Strong Magnetic Field driven Spin Density Waves in Pressured Black Phosphorus

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1. Research Motivations: experimental aspects

A New 2D Material: Black phosphorus

ARTICLES
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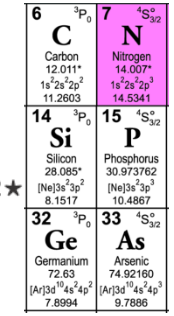
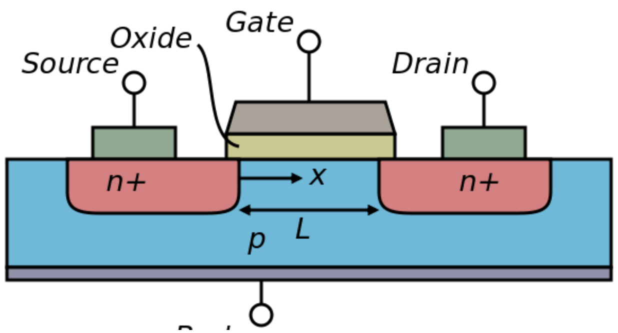
nature nanotechnology

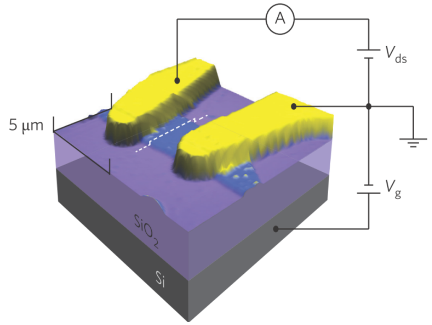


Black phosphorus field-effect transistors

Likai Li[1], Yijun Yu[1], Guo Jun Ye[2], Qingqin Ge[1], Xuedong Ou[1], Hua Wu[1], Donglai Feng[1], Xian Hui Chen[2]* and Yuanbo Zhang[1]*

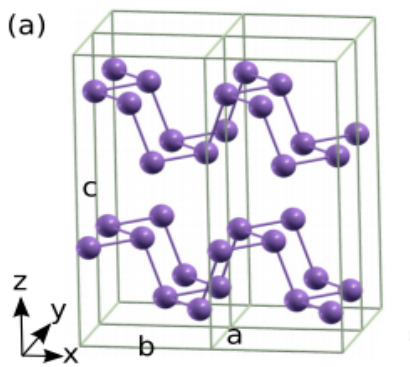
Two-dimensional crystals have emerged as a class of materials that may impact future electronic technologies. Experimentally identifying and characterizing new functional two-dimensional materials is challenging, but also potentially rewarding. Here, we fabricate field-effect transistors based on few-layer black phosphorus crystals with thickness down to a few nanometres. Reliable transistor performance is achieved at room temperature in samples thinner than 7.5 nm, with drain current modulation on the order of 10^5 and well-developed current saturation in the *I*–*V* characteristics. The charge-carrier mobility is found to be thickness-dependent, with the highest values up to ~1,000 $cm^2\ V^{-1}\ s^{-1}$ obtained for a thickness of ~10 nm. Our results demonstrate the potential of black phosphorus thin crystals as a new two-dimensional material for applications in nanoelectronic devices.

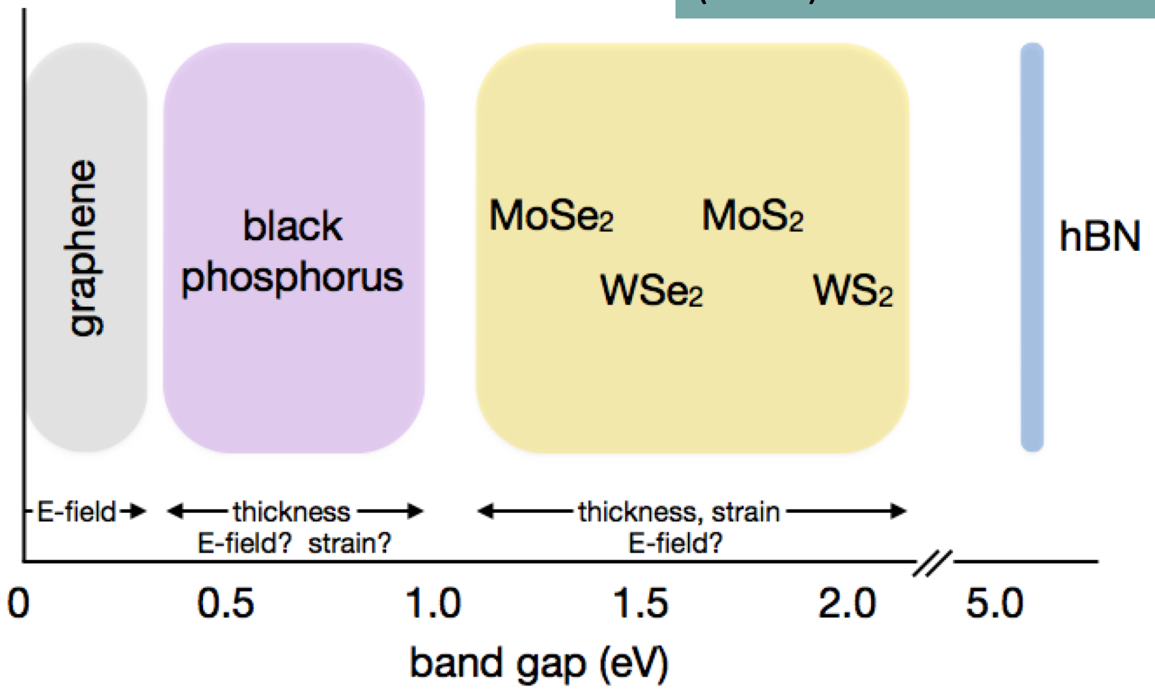




BP： direct band gap optical & electronic properties

Wei Ji, Nature Commun. (2014)





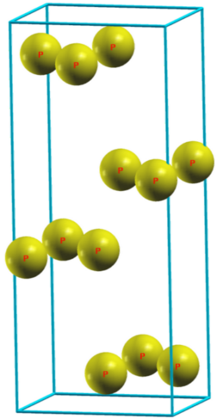
Superior electrical properties: high mobility (~1000cm^2/Vs), very large turn-off ratio (~10000)， comparable to traditional Si

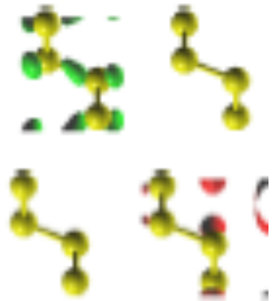
Topological origin of 3D Dirac Sememetal ?

