Ferromagnetic ground-state of a monolayer MoS_2

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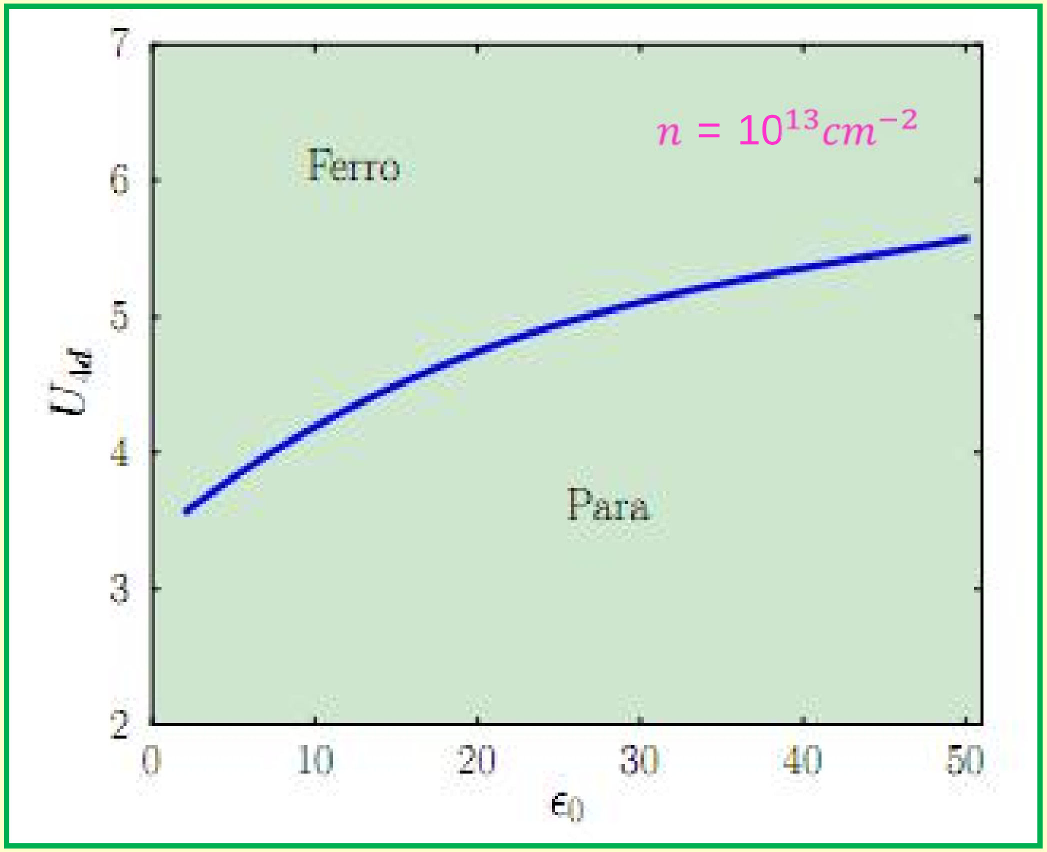
In collaboration with H Rostami

IPM Spring conference, 1-2 Khordad 92

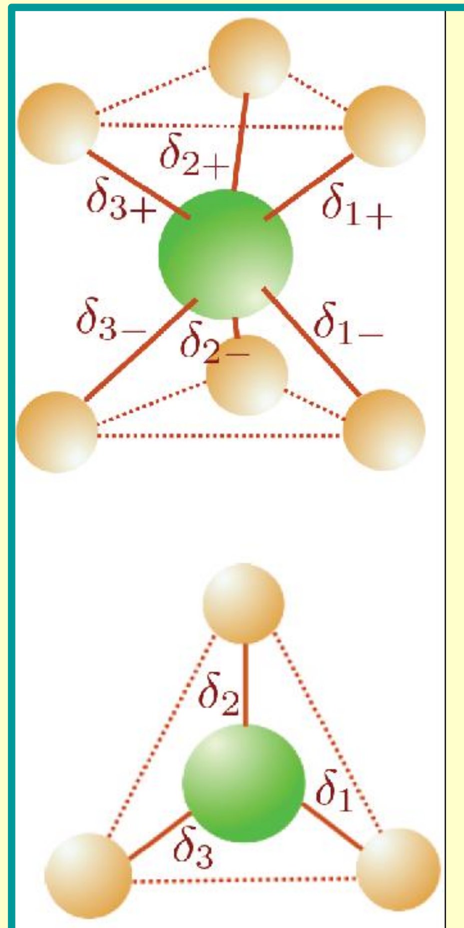
My purpose I: Phase diagram



H. Rostami and R. Asgari to be submitted (2013)

My purpose II: Two band Hamiltonian

$$
\begin{aligned}
H_{\tau s} &= \frac{\Delta}{2}\sigma_z + \lambda\tau s\frac{1-\sigma_z}{2} + t_0 a_0 \mathbf{q}\cdot\sigma_\tau \\
&+ \frac{\hbar^2|\mathbf{q}|^2}{4m_0}(\alpha+\beta\sigma_z) \\
&+ t_1 a_0^2 \mathbf{q}\cdot\sigma_\tau^* \sigma_x \mathbf{q}\cdot\sigma_\tau^*,
\end{aligned}
$$



Rostami, Moghaddam, Asgari arXiv:1302.5901

Outlook

1. Introduction

   brief overview on optical and electronic properties

2. Mean-field approximation

   two-band model Hamiltonian

   Mean-field approach

   Magnetic phase diagram

   Band-gap renromalization

3. Conclusion

   Electron-electron interaction

   Phase-diagram as function inter-interaction, charge density and dielectric constant

Why 2D Systems?

New and exciting physics

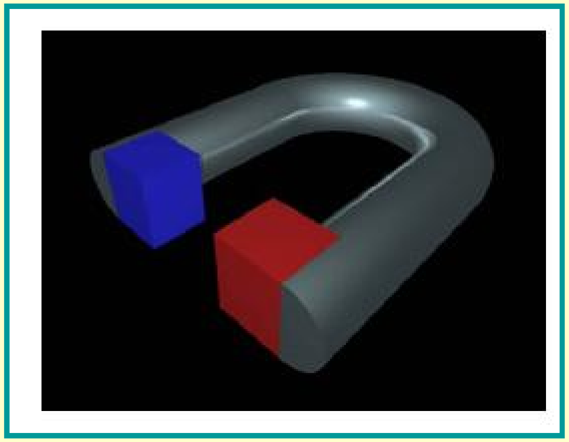
Correlated charge and spin

technologically useful properties

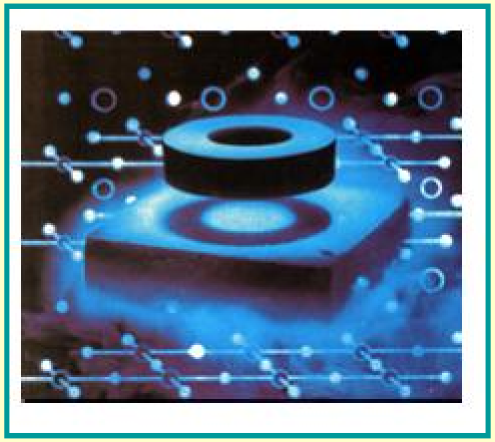
Phases of matter

-In classical world we have solid, liquid and gas phases

-In quantum world we have metals, insulators, magnetisms , superconductors, *etc* : spontaneous symmetry breaking



Broken rotational symmetry



Broken gauge symmetry

Qi and Zhang PRB 2008

New phases of matter in 2D quantum electron systems

-Quantum Hall effect

QHE without magnetic field?
Majorana fermions?

- Super fluidity and superconductors

Sc without BCS-like paradigm?
New routes to HTCS?

-Localization, disorder and quantum magnetism

Spin-liquid,
fractionalization

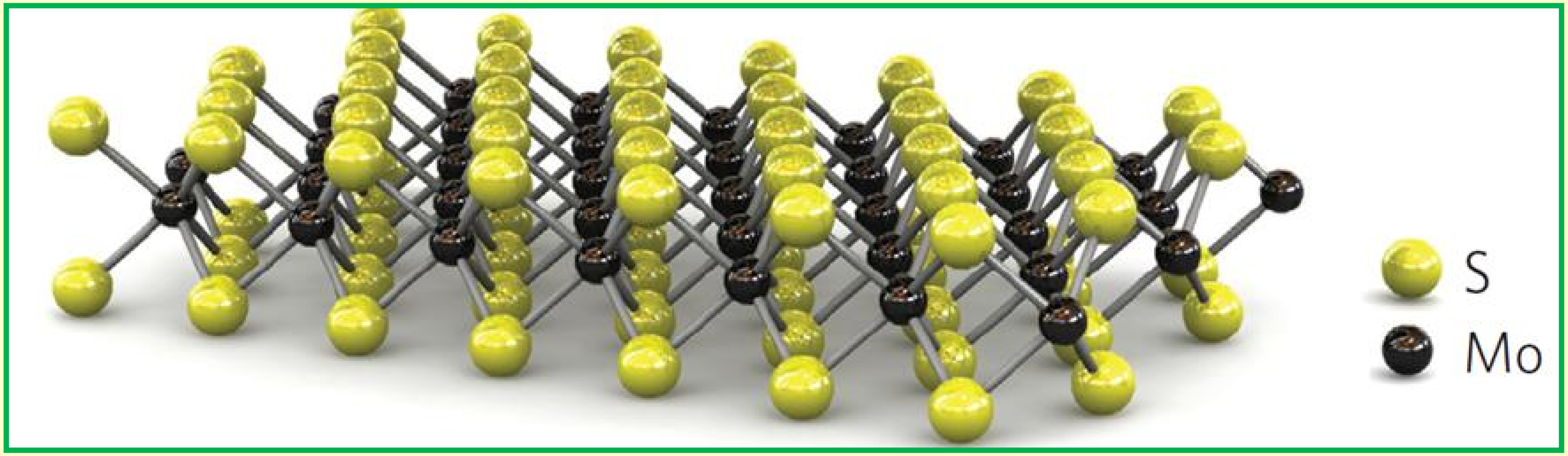
-Quantum phase transition, condensation

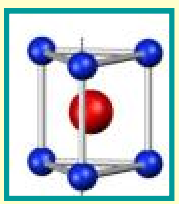
Q- phase transition,
New universality classes

