Supplemental Material for

Electronic strcture and magnetothermal properties of two-dimensional ScCl

Hao-Jia Wu [1], Dan Wang [1], Hua-Yun Geng [2], Xiang-Rong Chen [1,*]

[1] College of Physics, Sichuan University, Chengdu 610064, China;

[2] National Key Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, CAEP, Mianyang 621900, China

Abstract：Two-dimensional ferromagnetic materials with intrinsic half-metallic properties have strong application advantages in nanoscale spintronic applications. Our density functional theory calculations show that monolayer ScCl is ferromagnetic metallic materials when undoped (n = 0), the transition from metal to half-metal will occur with the continuous doping of holes. On the contrary, as the concentration of doped electrons increases, the system will exhibit metallic characteristics, which is particularly evident in the variation trend of spin polarizability. In the section on the Fermi surface, it is also shown how doped carriers affect the shape of the Fermi surface and the Fermi velocity of the electrons. Most importantly, our Monte Carlo simulations show that the ScCl monolayer is particularly regulated by the carrier concentration (n) and magnetic field (h). The trends of energy and magnetic exchange coupling in

* Corresponding author. E-mail: xrchen@scu.edu.cn

different magnetic configurations (AFM phase and FM phase) with different doping concentrations are given. When n < -0.16, the material is not only a half-metallic material that is easy to flip the magnetic axis, but also proves to be a ferromagnetic candidate material that works stably at room temperature from the perspective of dynamic stability. In addition, the origin of magnetocrystalline anisotropy is further analyzed, and the contribution of different orbits to spin-orbit coupling is given. In the section of size effect, we note that when the magnetic field is small (h < 1T), the change of size has a significant effect on the ferromagnetic phase transition. However, when the system size is larger (size > 15nm), the T_C is less sensitive to the magnetic field. In addition, hole doping and size effect have a great influence on the hysteresis loops of the system, but when the hole doping to a certain degree (n < -0.16), the influence on the hysteresis loops will reach saturation. These interesting magnetic phenomena and easily adjustable physical properties also show us that monolayer ScCl will be a promising functional material.

Keywords: Electronic structure; Magnetothermal properties; Spin polarization; Curie temperature; Magnetocrystalline anisotropy energy