Topology of Crystal Structure**: nonsymmorphic symmetry**

Under ambient & pressure, **space group of BP, Cmca,**

Symmetry operation elements**: glide planes**





Gibson & Cava, et al. 2015, Phys. RevB. 91. 205128

CASE III: 3D DIRAC SEMIMETALS FROM GLIDE PLANES AND SCREW AXES

The effects of "non-symmorphic" symmetry, or space groups containing glide planes and/or screw axes, on the electronic band structure of solids has been known for a long time [45]. The essence is that the presence of these symmetry elements makes it such that the normally two-fold degenerate bands must touch at four fold degenerate points at certain special points at the surface of the Brillouin zone, and that some of these degeneracies are not

Why 3D Dirac Semimetals interested ?

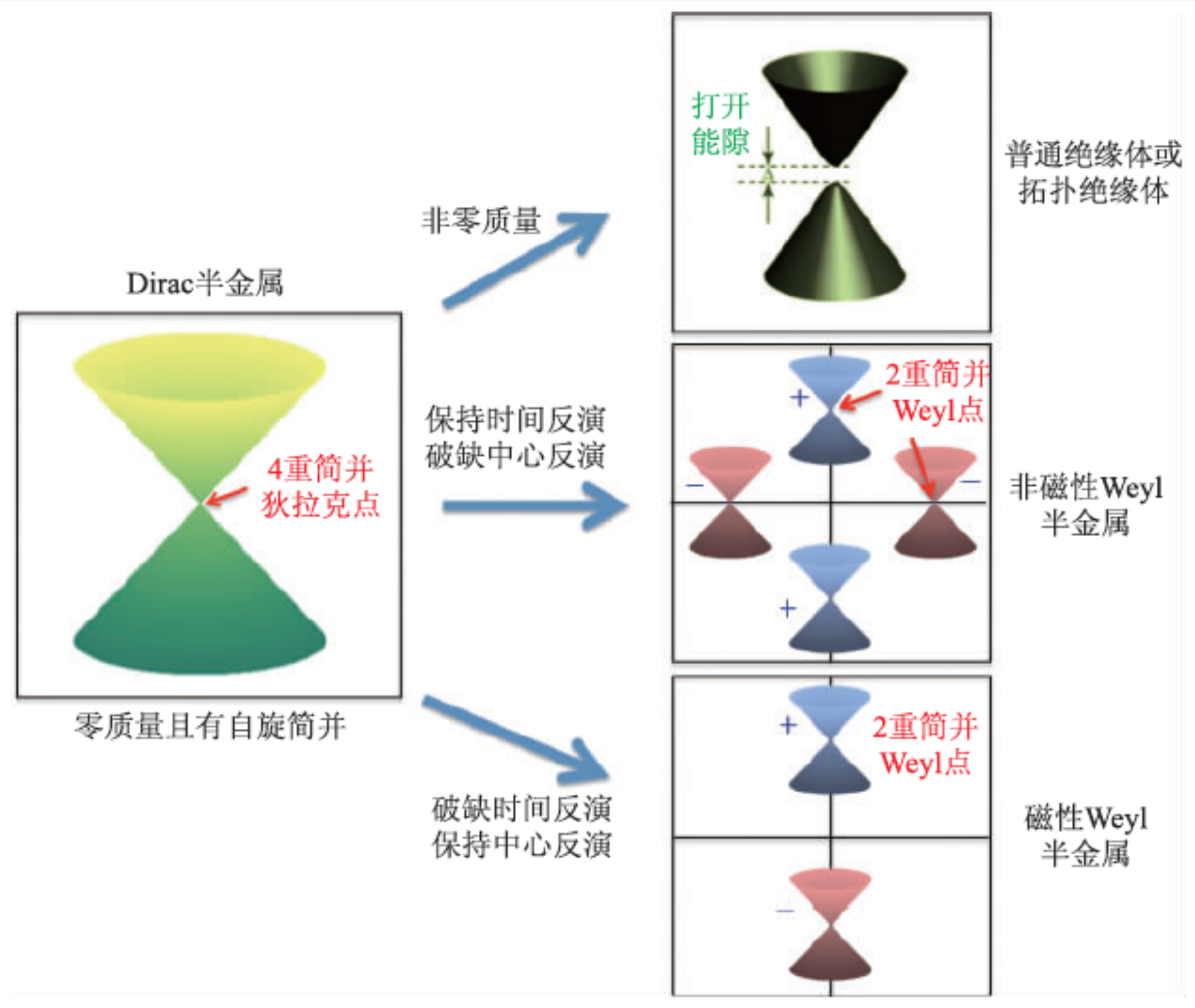


图1 三维狄拉克半金属、拓扑或普通绝缘体、最简单的非磁性和磁性Weyl半金属之间的关系

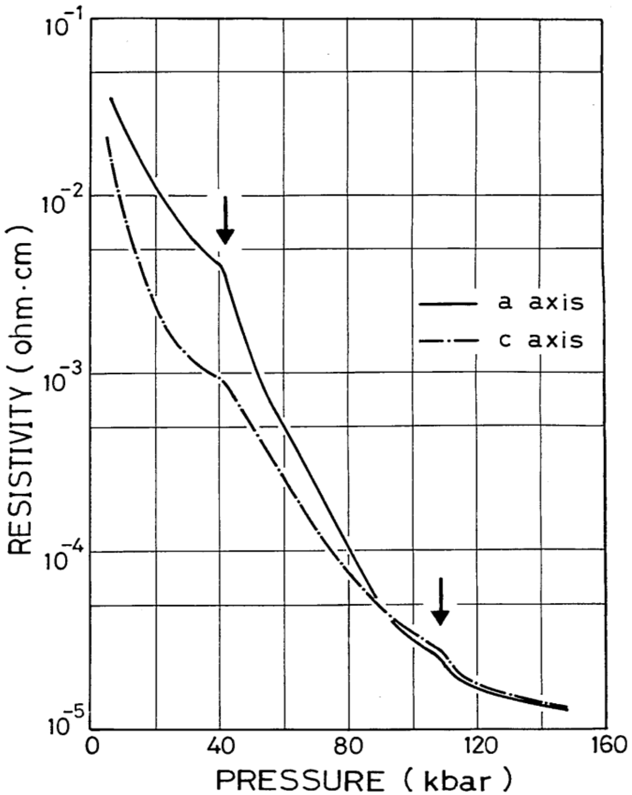
Weng, Fang, Dai

<<Physics>>,

2015

BP in hydrostatic pressure: Phase diagram & S-M transition