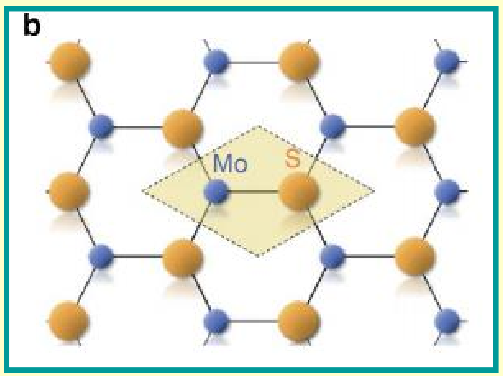
Classification of 2D systems

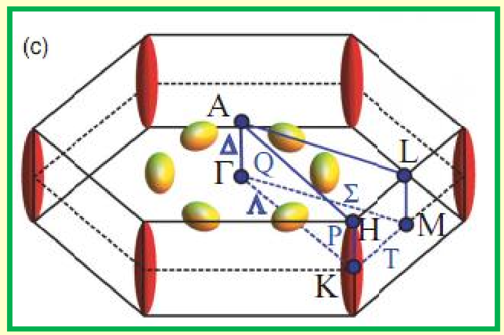
- Layered van der Waals solids
- Layered ionic solids
- Surface growth of nanolayer materials
- 2D artificial systems
- 2D topological insulator solids

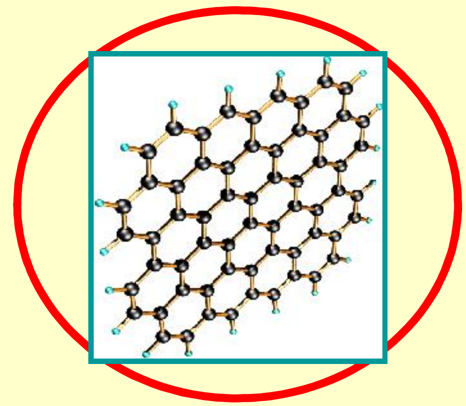
TMDCs: MoS_2 crystal







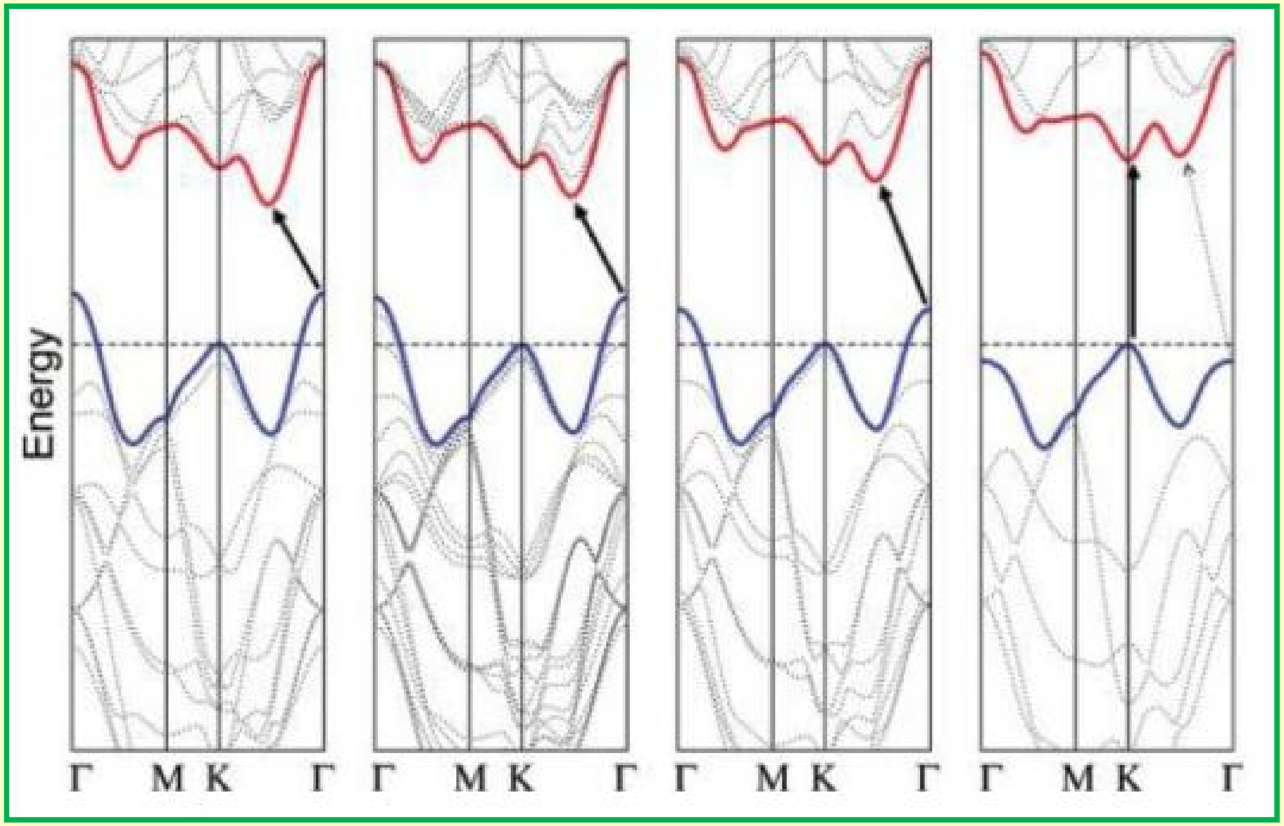




Wilson and Yaffe, Adv. Phys. **18**, 193 (1969)
Romley, Murray,Yoffe, J. Phys. C **5** (1972)
Mattheis, Phys. Rev. B **8**, 3719 (1973)
Helveg, et al Phys. Rev. Lett. **84**, 951 (2000)

kobayashi, Yamauchi, Phys. Rev. B **51**, 17085 (1995)

Bulk, quadri-, bi- and monolayer

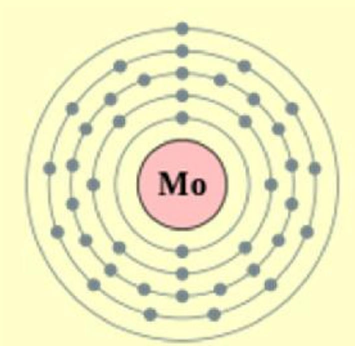


TMDCs: MoS_2 crystal

Photoluminescence properties

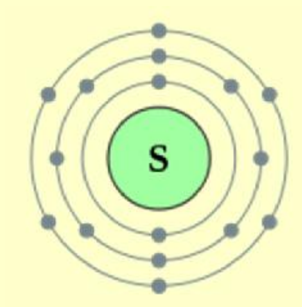
[Kr] $5s^1\ 4s^2p^6d^5$

2 ,8 ,18 ,13 ,1



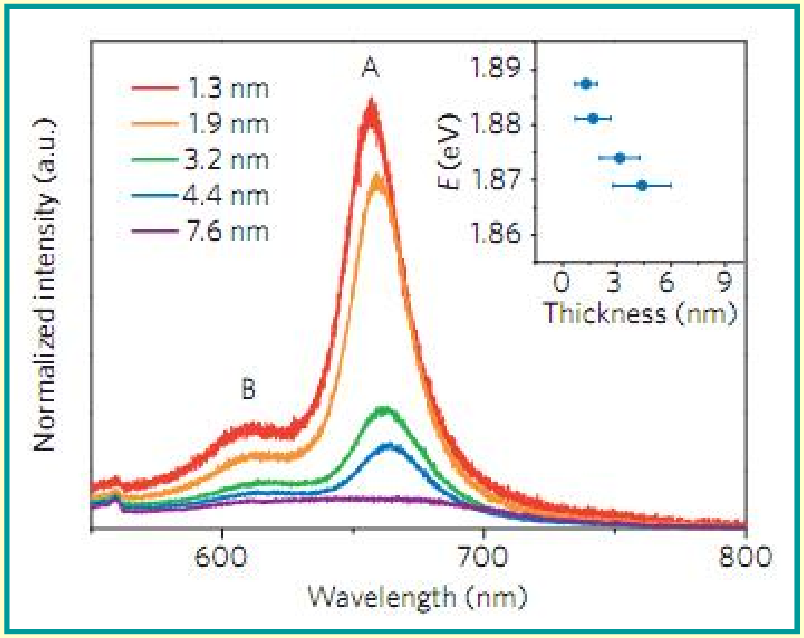
[Ne] $3s^2\ 3p^4$

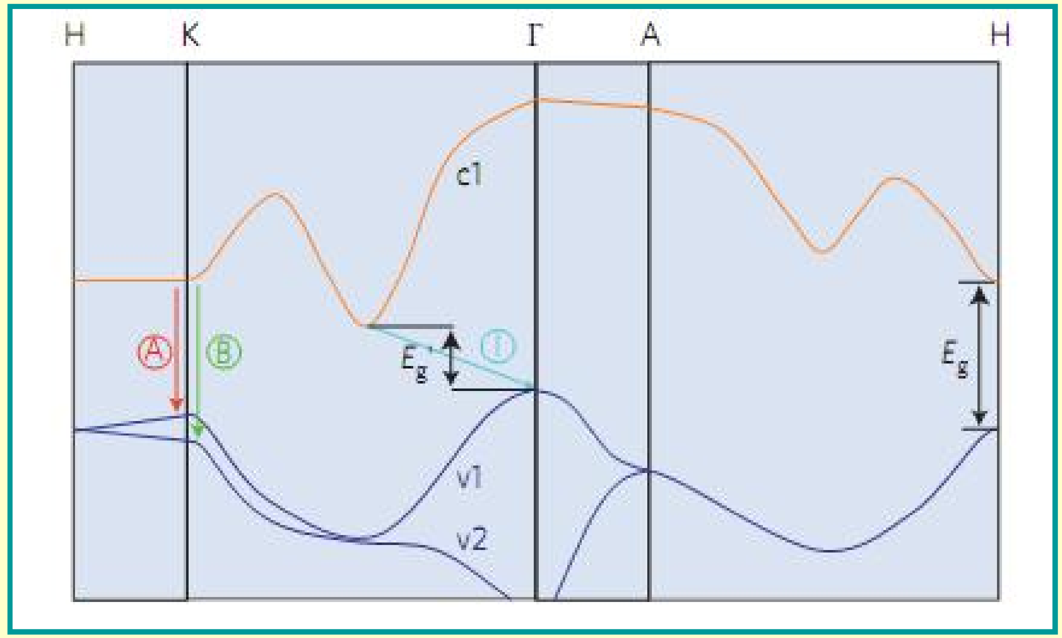
2 ,8 ,6



Wang, Kalantar Zadeh, Kis, Coleman, Strano, Nature Nanotech. **7**, 699 (2012)