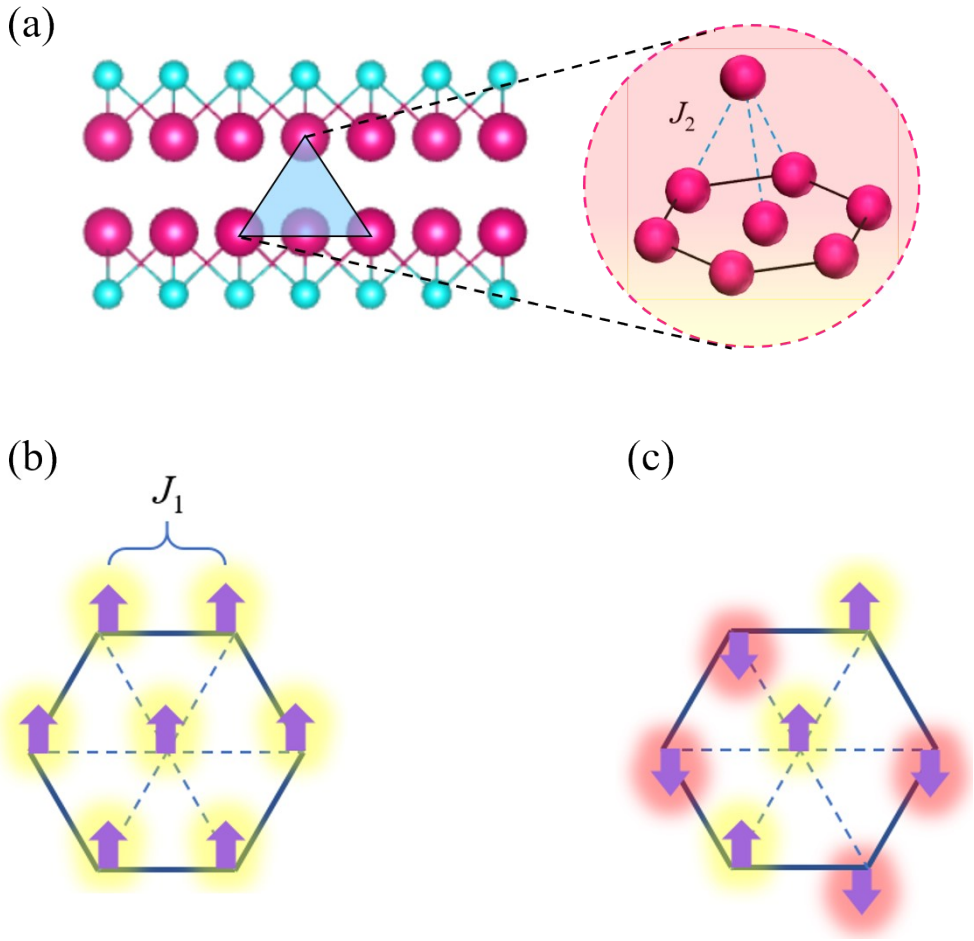

Fig. S1. (Color online) (a)-(c) The magnetic exchange coupling in monolayer ScCl is shown. The Hamiltonian corresponding to different magnetic configurations (FM and AFM phase) can be written out. The Hamiltonian of the FM phase is: $E_1 = E_0 - \frac{1}{2}\times 6\times 4\times\left(\frac{1}{2}\right)^2 \times J_1 = E_0 - 3J_1$; while the Hamiltonian of the AFM phase can be expressed as: $E_2 = E_0 - \frac{1}{2}\times(-2)\times 2\times\left(\frac{1}{2}\right)^2 \times J_1 - \frac{1}{2}\times(-2)\times 2\times\left(\frac{1}{2}\right)^2 \times J_1 = E_0 + J_1$. Based on the above expression, the nearest neighbor exchange can be obtained as: $J_1 = \frac{E_2 - E_1}{4}$, where E_0 is the total energy excluding the magnetic coupling.