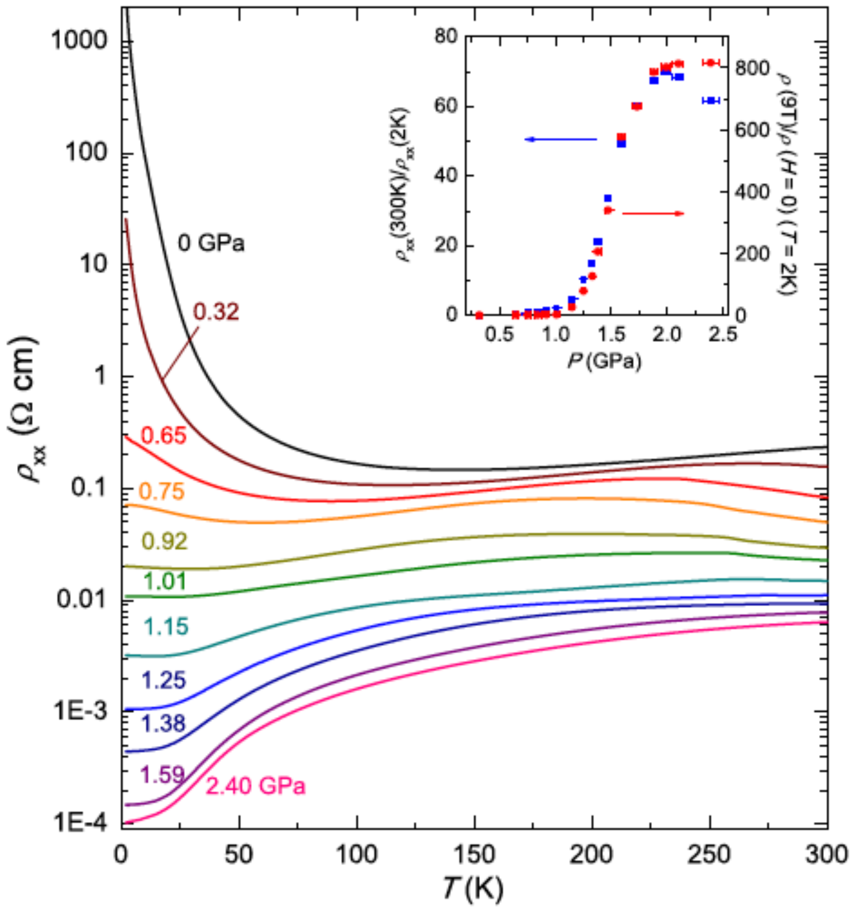
Phase Diagram



4.2 GPa: orthorhombic -- > rhombohedral
10.8 GPa: rhombohedral -- > simple cubic

Japanese Journal of Applied Physics
Vol. 23, No. 1, January, 1984 pp. 15–19

Resistivity - T



Semicond.-metal transition P_c ~ 1 Gpa

X.-H. Chen group, PRL 115, 186403 (2015)

Research Motivations:

What happen in BP: pressure + magentic field

- Nontrivial topological properties of 3D Dirac semimetal?
- (a). Band inversion, Dirac points & linear energy spectrum ?
- (b). 3D form of 2D graphene: gapless topological semimetals
- (c). In the critical point of various topological materials
- (d). Fermi arc on surface, large g factor, linear MR, ….

- 3D Dirac Semimetals, derived through modifying field/parameters:
- (e). Topological Insulators
- (f). Weyl semimetals
- (i). Topological SC: gapless zero energy mode : Majorana fermions
- (j)……

2. Electronic structures under pressure

Methods: VASP, Quatum Essepresso, WIEN2K,

Exchange-correlation potential:

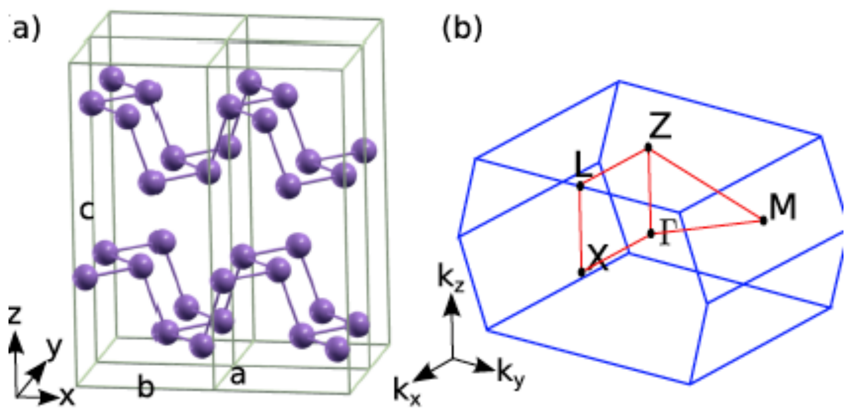
- PBE

Band gap corrections

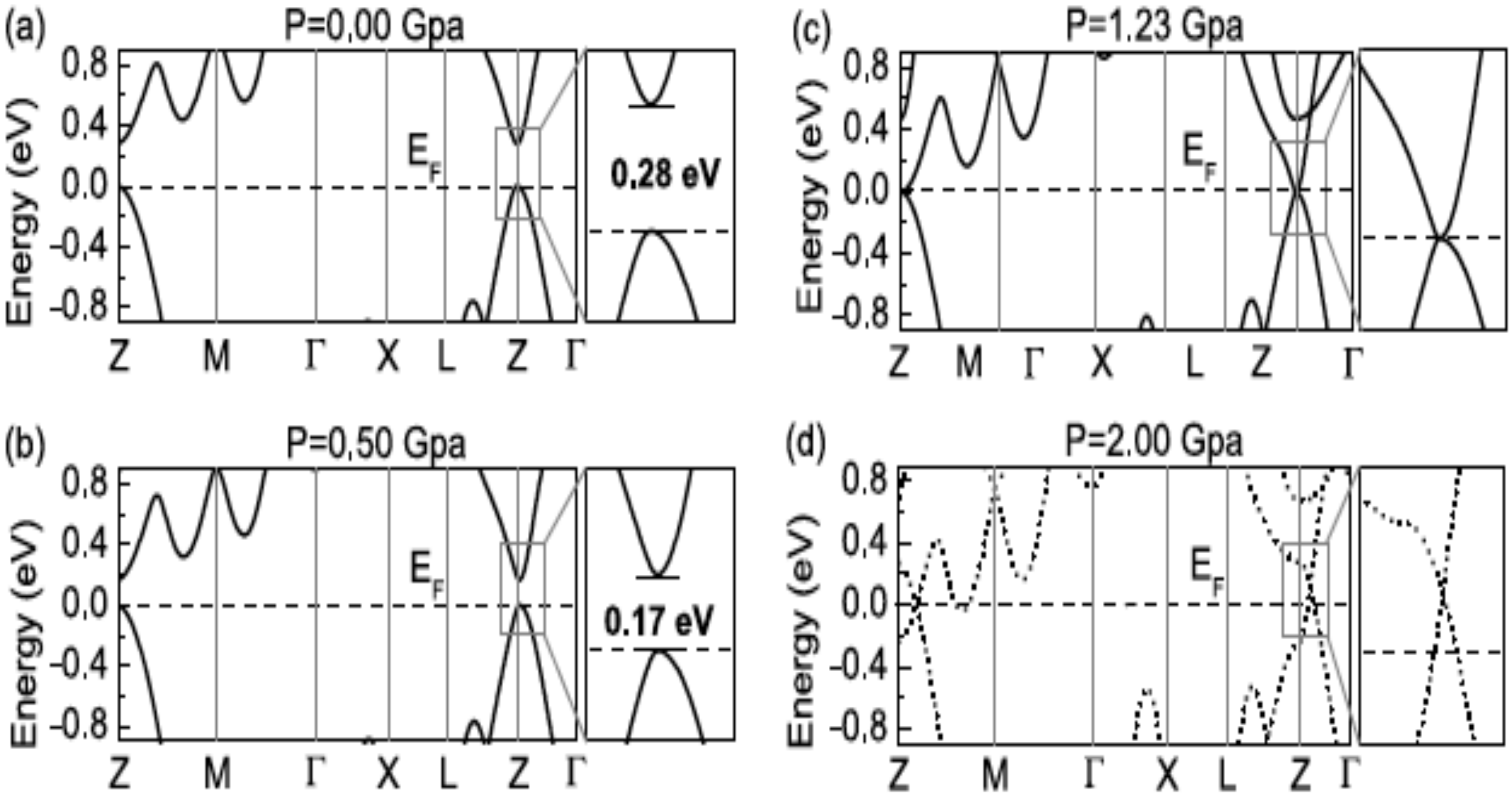
- mBJ
- HSE

Structure optimization

- Vdw: opt-vdw



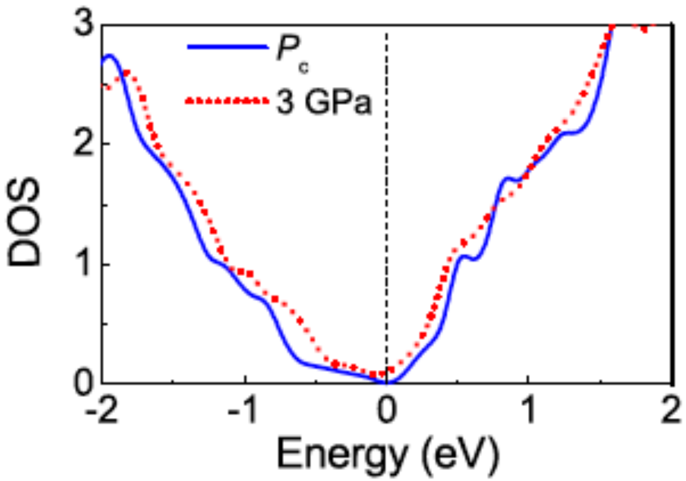
Evolutions of Band structures with pressure



S-M transition: P_c=1.23 eV

DOS & Dirac Cones： 3D Dirac Semimetal

P=1.23 Gpa: 3D Dirac Semimetal



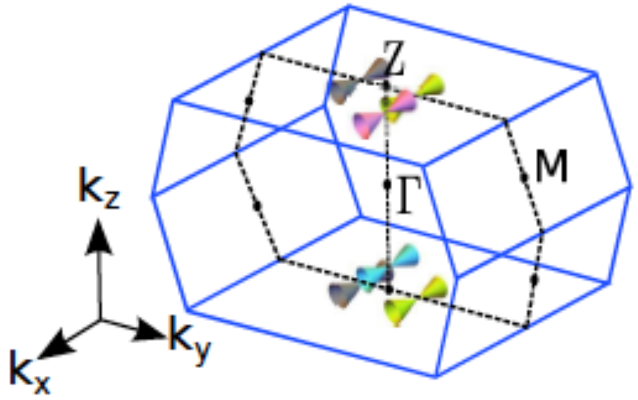
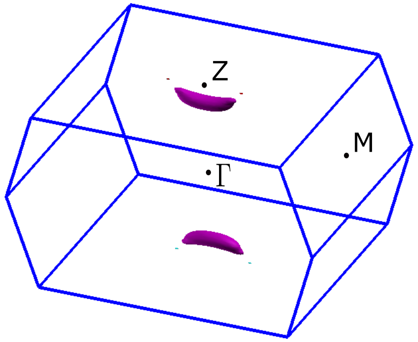


TABLE II. Effective masses of black phosphorus under various hydrostatic pressures and comparison with Refs. [11,37].