Spectroscopy: few layers

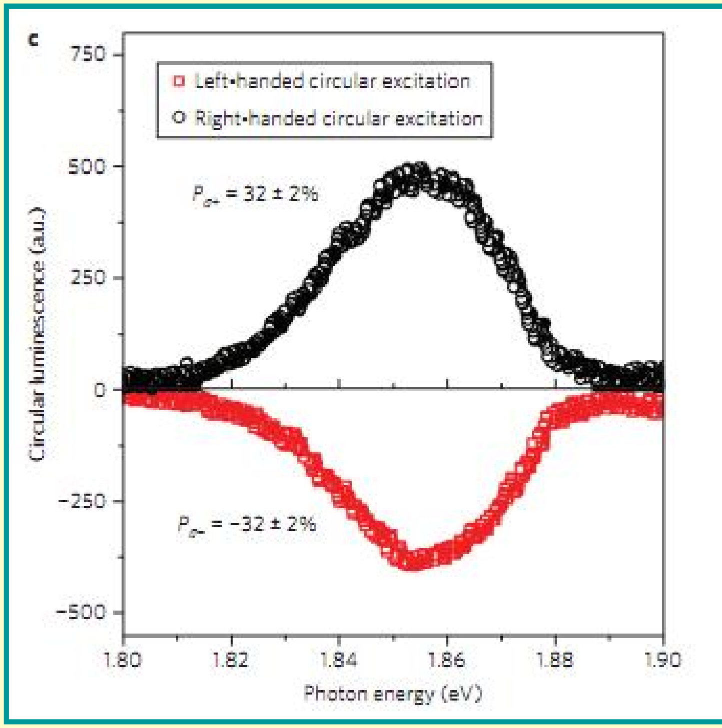


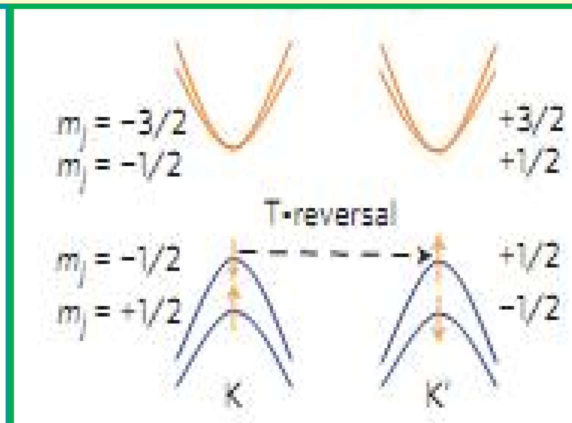


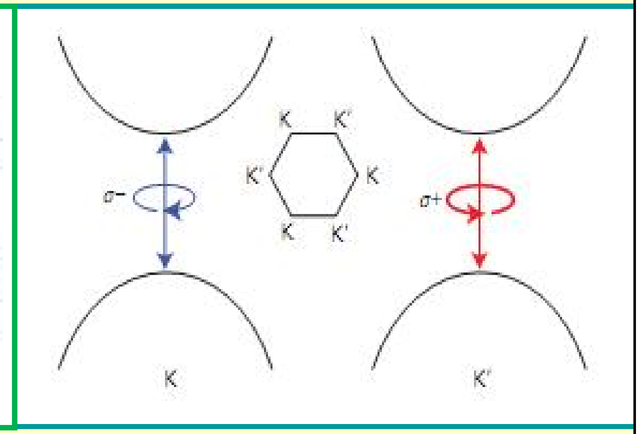
Eda, *et al*, Nano Lett. **11**, 5111 (2011)

Mak *et al*, Phys. Rev. Lett. **105**, 136805 (2010)

Valley polarization







$$\Delta m = \pm 1$$

$$P = \frac{|P_{+}^{vc}|^2 - |P_{-}^{vc}|^2}{|P_{+}^{vc}|^2 + |P_{-}^{vc}|^2}$$

$$P_{\pm}^{vc}(k) = < u_c(k) \,|\, p_x + i p_y \,|\, u_v(k) >$$

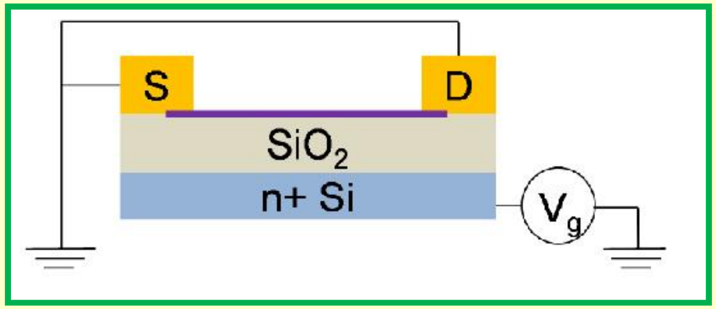
$$|P_{\pm}^{vc}(k)|^2 \propto \left(1 \pm \tau \frac{\Delta'}{\sqrt{\Delta'^2 + 4a^2 t^2 k^2}}\right)^2$$

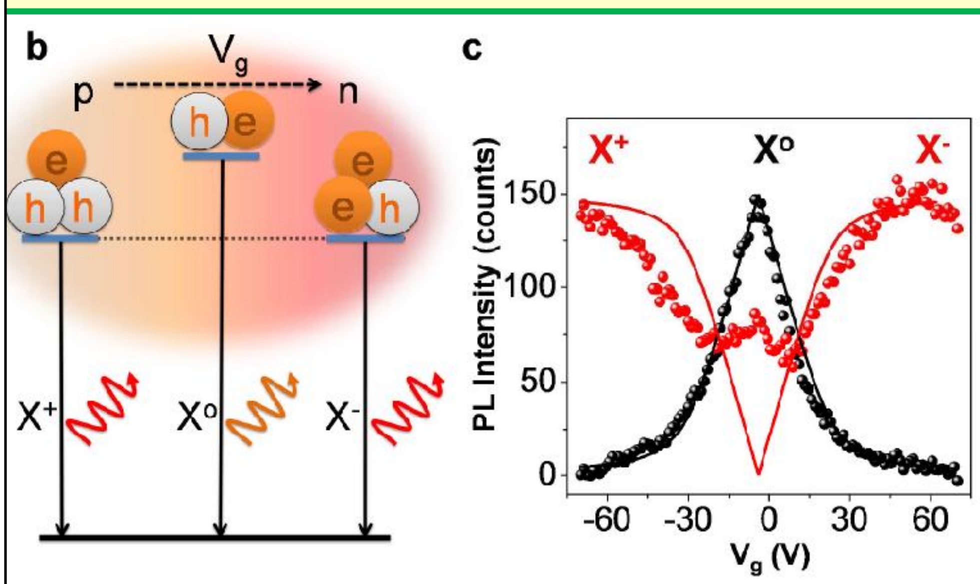
$$\Delta' = \Delta - \tau\, s\, \lambda$$

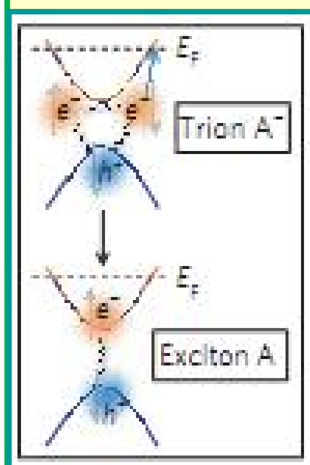
Zeng, *et al*, Nature Nano **7**, 490 (2012)

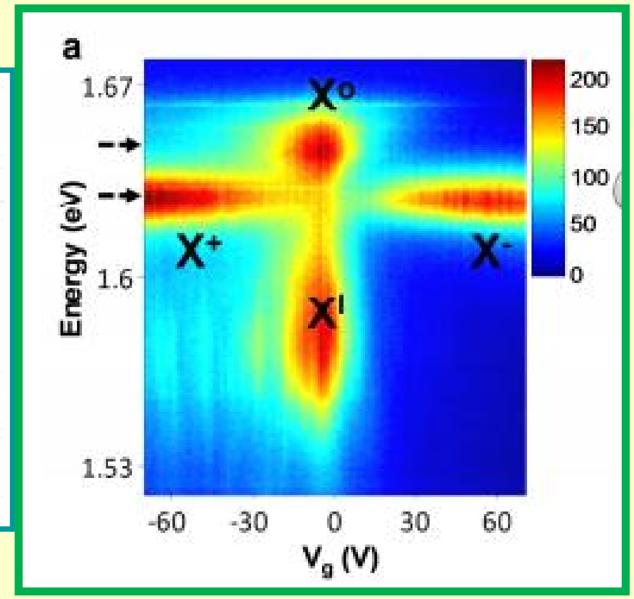
T. Cao, *et al* Nature Commuin. DoI: 10.1038/ncomms1882 (2012)

Charged excitons ($MoSe_2$: Trion)









K. F. Mak *et al*, Nature Materials **12**, 207 (2013)

J. S. Ross *et al*, Nature Communi. **4**, 1474(2013)

TMDCs: MoS_2 crystal

Nanoelectronic properties

Scattering mechanisms

- Charged impurities(Coulomb scattering)
- Neutral defects (short range scattering)
- Surface interface phonon scattering
- Ripples and roughness scattering
- Acoustic and optical phonons scattering