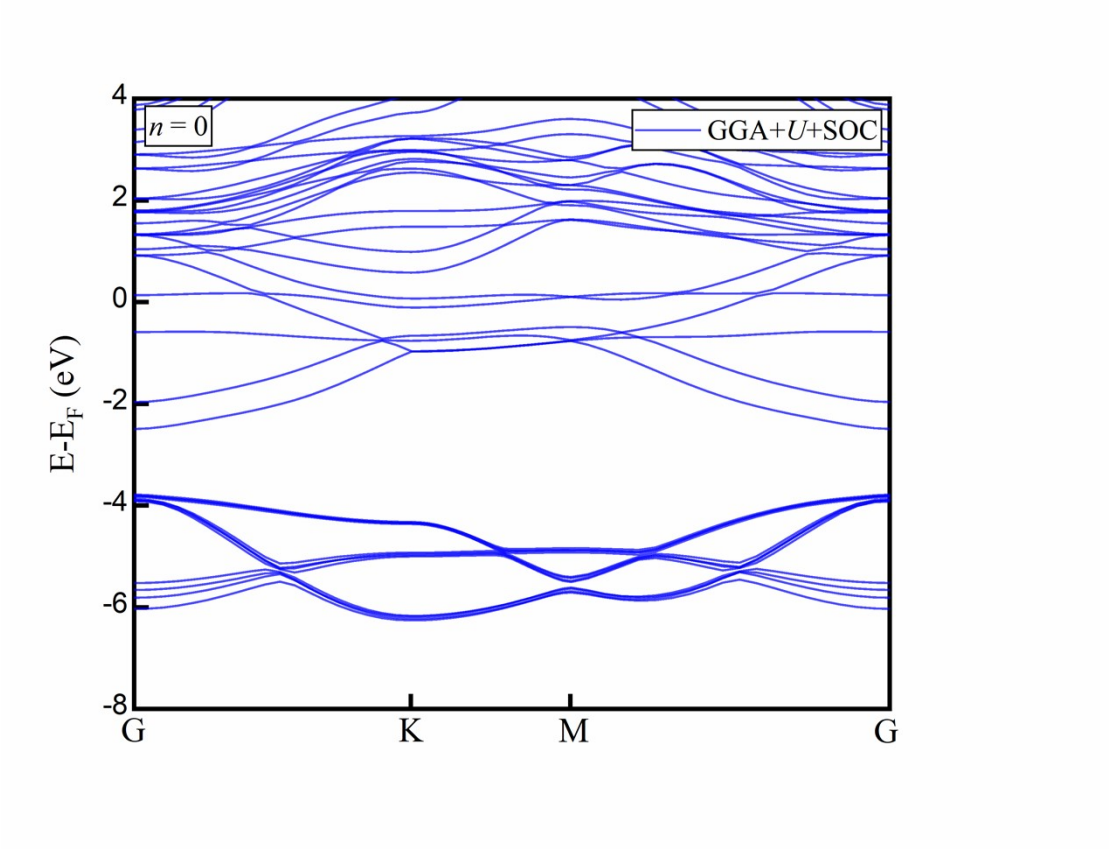

Fig. S2. (Color online) The band structure of monolayer ScCl obtained based on GGA+*U*+SOC method