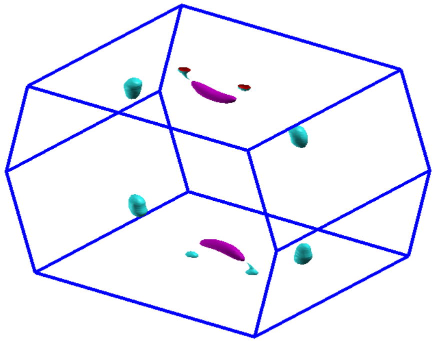
	P(GPa)	m_x^*/m_0	m_y^*/m_0	m_z^*/m_0
	0.00	0.14(0.12 [11], 0.08 [37])	1.26(1.15 [11], 1.03 [37])	0.16(0.15 [11], 0.13 [37])
e	0.50	0.09	1.24	0.14
	1.00	0.05	1.21	0.13
	0.00	0.12(0.11 [11], 0.07 [37])	0.90 (0.71 [11], 0.65 [37])	0.34 (0.30 [11], 0.28 [37])
h	0.50	0.08	0.82	0.32
	1.00	0.04	0.78	0.31

Fermi surface evolution with pressure: Lifshitz transition

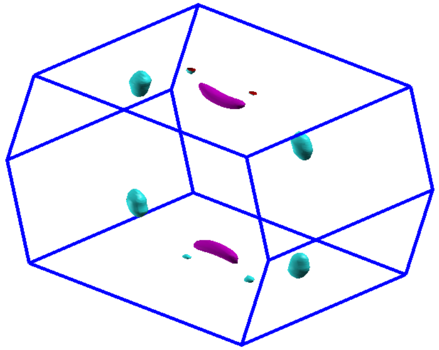
P=1.5 GPa



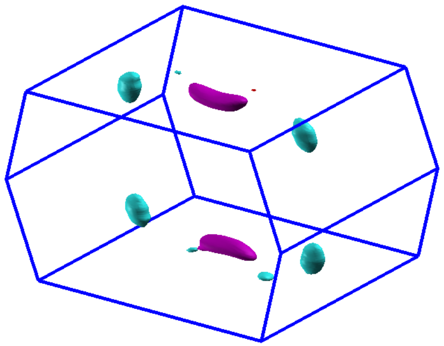
P=2.0 GPa



P=3.0 GPa

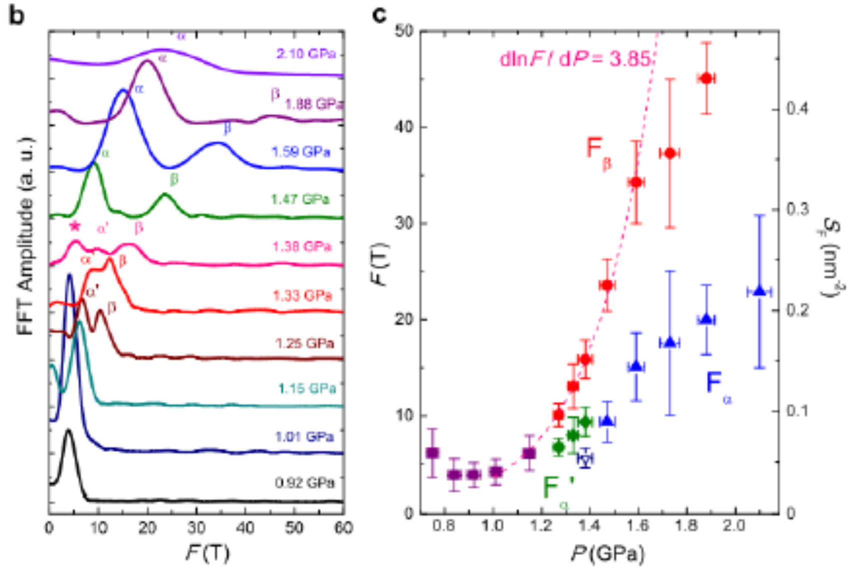


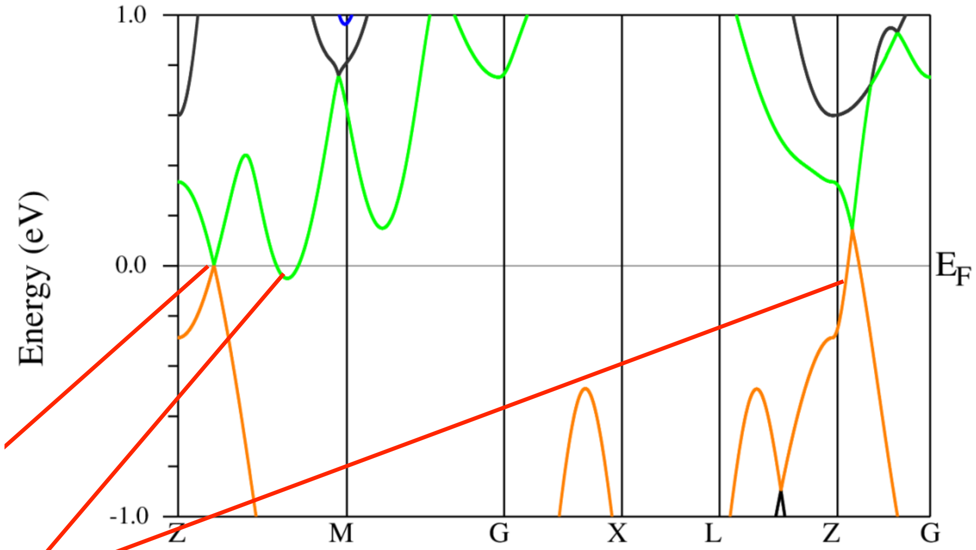