2D Semiconductor

$$\mu_{charged} \approx \left(m_e^*\right)^{-1/2} T^{3/2}$$

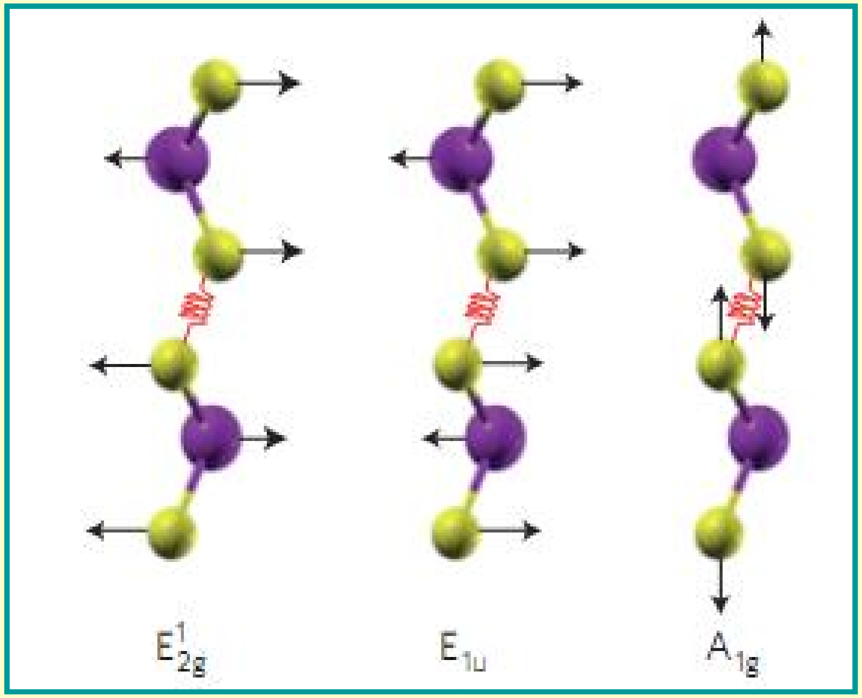
$$\mu_{optical} \approx \left(m_e^*\right)^{-5/2} T^{-1} \left[e^{\frac{\omega_{op}}{T}} - 1 \right]$$

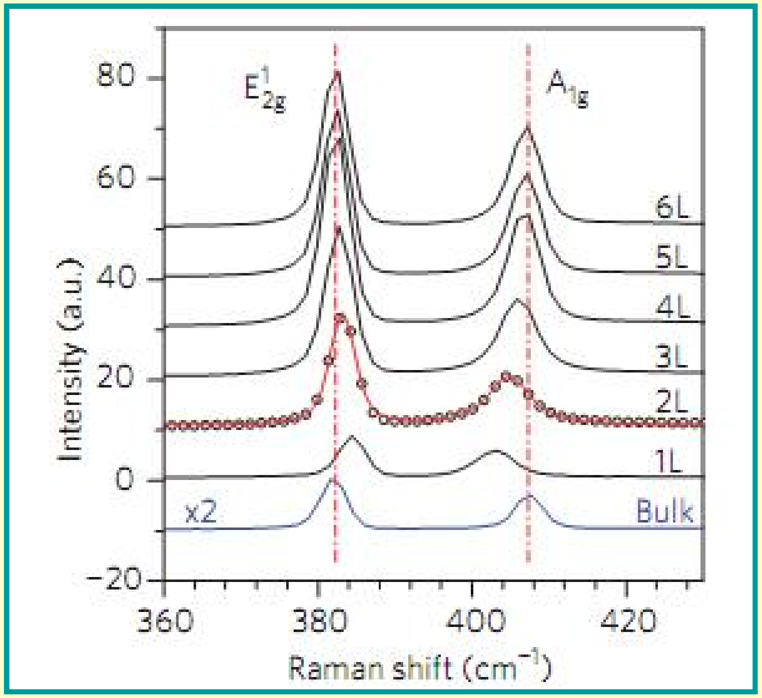
$$\mu_{acoustic} \approx \left(m_e^*\right)^{-5/2} T^{-3/2}$$

$$\mu(T) \approx \begin{cases} T \prec\prec 1 & 10^4 \quad (1978) \\ T \prec\prec 1 & 3\times 10^6 \quad (2000) \\ T = 300 & 1000 \quad (2000) \end{cases}$$

Typical electron mobility for Si at room temperature (300 K) is 1400 $cm^2/(V\cdot s)$ and the hole mobility is around 450 $cm^2/(V\cdot s)$.

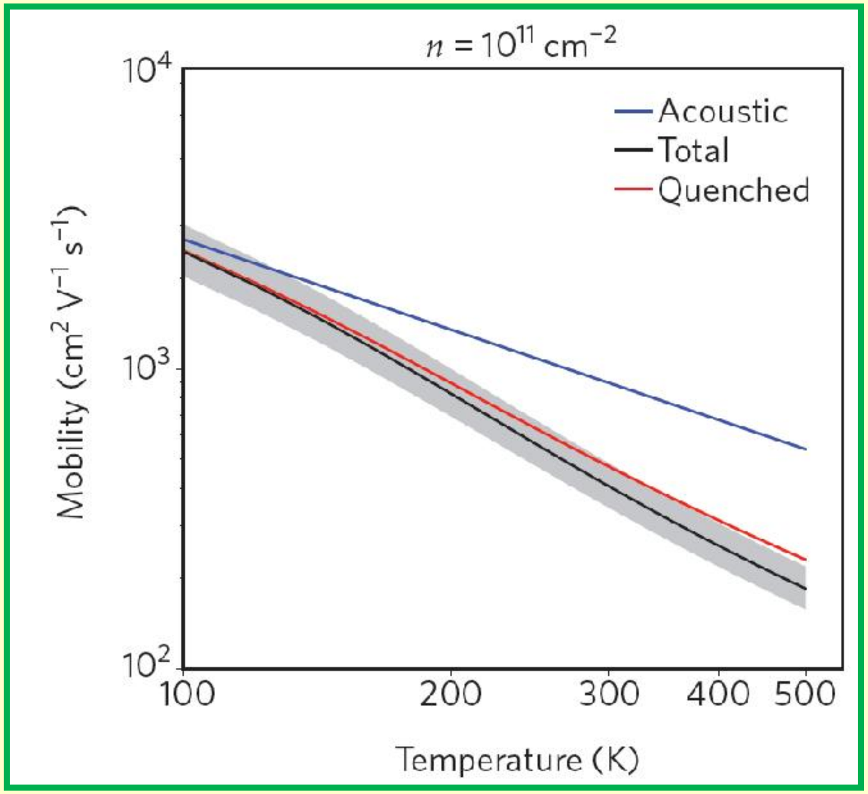
Phonons, Raman Spectroscopy

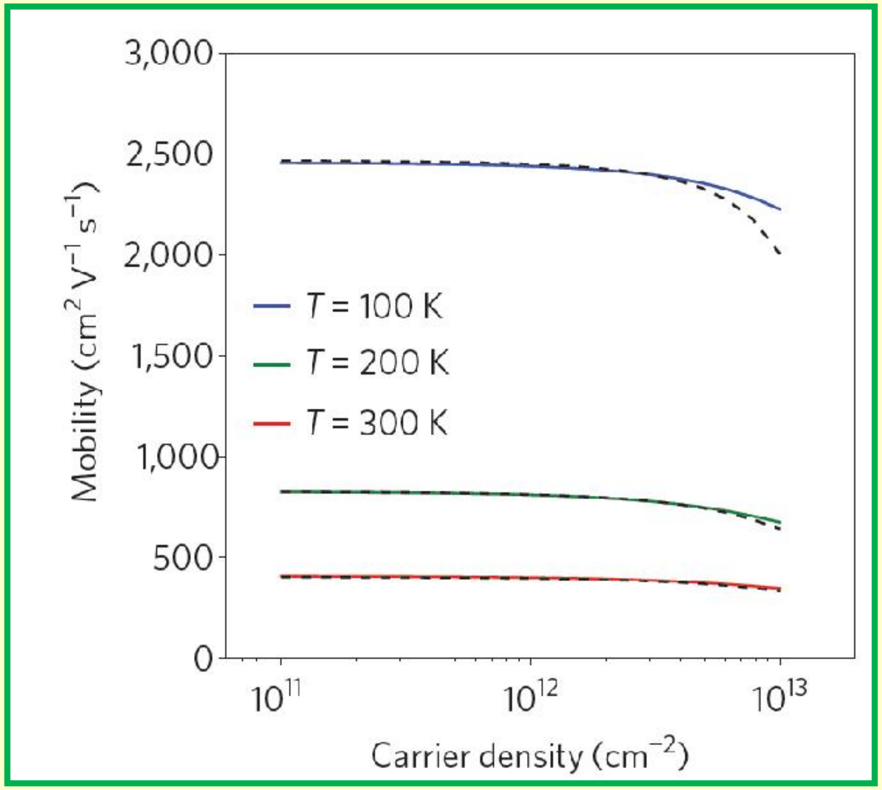




Molina-Sanchez, Wirtz, Phys. Rev. B **84**, 155413 (2011)
Lee *et al*., Acs Nano, **4**, 2695 (2010)

