Band structure of magnetic materials

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Outlook

- Introduction to electronic structure theory (tight-binding method)
- Magnetic systems – mean-field approximation
- Electronic structure of selected materials
- Correlation effects

Introduction to electronic structure theory

Reference textbook: A.P. Sutton, Electronic Structure of Materials (Calderon Press, 1993)

Electronic Hamiltonian

$$[T_e + V_{ee} + V_{Ne}]\Psi(\{\vec{r}\}) = E\Psi(\{\vec{r}\})$$

$T_e(\vec{r}) = -\sum_j^N \frac{\hbar^2\nabla_j^2}{2m_j}$ Electrons kinetic Energy

$V_{ee}(\vec{r}) = \frac{1}{2}\sum_{i\neq j}^N \frac{e^2}{r_{ij}}$ Electron-Electron Interaction

$V_{eN}(\vec{r},\vec{R}) = -\frac{1}{2}\sum_{i,I}^{N,M} \frac{e^2 Z_I}{R_{iI}}$ Electron-Nucleus Interaction

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Electronic Hamiltonian

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Electronic Hamiltonian

$$-\frac{\hbar^2\nabla^2}{2m}\psi(\vec{r}) - \frac{1}{2}\sum_{I}^{M}\frac{e^2 Z_I}{r_I}\psi(\vec{r}) = E\psi(\vec{r})$$

Schrödinger equation

$$H(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

Schrödinger equation

$$H(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

$$H(\vec{r})\langle\vec{r}|\psi\rangle = E\langle\vec{r}|\psi\rangle$$

Basis set expansion

$$H(\vec{r})\langle\vec{r}|\psi\rangle = E\langle\vec{r}|\psi\rangle$$

Each state can be expanded onto a complete orthonormal basis set $|\phi_i\rangle$

$$|\psi\rangle = \sum_i^M |\phi_i\rangle\langle\phi_i|\psi\rangle = \sum_i^M c_i|\phi_i\rangle$$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}$$
$$\langle\phi_i|\psi\rangle = c_i$$

Basis set expansion

$$H(\vec{r})\sum_{j}^{M}\langle\vec{r}|\phi_j\rangle\langle\phi_j|\psi\rangle = E\sum_{j}^{M}\langle\vec{r}|\phi_j\rangle\langle\phi_j|\psi\rangle$$

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If I now multiply both side by $\langle\phi_i|\vec{r}\rangle = \phi_i^*(\vec{r})$ and take $\int d\vec{r}$

$$\sum_{j=1}^{M}\Big[\int d\vec{r}\phi_i^*(\vec{r})H(\vec{r})\phi_j((\vec{r})\Big]c_j = E\sum_{j=1}^{M}c_j\Big[\int d\vec{r}\phi_i^*(\vec{r})\phi_j((\vec{r})\Big]$$

Basis set expansion

$$H(\vec{r})\sum_{j}^{M}\langle\vec{r}|\phi_j\rangle\langle\phi_j|\psi\rangle = E\sum_{j}^{M}\langle\vec{r}|\phi_j\rangle\langle\phi_j|\psi\rangle$$

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$$\sum_{j=1}^{M}\underbrace{\Big[\int d\vec{r}\phi_i^*(\vec{r})H(\vec{r})\phi_j((\vec{r})\Big]}_{\langle\phi_i|H|\phi_j\rangle}c_j = E\sum_{j=1}^{M}c_j\underbrace{\Big[\int d\vec{r}\phi_i^*(\vec{r})\phi_j((\vec{r})\Big]}_{\langle\phi_i|\phi_j\rangle}$$

Basis set expansion

$$\sum_{j=1}^{M} \underbrace{\left[\int d\vec{r}\phi_i^*(\vec{r})H(\vec{r})\phi_j((\vec{r})\right]}_{H_{ij}} c_j = E \sum_{j=1}^{M} c_j \underbrace{\left[\int d\vec{r}\phi_i^*(\vec{r})\phi_j((\vec{r})\right]}_{\delta_{ij}}$$

Schrödinger matrix equation

$$\sum_{j=1}^{M} H_{ij} c_j = E c_i$$

Schrödinger matrix equation

$$\mathbb{H}\mathbb{C} = E\mathbb{1}\mathbb{C}$$

$$\mathbb{H} = \begin{vmatrix} H_{11} & H_{12} & \dots & H_{1M} \\ H_{21} & H_{22} & \dots & H_{2M} \\ \dots & \dots & \dots & \dots \\ H_{M1} & H_{M2} & \dots & H_{MM} \end{vmatrix} \qquad \mathbb{C} = \begin{vmatrix} c_1 \\ c_2 \\ \dots \\ c_M \end{vmatrix}$$