P=4.0 GPa

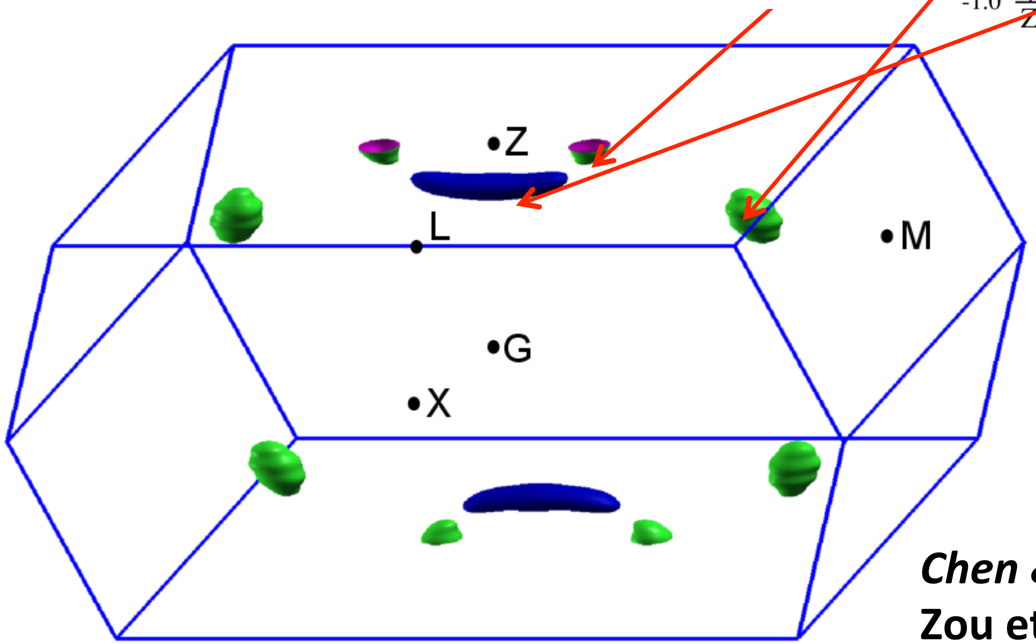


Pockets type	β (hole)	α (electron)	α^* (electron)
S_F (nm^{-2})	1.06[a] (0.42)[b]	0.4[a] (0.22)[b]	0.23[a] (0.16)[c]
Inequivalent numbers	2	4	2
Total S_F (nm^{-2})	2.12	1.60	0.46

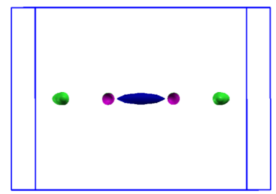
Fermi surfaces & Band structures



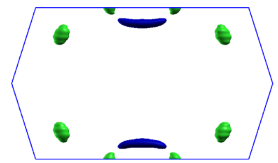




Top view



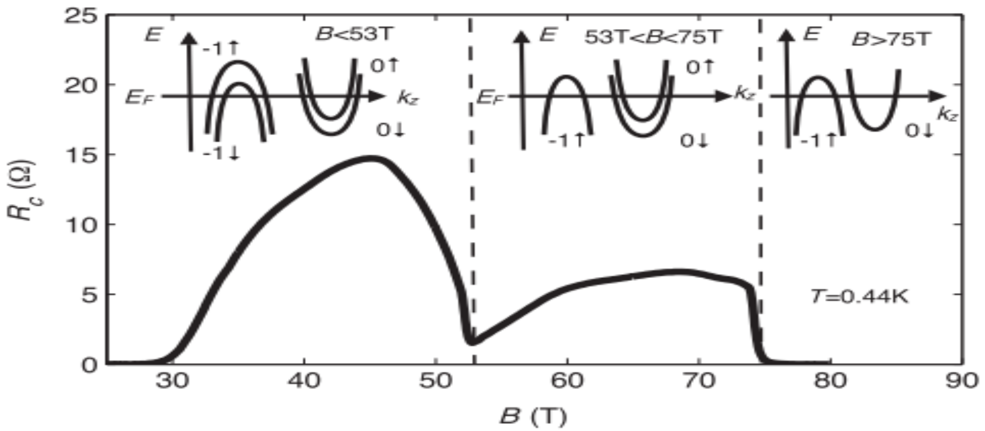
Side view



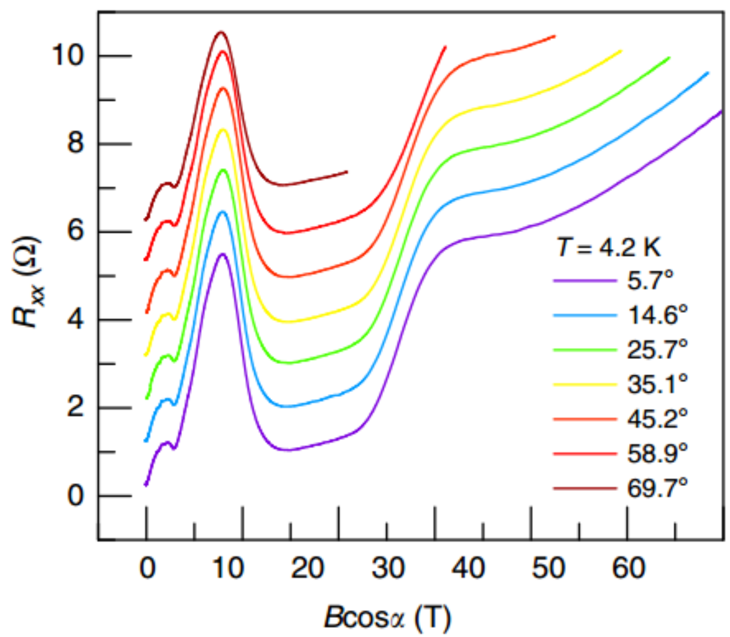
***Chen & Zou., Phys. Rev. Lett*. 115**, 186403 (2015)
Zou et al. in Phys. Rev. B 95, 195434 (2016).