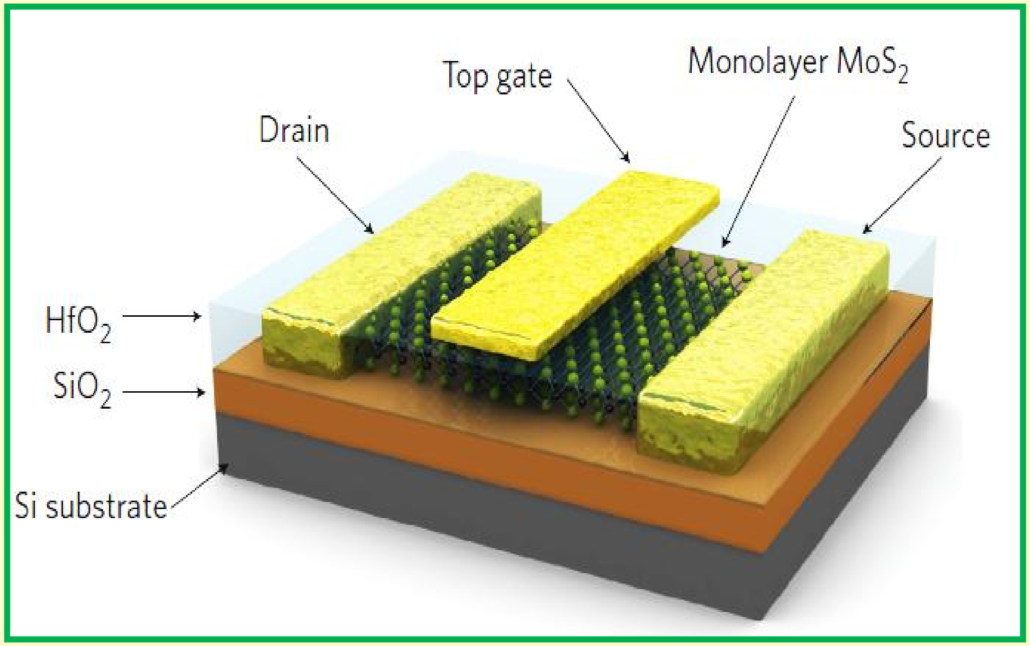
Mobility: evidence

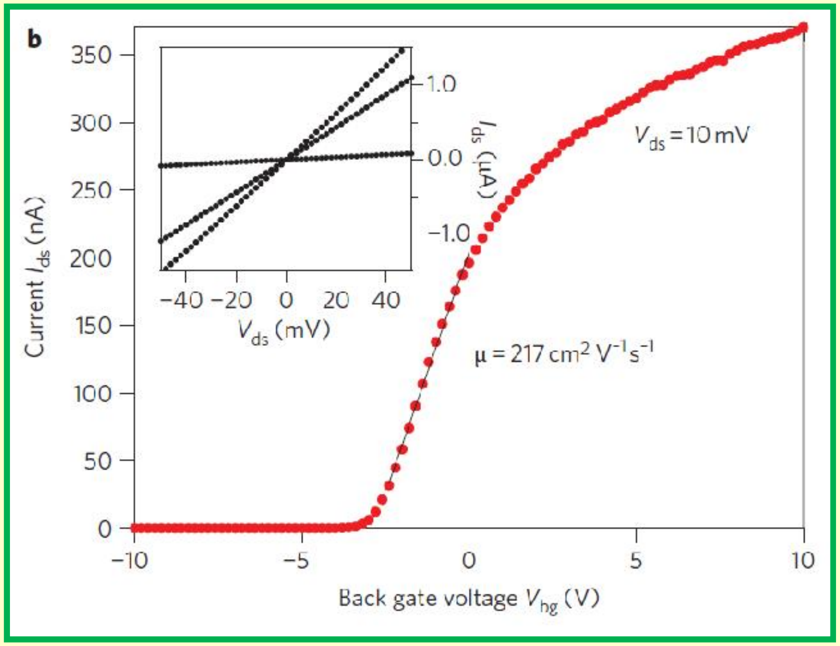




Kaasbjerg, *et al Phy. Rev. B* **85**,115317 (2012)

MoS2 Transistor



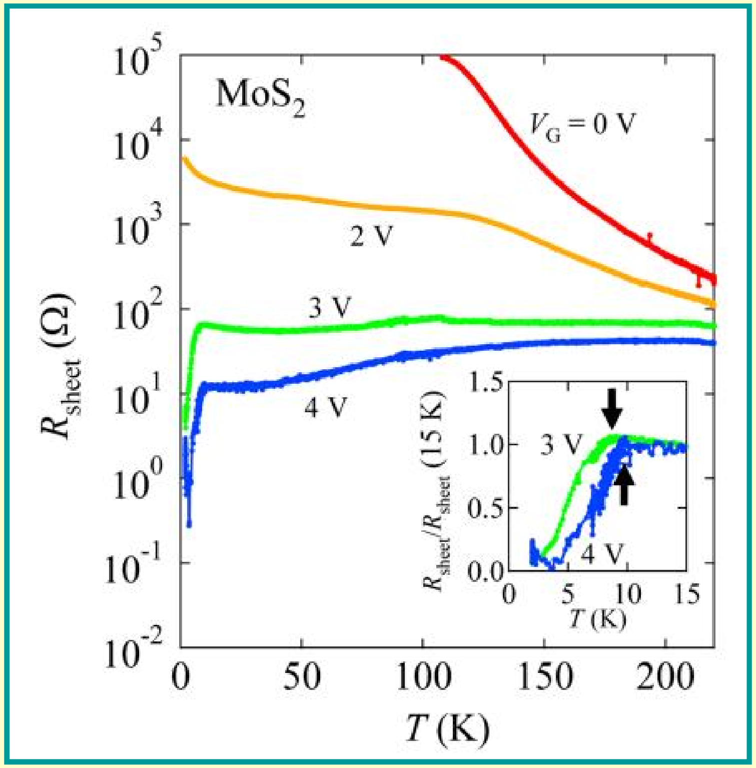


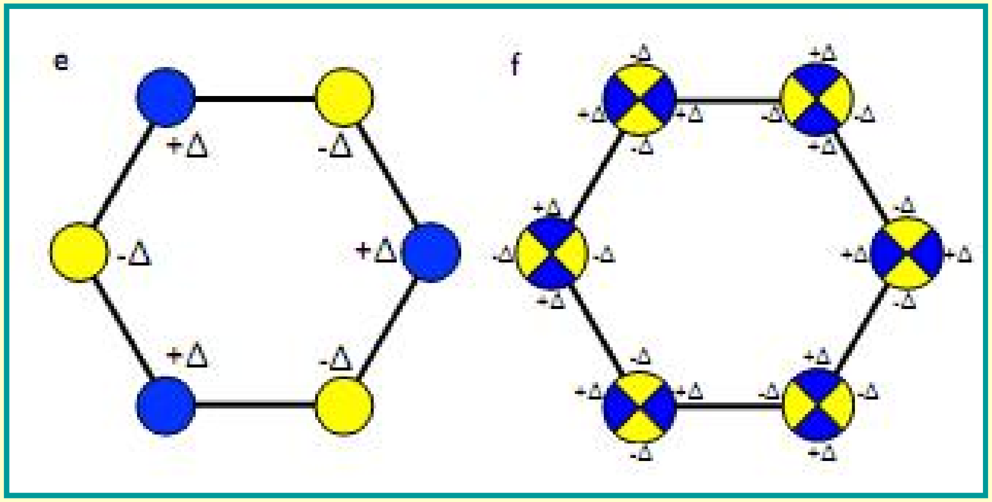
Beritnell, *et al* Science **335**, 947 (2012)

Yoon *et al*, Nano Lett. **11**, 3768 (2011)

Radisavljevic, Nature Nano, **6,** 147 (2011)

Superconductivity





Ztaniguchi *et al*, Appl. Phys. Lett. **101**, 042603 (2012)

Roldan, Cappelluti and Guinea, arXiv: 1301.4836

Outlook

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    Mean-field approach

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    Phase-diagram as function inter-interaction and dielectric constant

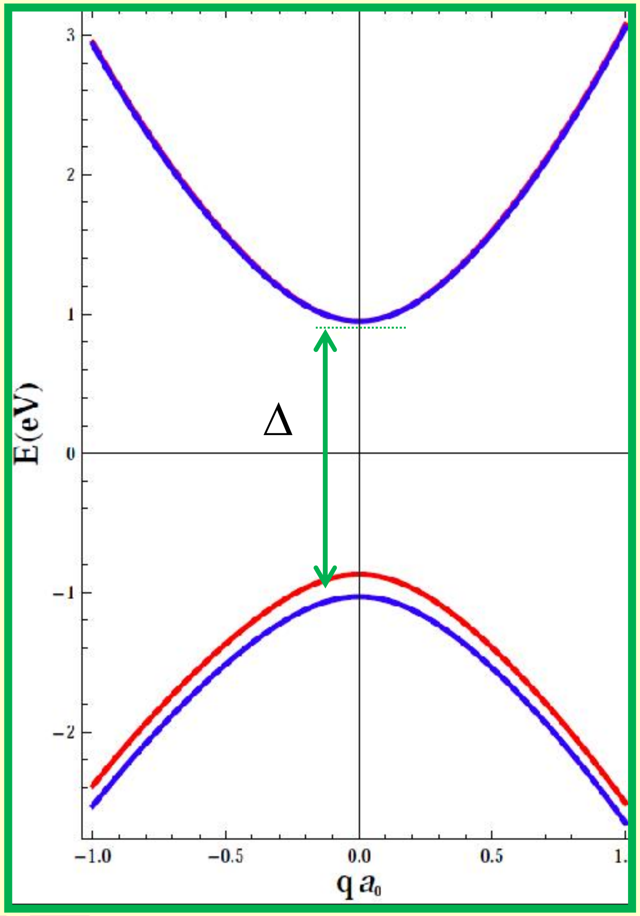
Low energy Field theory

Don't miss a talk given by Rostami today at 17:20

Low-energy Hamiltonian

$$
\begin{aligned}
H_{\tau s} &= \frac{\Delta}{2}\sigma_z + \lambda\tau s\frac{1-\sigma_z}{2} + t_0 a_0 \mathbf{q}\cdot\sigma_\tau \\
&+ \frac{\hbar^2|\mathbf{q}|^2}{4m_0}(\alpha + \beta\sigma_z) \\
&+ t_1 a_0^2 \mathbf{q}\cdot\sigma_\tau^* \sigma_x \mathbf{q}\cdot\sigma_\tau^*,
\end{aligned}
$$

$$
\begin{aligned}
t_0 &= 1.68eV \\
t_1 &= 0.1eV \\
\alpha &= 0.43 \\
\beta &= 2.21
\end{aligned}
$$