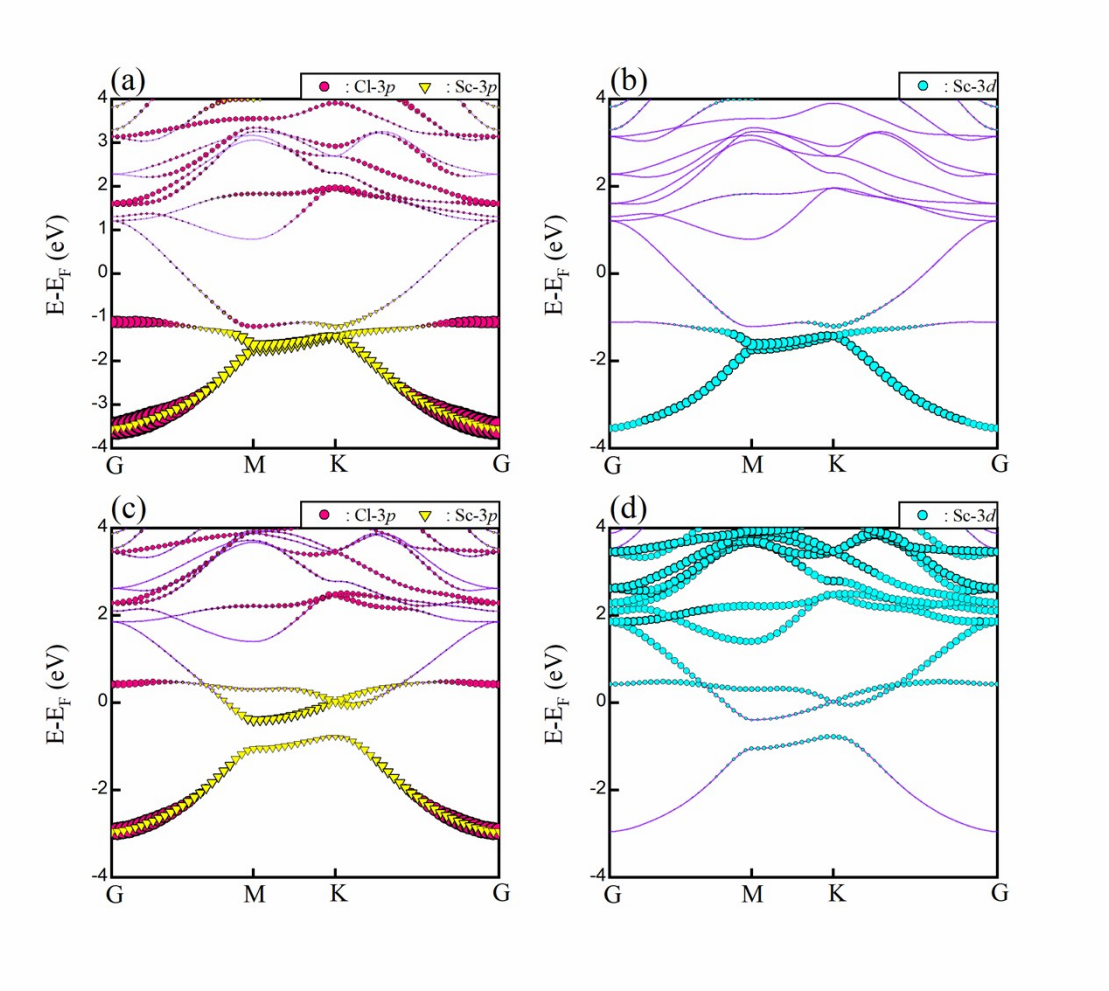

Fig. S3. (Color online) (a)-(b) The spin-down band of monolayer ScCl obtained based on HSE06 method, the spheres of different sizes represent the orbital projections of different atoms. (c)-(d) The spin-up band of monolayer ScCl obtained based on HSE06 method.

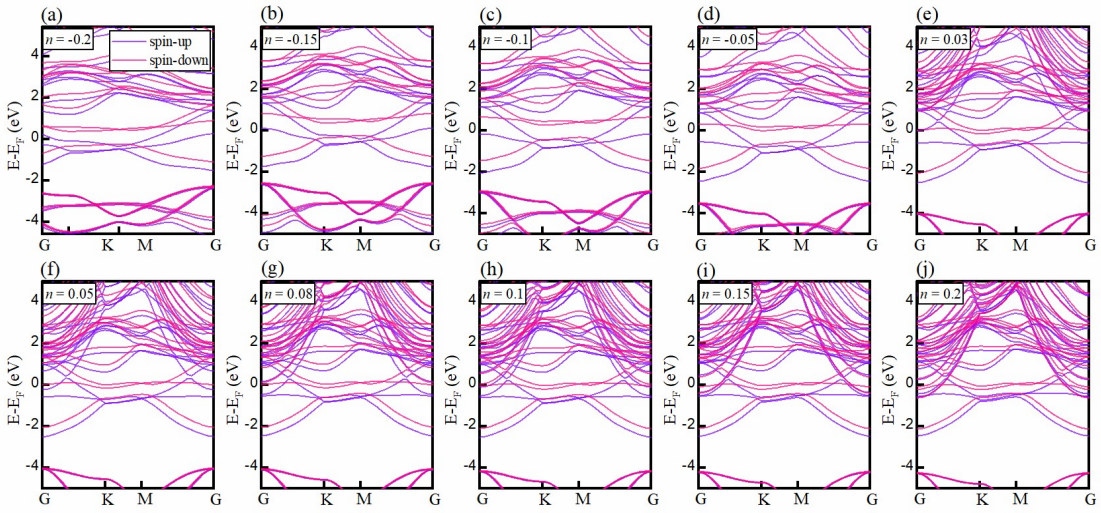

Fig. S4. (Color online) (a)-(d) Band structure of monolayer ScCl at different hole concentrations; (e)-(j) Band structure at different electron concentrations. The purple lines represent spin-up bands and the red lines represent spin-down bands.

