr with spin-polarized and vertical electric field of E=0.5V/Å, E=0.0V/Å and E=-0.6V/Å respectively.

(d) SOC-induce phase transition



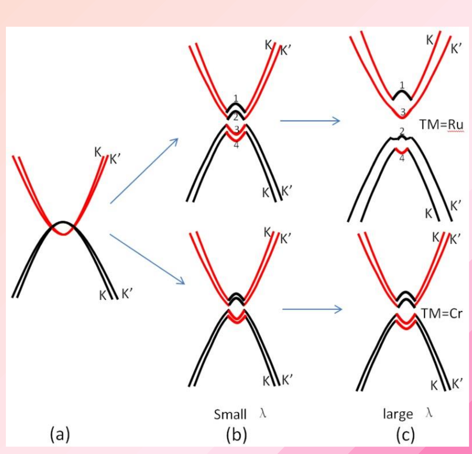


FIG.8.Ru-(3x3) silicene with different SOC strength.
FIG.9.physical picture

(b) Quantum Valley Hall Effect

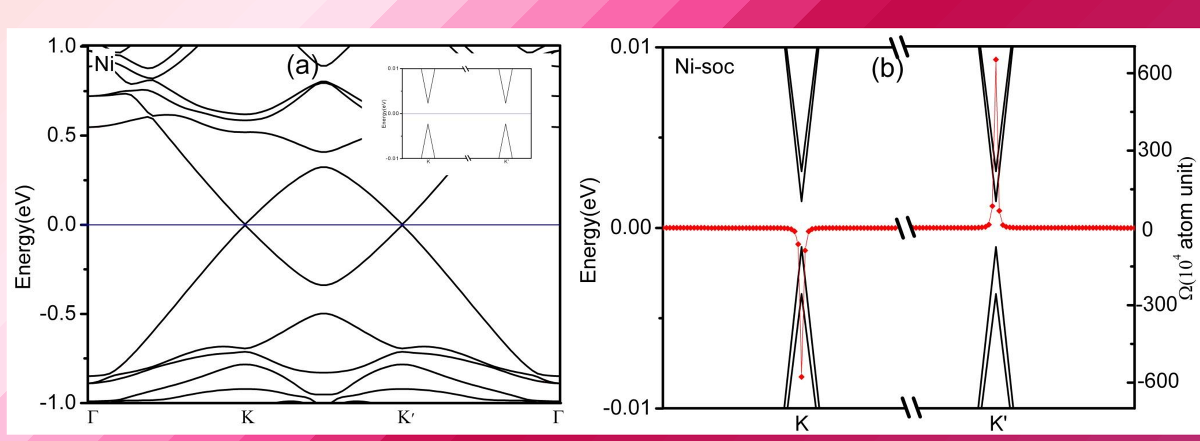


FIG.6.(a): The calculated band structure of Ni adsorbed at the hollow site on 4x4 supercell of silicene with spin-polarized. (b): The magnification of bands including spin-orbit coupling around K and K' Dirac points near the Fermi-energy, and the red dots give the Berry curvature Ω(k) along the high symmetry lines.

IV. Summary

We find TM adatoms adsorbed at the hollow adsorption site on 3x3 and 4x4 supercell of silicene could realize the QAH and QVH effect, and the SOC induced nontrivial bulk band gap in 4d TM(Nb,Ru)@silicene systems is larger than 3d TM@silicene, and maybe more suitable for experiment observation.