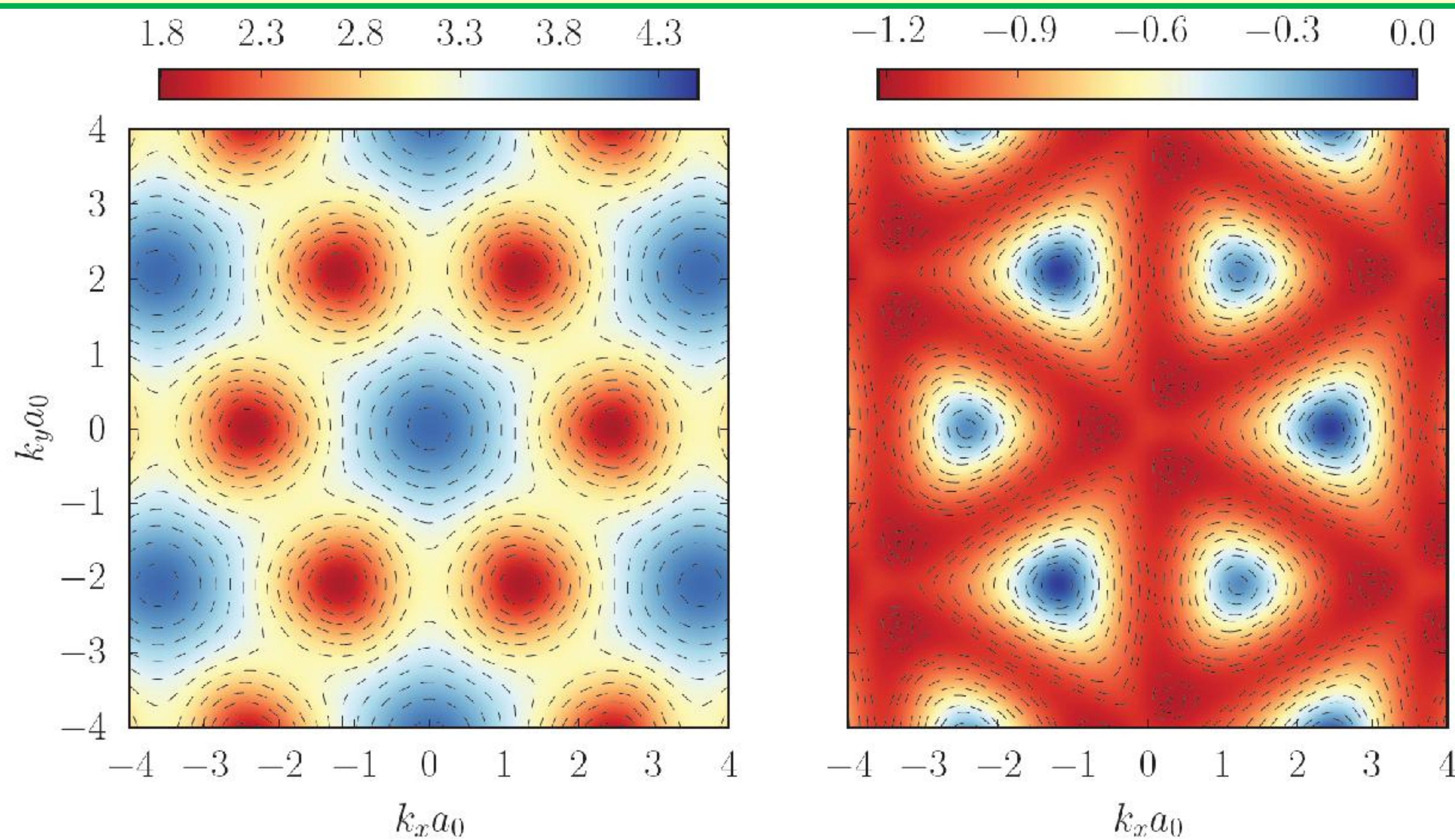
$$\alpha = \frac{m_0}{m_+}$$

$$\beta = \frac{m_0}{m_-} - \frac{4\, m_0 a_0^2 t_0^2}{(\Delta - \lambda)\hbar^2}$$

$$m_\pm = \frac{m_e m_h}{m_h - m_e}$$

Rostami, Moghaddam, Asgari arXiv:1302.5901

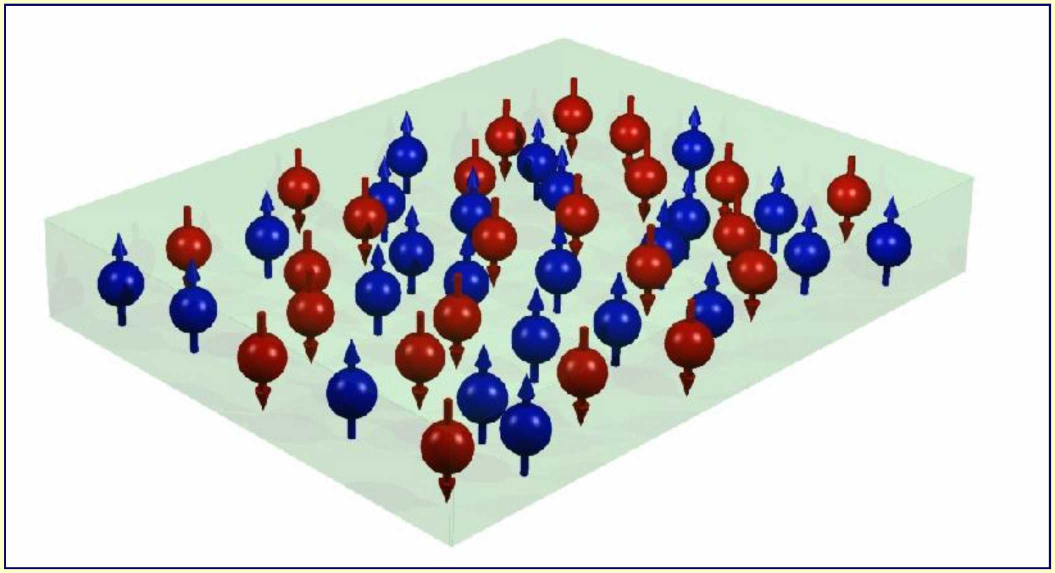
Trigonal Warping (beyond Low energy)



Rostami, Moghaddam, Asgari arXiv:1302.5901

....Ground-state properties...

The quasi-2D electron liquid (jellium)



Coulomb interaction

$$\frac{e^2}{\epsilon_0 r}$$

4 parameters @
zero magnetic field
and
spin-orbit coupling

$$n_{2d}, \epsilon_0, U_{4d}, \xi$$

Low energy model Hamiltonian: MoS_2

$$\mathcal{H}_0 = \sum_{k,\tau,s,\alpha',\beta'} \psi^{\dagger}_{k,\tau,s,\alpha'} \mathcal{H}_{\alpha'\beta'} \psi_{k,\tau,s,\beta'}$$

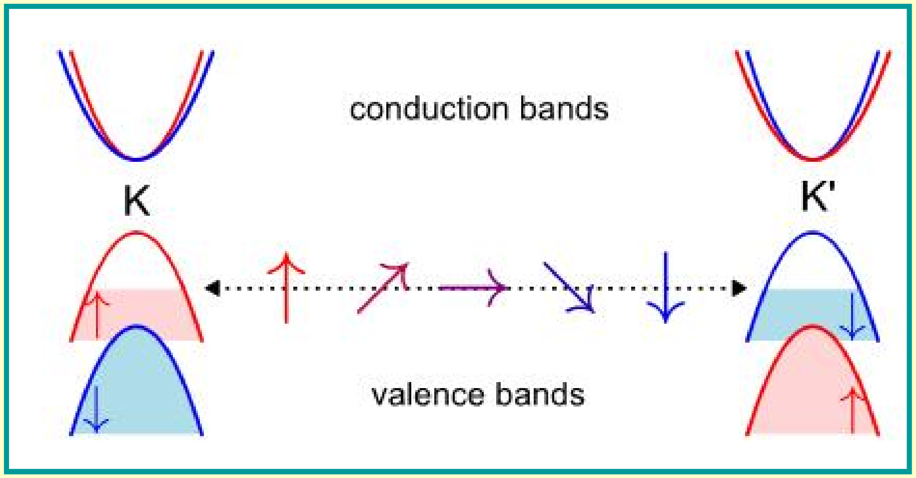
$$\mathcal{H} = \frac{\Delta}{2}\sigma_z + \lambda\tau s \frac{1-\sigma_z}{2} + t_0 a_0 k \cdot \sigma_\tau + \frac{\hbar^2 k^2}{4m_0}(\alpha + \beta\sigma_z)$$

$$U = U_{4d} \times S$$

$$\mathcal{V}_{intra} = \frac{1}{2S} \sum_{kk',\tau s s',\alpha\beta} \sum_{q \neq 0} v_q \psi^{\dagger}_{k-q,\tau s,\alpha} \psi^{\dagger}_{k'+q,\tau s',\beta} \psi_{k',\tau s',\beta} \psi_{k,\tau s,\alpha}$$

$$\mathcal{V}_{inter} = \frac{U}{2S} \sum_{kk'q,\tau s,\alpha\beta} \psi^{\dagger}_{k-q,\tau s,\alpha} \psi^{\dagger}_{k'+q,\bar{\tau}\bar{s},\beta} \psi_{k',\bar{\tau}\bar{s},\beta} \psi_{k,\tau s,\alpha}$$

$$v_q = \frac{2\pi e^2}{\epsilon_0 (q_{TF} + |q|)}$$



$$q_{TF} = \frac{2\pi e^2 D(\varepsilon_F)}{\epsilon_0}$$

Mean-field theory

$$\mathcal{H}_{MF} = \mathcal{H}_0 - \frac{1}{S} \sum_{k,k',\tau,s,\alpha,\beta} \psi^{\dagger}_{k,\tau,s,\alpha} v_{k-k'} \rho_{\alpha\beta}(k', \tau s) \psi_{k,\tau,s,\beta}$$

$$+ \frac{U}{S} \sum_{k,k',\tau,s,\alpha} trace[\rho(k', \tau' s')]\, \psi^{\dagger}_{k,\tau,s,\alpha} \psi_{k,\tau,s,\alpha}$$

$$\rho_{\alpha\beta} = \langle \psi_0 | \psi^{\dagger}_{k,\tau,s,\alpha} \psi_{k,\tau,s,\beta} | \psi_0 \rangle$$

H. Rostami and R. Asgari to be submitted (2013)

Mean-field theory

$$\mathcal{H}_{HF} = B_0^{\tau s}(\mathbf{k})\sigma_0 + \mathbf{B}^{\tau s}(\mathbf{k}) \cdot \boldsymbol{\sigma}_\tau$$

$$B_0^{\tau s}(\mathbf{k}) = \frac{1}{2}\lambda\tau s + \frac{\hbar^2 k^2}{4m_0}\alpha - \frac{1}{2}\int \frac{d^2k'}{(2\pi)^2} v_{k-k'}\{n^c_{k',\tau s} + n^v_{k',\tau s}\} + U\int \frac{d^2k'}{(2\pi)^2}\{n^c_{k'\bar{\tau}\bar{s}} + n^v_{k'\bar{\tau}\bar{s}}\}$$

$$B_z^{\tau s}(\mathbf{k}) = \frac{\Delta - \lambda\tau s}{2} + \frac{\hbar^2 k^2}{4m_0}\beta - \frac{1}{2}\int \frac{d^2k'}{(2\pi)^2} v_{k-k'}\{\frac{(t_0a_0)^2k'^2 - D_+^2}{(t_0a_0)^2k'^2 + D_+^2} n^c_{k',\tau s} + \frac{(t_0a_0)^2k'^2 - D_-^2}{(t_0a_0)^2k'^2 + D_-^2} n^v_{k',\tau s}\}$$