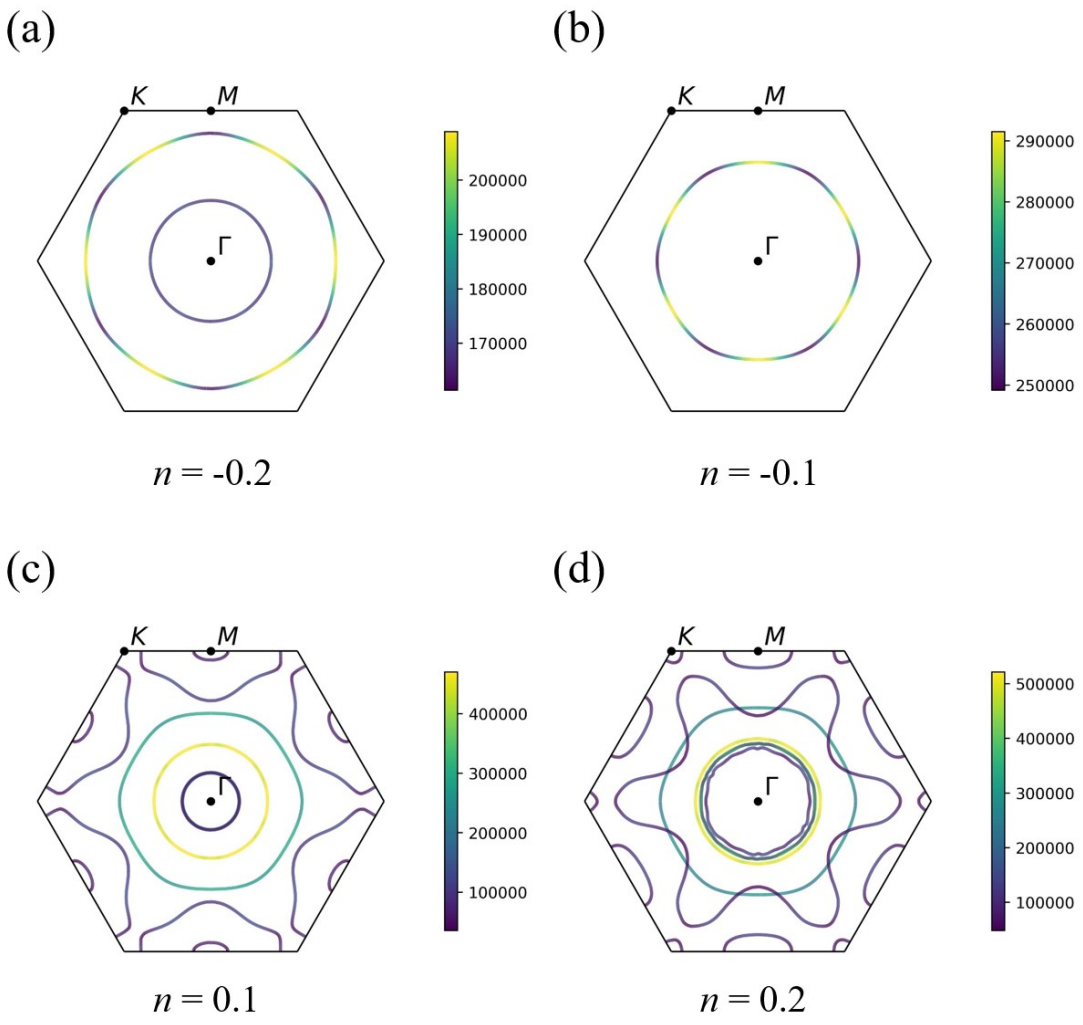

Fig. S5. (Color online) (a)-(d) The Fermi surface of monolayer ScCl at different concentrations. The color bars represent the Fermi velocity of the electron projected onto the Fermi surface.