Schrödinger matrix equation

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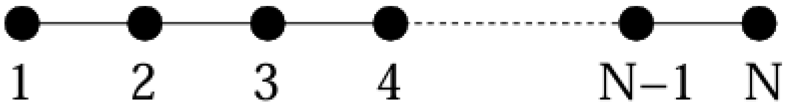
Basis set: **atomic orbitals**

Example: chain of H atoms



Basis orbital: 1s orbital

$$H_{ij} = \begin{cases} \epsilon_0 & \text{if} \quad i = j \\ \gamma & \text{if} \quad j = i \pm 1 \\ 0 & \text{elsewhere} \end{cases}$$

"on-site" energy

"hopping" parameter

$\gamma < 0$

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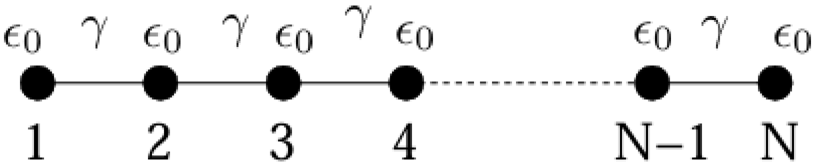

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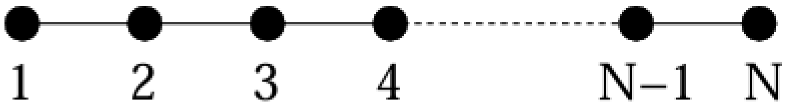

$$\begin{pmatrix} \epsilon_0 & \gamma & 0 & \dots & \dots \\ \gamma & \epsilon_0 & \gamma & \dots & \dots \\ 0 & \gamma & \epsilon_0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \dots \\ \psi_n \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \dots \\ \psi_n \end{pmatrix}$$

Python code


```
import numpy as np
import matplotlib.pyplot as plt

N = 20
epsilon = 0
t = -1

def diagonalize_H(N):

    diag_main = np.full(N, epsilon)  # Main diagonal
    diag_off = np.full(N - 1, t)  # Off-diagonal elements
    # Construct the Hamiltonian matrix (tridiagonal)
    H = np.zeros((N, N))  # Hamiltonian matrix

    # Fill the main diagonal (kinetic + potential energy)
    for i in range(N):
        H[i, i] = diag_main[i]

    # Fill the off-diagonal elements (kinetic energy part)
    for i in range(N - 1):
        H[i, i + 1] = diag_off[i]  # Upper diagonal
        H[i + 1, i] = diag_off[i]  # Lower diagonal


    # Solve the eigenvalue problem
    eigenvalues, eigenvectors = np.linalg.eigh(H)

    return eigenvalues, eigenvectors

eigenvalues, eigenvectors = diagonalize_H(N)

print("Eigenenergies")
print(eigenvalues)
```