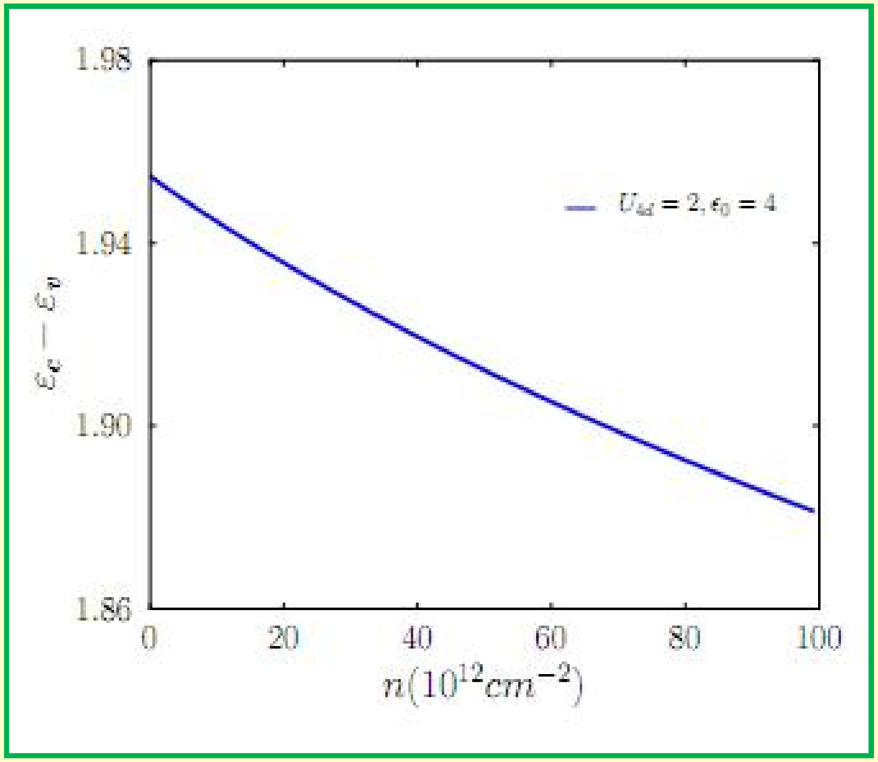
$$B_x^{\tau s}(\mathbf{k}) - iB_y^{\tau s}(\mathbf{k}) = (t_0a_0)k(\cos\phi - i\sin\phi) + \int \frac{d^2k'}{(2\pi)^2} v_{k-k'}\{\frac{(t_0a_0)k'D_+}{(t_0a_0)^2k'^2 + D_+^2} n^c_{k',\tau s} + \frac{(t_0a_0)k'D_-}{(t_0a_0)^2k'^2 + D_-^2} n^v_{k',\tau s}\}(\cos\phi' - i\sin\phi')$$

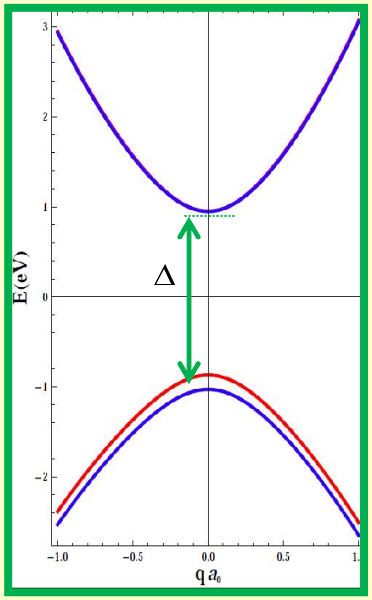
$$D_\pm = \frac{\Delta}{2} + \frac{\hbar^2 k^2}{4m_0}(\alpha + \beta) - E_\pm$$

$$E_\pm = \pm\sqrt{(\frac{\Delta - \lambda\tau s}{2} + \frac{\hbar^2 k^2}{4m_0}\beta)^2 + (t_0a_0)^2k^2} + \frac{1}{2}\lambda\tau s + \frac{\hbar^2 k^2}{4m_0}\alpha$$

$$k_{F\sigma} = k_F(1 + \sigma\xi)^{1/2}$$

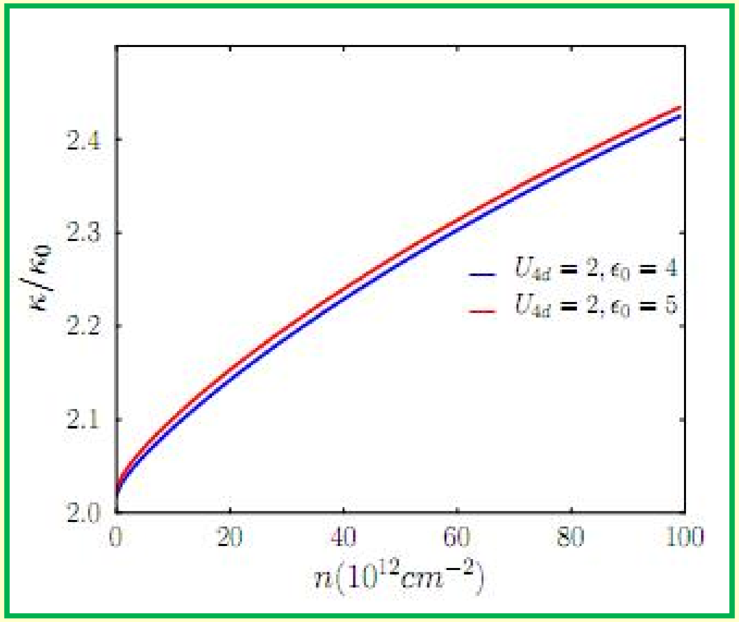
Band-gap renormalization

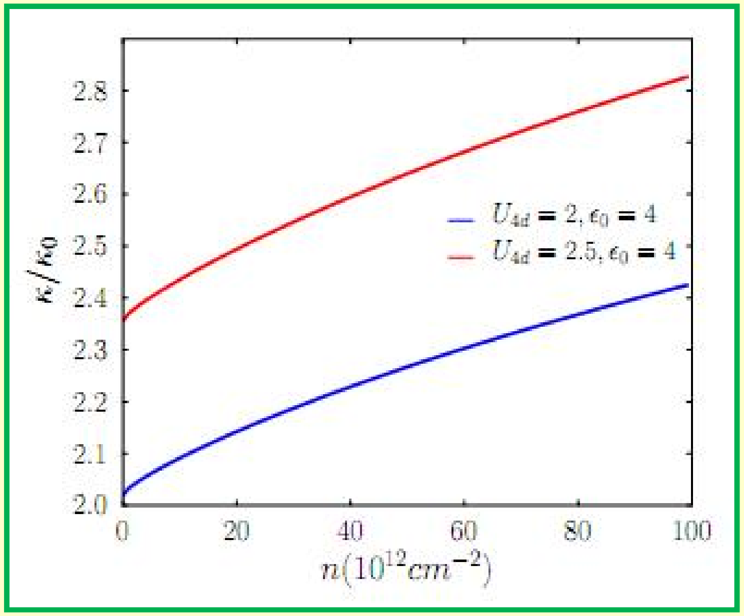




H. Rostami and R. Asgari To be submitted (2013)

Charge compressibility: MoS_2



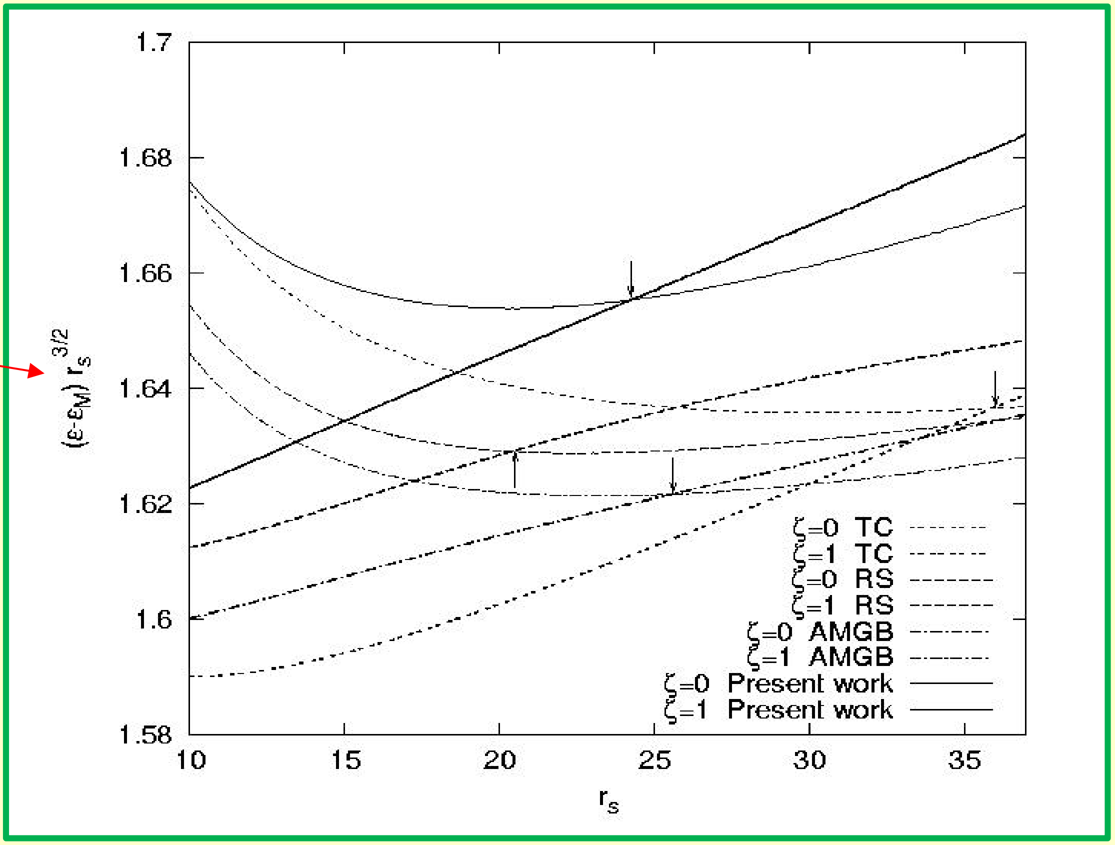


$$\frac{1}{n^2\kappa}=\frac{\partial\mu}{\partial n}$$

H. Rostami and R. Asgari To be submitted (2013)

paramagnetic to fully spin-polarized quantum phase transition of a 2D EG

$r_s a_B = (\pi n)^{-1/2}$



TC: B. Tanatar and D. M. Ceperley, Phys. Rev. B **39**, 5005 (1989)
RS: F. Rapisarda and G. Senatore, Aust. J. Phys. **49**, 161 (1996)
AMGB : C. Attaccalite, *et al.*, Phys. Rev. Lett **88**, 256601 (2002)
Present: R. Asgari, B. Davoudi, M. Tosi, SSC **131**, 301 (2004)