3. 3D Dirac Semimetal in Pressured BP: Strong Magnetic Field Effect

Layered Graphite Semimetal



ZrTe5: 3D Dirac Semimetal



Anomolous increase in Rxx:

Why? Exciton condensation

Charge density wave

Spin density wave

… still hotly debated

Model Hamiltonian of 3D Dirac Semimetal BP

Similar to ZrTe5, bulk BP has symmetry of D_2h point group below P<4.5 Gpa:

At P around Pc for 3D Dirac semimetal, we have linear Dirac spectrum

$$m_{xz}: \quad \Psi_{(k_x,k_y,k_z)} \rightarrow -\tau^z \cdot i\sigma^y \cdot \Psi_{(k_x,-k_y,k_z)},$$

$$m_{yz}: \quad \Psi_{(k_x,k_y,k_z)} \rightarrow i\sigma^x \cdot \Psi_{(-k_x,k_y,k_z)},$$

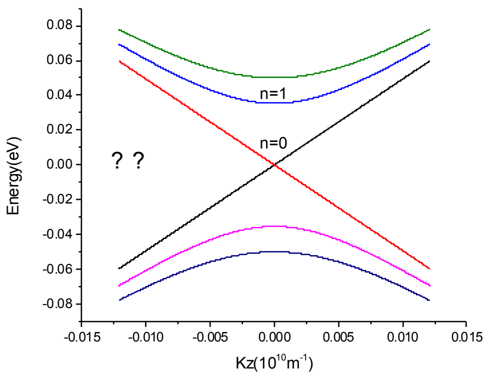
$$I: \quad \Psi_{(k_x,k_y,k_z)} \rightarrow \tau^z \cdot \Psi_{(-k_x,-k_y,-k_z)},$$

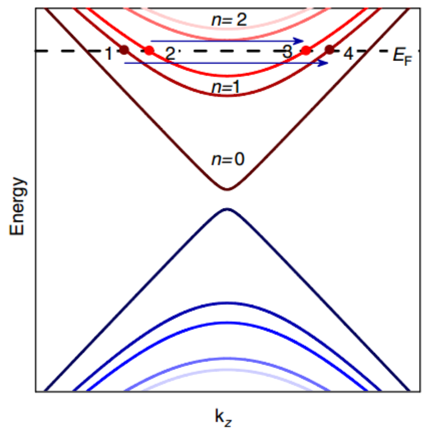
$$\mathcal{T}: \quad \Psi_{(k_x,k_y,k_z)} \rightarrow \mathcal{K} \cdot i\sigma^y \cdot \Psi_{(-k_x,-k_y,-k_z)}.$$

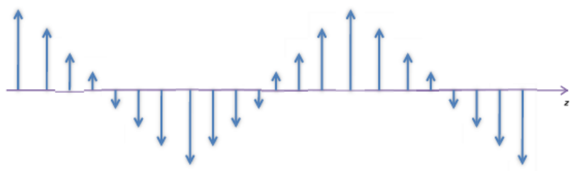
$$H_0(k) = \mathrm{h}(v_x k_x \tau_x \sigma_z + v_y k_y \tau_y + v_z k_z \tau_x \sigma_x)$$

Landau Guage: Landau level quantization in xy plane; free motion in z-axis

$$H = \sum_{k,\sigma} \left(\sqrt{v_z^2 \mathrm{h}^2 k^2 + 2\mathrm{h} v_x v_y eBn}\right) a_{k,\sigma}^{+} a_{k,\sigma} + \frac{U}{N} \sum_{k,k',q,\sigma} a_{k,\sigma}^{+} a_{k+q,\sigma} a_{k',-\sigma}^{+} a_{k'-q,-\sigma}$$







ry Figure 15. The spin density from the $n = 0$ Landau level.

Focus on the quantum limit: Landau level index n=0

(a) on-site Coulomb Interaction:

$$H = \sum_{k,\sigma} v_z \hbar |k| a^+_{k,\sigma} a_{k,\sigma} + \frac{U}{N} \sum_{k,k',q,\sigma} a^+_{k,\sigma} a_{k+q,\sigma} a^+_{k',-\sigma} a_{k'-q,-\sigma}$$

SDW order parameter: $\Delta s(q = 2k_F) = \frac{U}{N} \sum_{k,\sigma} \sigma a^+_{k,\sigma} a_{k+q,\sigma}$

Chiral SDW order parameter: $\Delta s(q = 2k_F) = \frac{U}{N} \sum_{k} a^+_{k,\sigma} a_{k+q,-\sigma}$

n=0 SDW energy gap （a,b,c lattice constant）

$$|\Delta|_0 = 2E_F \exp\left(-\frac{(2\pi\hbar)^2 v_z}{eBUabc}\right) = 2E_F \exp\left(-\frac{B^*}{B}\right)$$

One gets critical magnetic field B* is about $10^4 \sim 10^5$ T, so the on-site repulsive Hubbard model is not applicable !

(b) Long-range Screened Coulomb Interaction:

$$V_c = \frac{1}{2}\int d^3\vec{r}_1 d^3\vec{r}_2 V_c(\vec{r}_1 - \vec{r}_2)\rho(\vec{r}_1)\rho(\vec{r}_2) \qquad V_c(\vec{r}_1 - \vec{r}_2) = \frac{e^2 \exp(-k_s|\vec{r}_1 - \vec{r}_2|)}{4\pi\varepsilon|\vec{r}_1 - \vec{r}_2|}$$

To replace the on-site U

Self-consistent equation for energy gap of SDW:

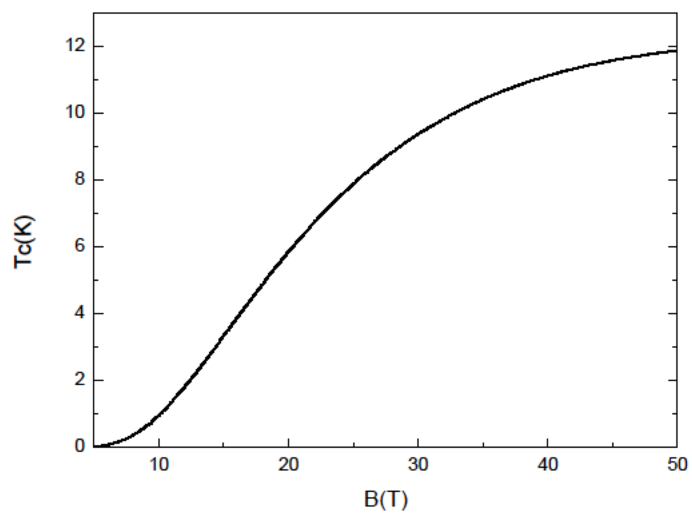
$$\frac{4\varepsilon_0\varepsilon_r\Delta_{k_{x,z}}}{e^2}=\frac{1}{(2\pi)^2}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}dk_x^{'}\int_{-k_F}^{k_F}dk_z^{'}\frac{\Delta_{k^{'}_{x,z}}}{2\sqrt{\left|\Delta_{k^{'}_{x,z}}\right|^2+(\mathrm{h}v_Fk_z^{'})^2}}\frac{\exp\{\frac{l_B^2[(k_z-k_z^{'})^2+k_s^2]}{2}\}}{\sqrt{(k_x-k_k^{'})^2+(k_z-k_z^{'})^2+k_s^2}}$$