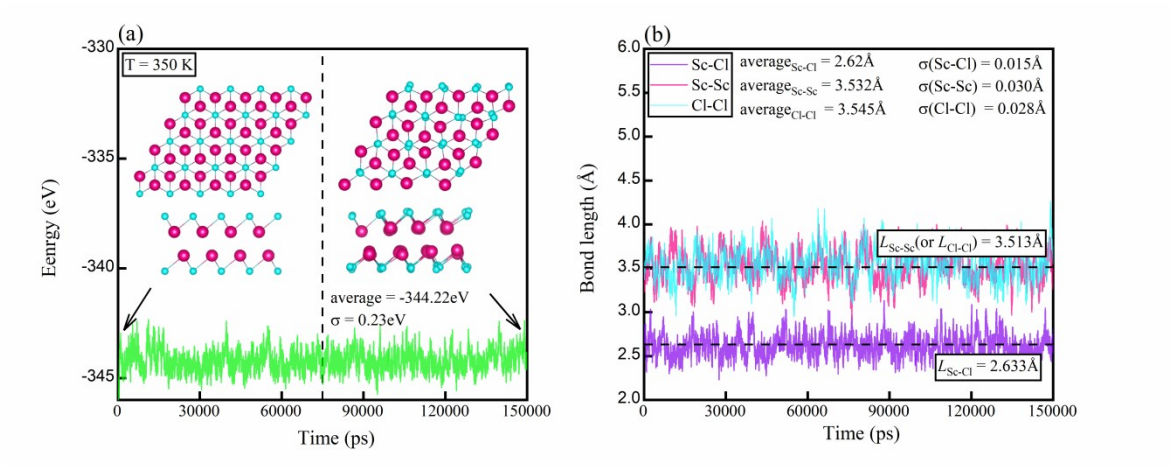

Fig. S6. (Color online) (a) Molecular dynamics simulation of monolayer ScCl at 350 K. (b) The evolution of bond length with time in AIMD simulation at 350 K.

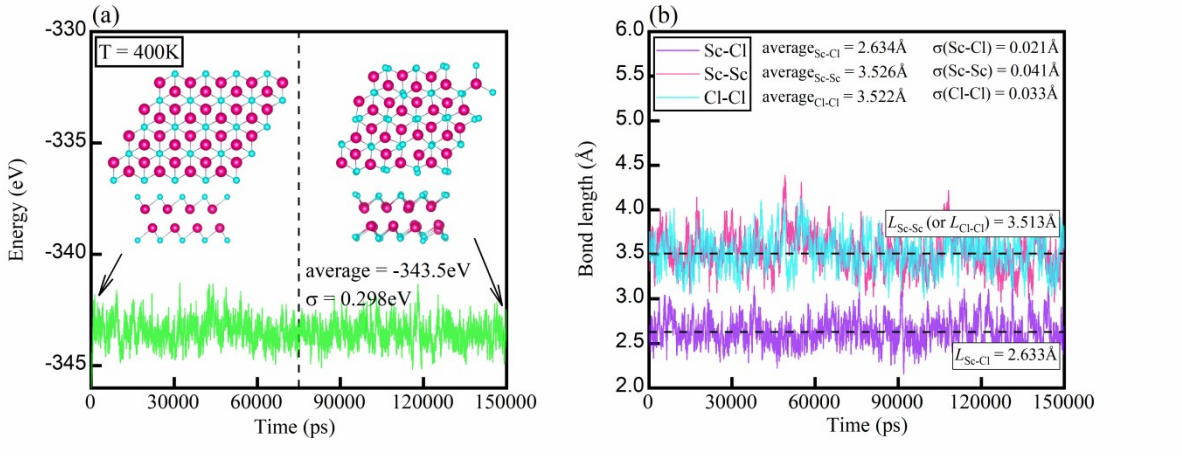

Fig. S7. (Color online) (a) Molecular dynamics simulation of monolayer ScCl at 400 K. (b) The evolution of bond length with time in AIMD simulation at 400 K.