Critical magnetic field: Graphene

$$\frac{B_c}{B_{c0}} = \frac{\sqrt{2}}{2\varepsilon_F}\left\{[(2\varepsilon_F^2+\Delta^2)^{1/2}-\Delta]+2\frac{\partial\delta\varepsilon_{xc}}{\partial\zeta}|_{\zeta=1}\right\}$$

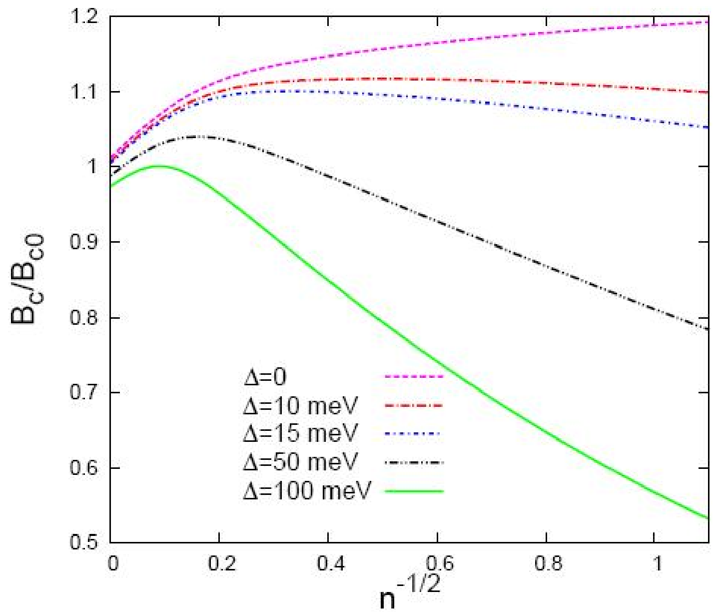


FIG. 2: (color online). Critical magnetic field as a function of inverse square root of density (in units of 10^{-6} cm) for various gap energies.

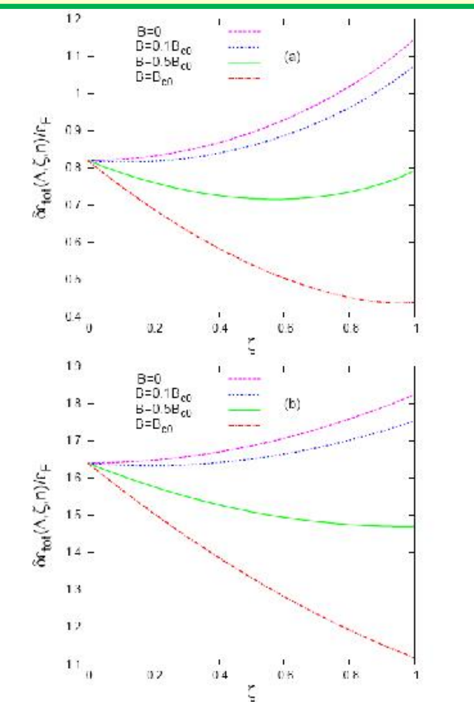
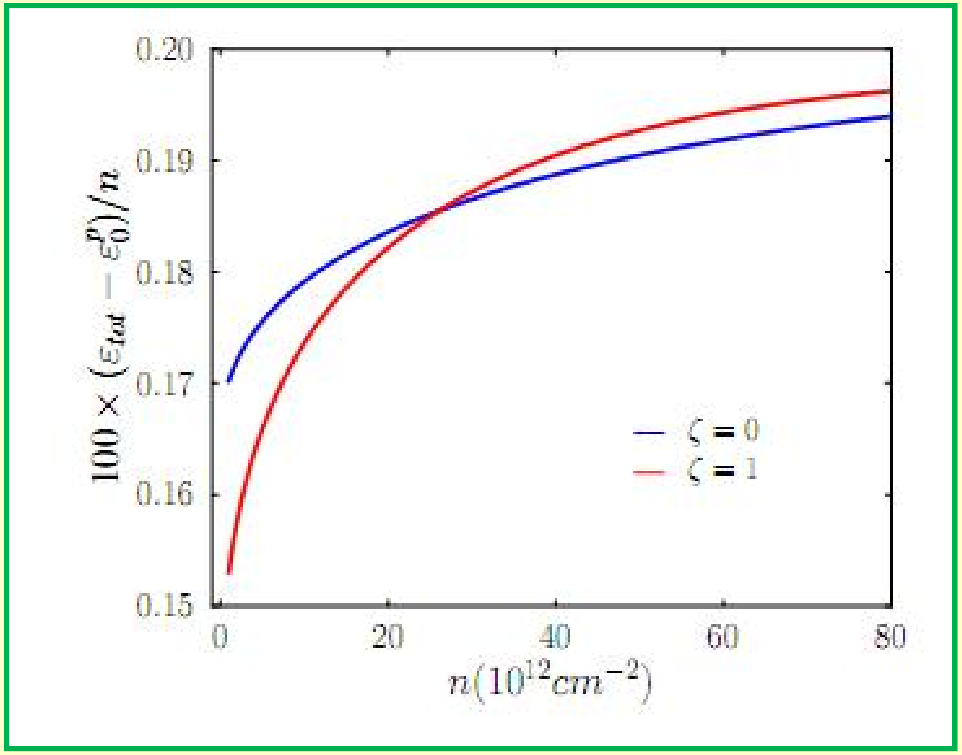


FIG. 3: (color online). Total energy as a function of spin polarization for various magnetic fields for (a): $\Delta = 0$ and (b): $\Delta = 100$meV at $\Lambda = 100$.

$$B_{c0} = \varepsilon_F / \sqrt{2}\mu_B$$

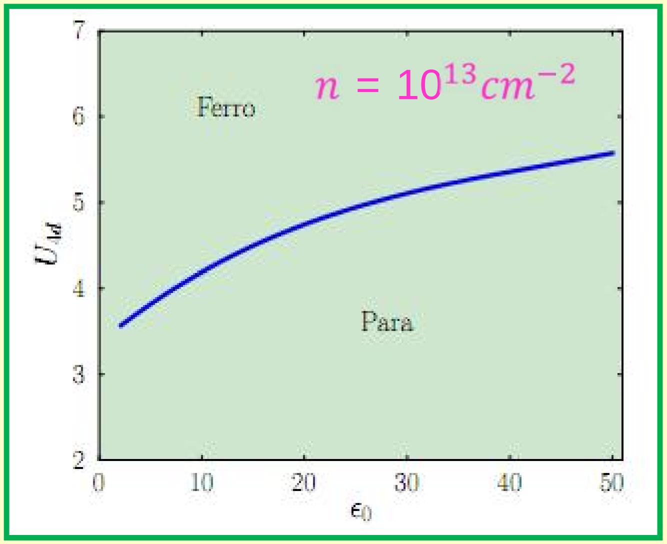
A. Qaiumzadeh & R. Asgari, *Phys. Rev. B* ***80***,035429(2009)

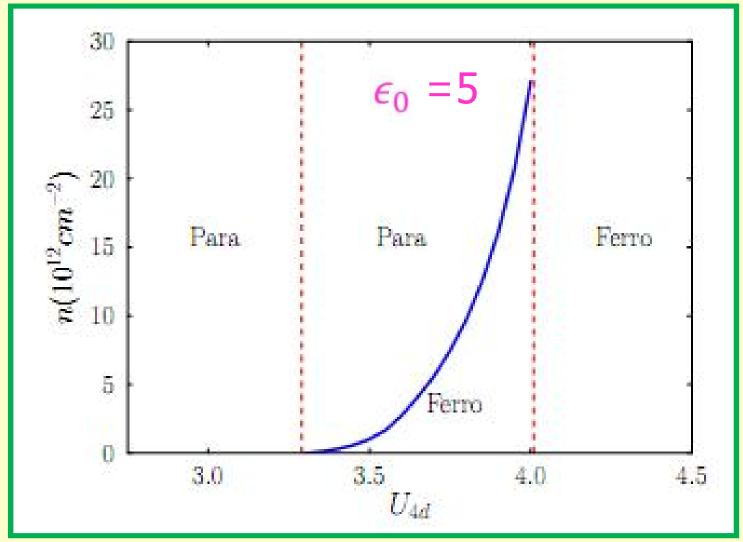
Magnetic phase diagram: MoS_2

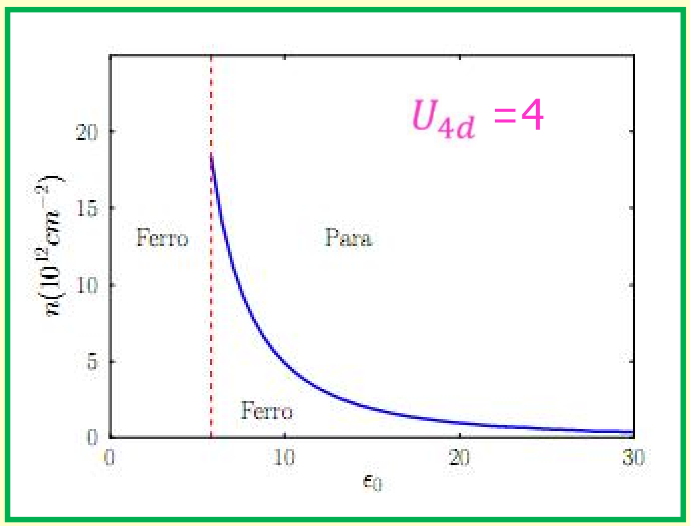


H. Rostami and R. Asgari To be submitted (2013)

Magnetic phase diagram: MoS_2







H. Rostami and R. Asgari To be submitted (2013)

Conclusion

1. Propose an mean-field Hamiltonian.
2. Band gap renormalization due to e-e interactions.
3. Magnetic phase diagram as function of electron density, dielectric constant and the inter-interaction
4. Magnetic phase diagram for a hole-doped system?
5. Phase diagram as a function of gated voltage?

Thanks for your attention