$$\times Erfc(\frac{l_B\sqrt{(k_x-k_k^{'})^2+(k_z-k_z^{'})^2+k_s^2}}{\sqrt{2}})\times\tanh(\frac{\sqrt{\left|\Delta_{k^{'}_{x,z}}\right|^2+(\mathrm{h}v_Fk_z^{'})^2}}{2k_BT})$$

$$\frac{4\varepsilon\Delta_{k_{x,z}}}{e^2}=\int\frac{dk_x^{'}dk_z^{'}}{(2\pi)^2}\frac{\Delta_{k^{'}_{x,z}}}{2\sqrt{\left|\Delta_{k^{'}_{x,z}}\right|^2+(\mathrm{h}v_zk_z^{'})^2}}\frac{\exp\{\frac{l_B^2[(k_z-k_z^{'})^2+k_s^2]}{2}\}}{\sqrt{\delta k^2+k_s^2}}Erfc(\frac{l_B\sqrt{\delta k^2+k_s^2}}{\sqrt{2}})$$

here the screening constant ks is comparable with Fermi wavevector $k_s=0.2\times10^9m^{-1}$, the relative dielectric constant =4， carrier $n=2.4\times10^{23}m^{-3}$ is taken from the experimental observation.

Why not CDW ? weak e-ph coupling in BP



SDW of 3D Dirac semimetals

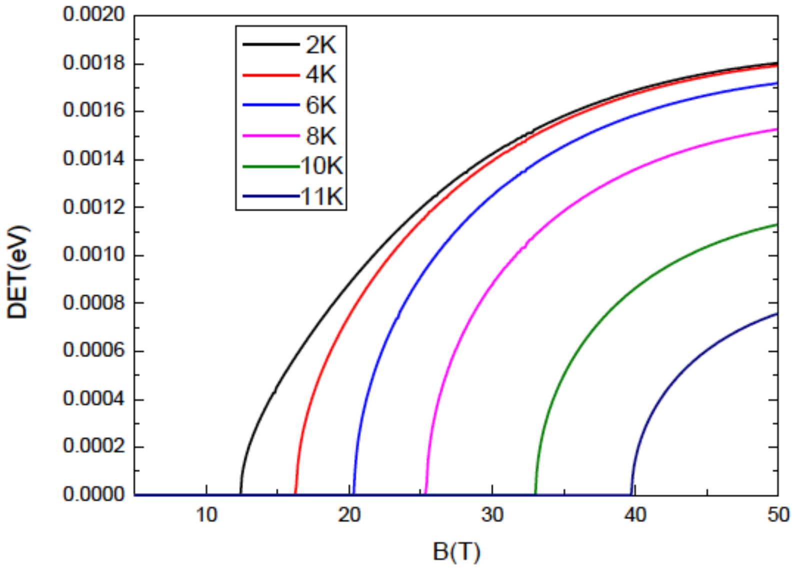


Fig.1a. Depend. of energy gap on applied field

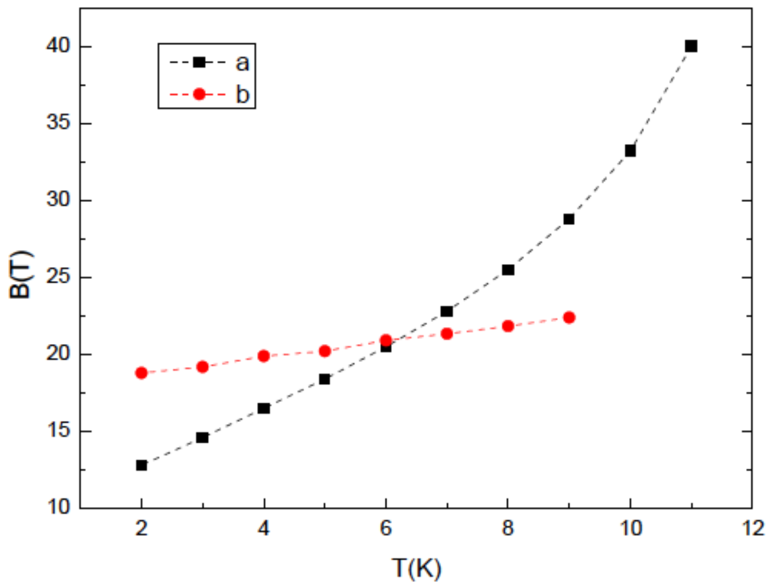


Fig.1b Depend. of critical field Bc on T
Black: theory. Red: recent exp.

Why SDW chiral ? Dirac particles are chiral, particular spins form density wave

we expect more exciting properties in the future.

4. Summary

Hydrostatic pressure effects: confirmed

- At P=0, gap ~ 0.27 eV (mBJ) or 0.34 (HSE)
- P_c =1.23 GPa: semicond.-metal transition ➔ Lifshitz transition
- P ~ 1.5 GPa: Dirac points appear near Z point
- P>2.5 GPa: 2 Fermi pockets (hole & electron) + a Dirac point

- **Strong Magnetic Field Effects: predicted**
- A 3D Dirac semimetal-SDW transition
- SDW critical magnetic field $B_c \approx 15$ T at T=2 K
- Critical field Bc approx. linearly increases with T

- Expect more rich quantum phases in 3D Dirac semimetals

Thanks for your attention !