Python code


```python
from scipy.linalg import eigh_tridiagonal
import matplotlib.pyplot as plt

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    eigenvalues, eigenvectors = eigh_tridiagonal(diag_main, diag_off)

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```

H_2 model ion

$$\begin{pmatrix} \epsilon_0 & \gamma \\ \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

H_2 model ion

$$\begin{pmatrix} \epsilon_0 & \gamma \\ \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

We have non-trivial solution only if:

$$\det \begin{pmatrix} \epsilon_0 - E & \gamma \\ \gamma & \epsilon_0 - E \end{pmatrix} = 0$$

$$(\epsilon_0 - E)^2 - \gamma^2 = 0$$

H_2 model ion

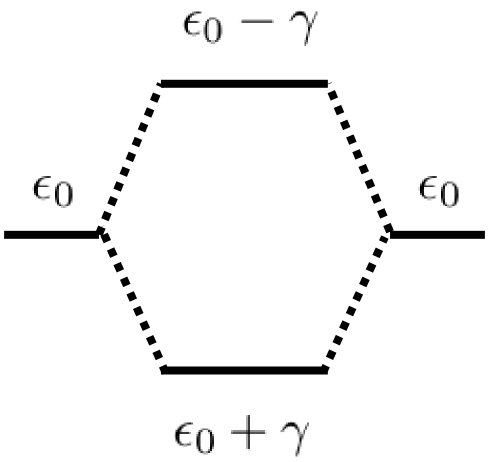
So we have two solutions:

$$\boxed{\begin{array}{c} E_{\mathrm{bond}} = \epsilon_0 + \gamma \\ \text{and} \\ \\ E_{\mathrm{anti}} = \epsilon_0 - \gamma \end{array}}$$

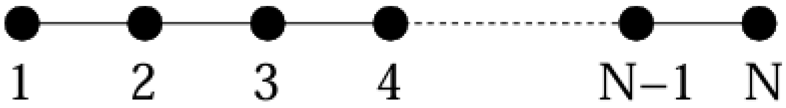
with corresponding eigenvectors

$$\Psi_{\mathrm{bond}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \Psi_{\mathrm{anti}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

H_2 model ion



Chain of H atoms



$$\begin{pmatrix} \epsilon_0 & \gamma & 0 & \dots & \dots \\ \gamma & \epsilon_0 & \gamma & \dots & \dots \\ 0 & \gamma & \epsilon_0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \gamma & \epsilon_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \dots \\ \psi_n \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \dots \\ \psi_n \end{pmatrix}$$

Chain of H atoms

Finally we have obtained the spectrum of the H_N molecule

$$E_m = \epsilon_0 + 2\gamma \cos\left(\frac{m\pi}{N+1}\right) \qquad m = 1, 2 \ldots N$$

and its eigenvalues $|\psi^m\rangle = \sum_j^N \psi_j^m |j\rangle$ where

$$\psi_j^m = \left(\frac{2}{N+1}\right)^{1/2} \sin\left(\frac{m\pi}{N+1} j\right)$$

Chain of H atoms

$\underline{N=2}$

$$E_m = \epsilon_0 + 2\gamma\cos\left(\frac{m\pi}{3}\right) \rightarrow \begin{cases} E_1 = \epsilon_0 + \gamma \\ E_2 = \epsilon_0 - \gamma \end{cases}$$

$$\psi_j^m = \left(\frac{2}{3}\right)^{1/2} \sin\left(\frac{m\pi}{3} j\right) \rightarrow \begin{cases} \psi_j^1 = 1/\sqrt{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \psi_j^2 = 1/\sqrt{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{cases}$$

Chain of H atoms

$N \to \infty$

This means that both N and $m \to \infty$ however:

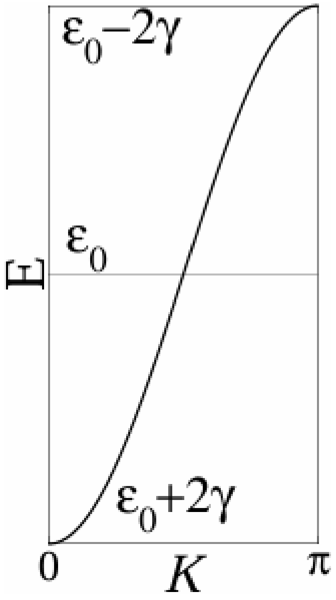
$$K = \frac{m\pi}{N+1} = \pi \frac{m}{N} \frac{1}{1+1/N} \to \pi \frac{m}{N}$$

so

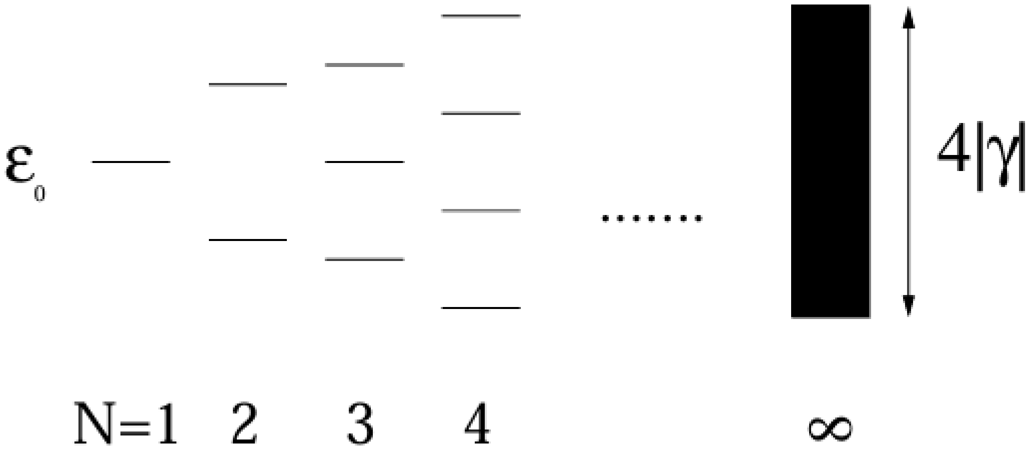
$$E_m \to E_K = \epsilon_0 + 2\gamma \cos K \quad \text{with} \quad 0 < K < \pi$$

This is called **energy band** or also **dispersion relation**. In this case:

$$E_{m+1} - E_m \to 0 \quad \text{and} \quad \Delta = E_\infty - E_0 = 4|\gamma|$$



From atomic levels to bands



Density of states

DOS is the *number of states* S *per unit energy* E

$$D(E) = \frac{\mathrm{d}S}{\mathrm{d}E} = \frac{\mathrm{d}S}{\mathrm{d}k} \cdot \left| \frac{\mathrm{d}k}{\mathrm{d}E} \right|$$

Density of states

$$E_k = \epsilon_0 + 2\gamma \cos ka, \quad k = \frac{2m\pi}{Na}$$

$$\frac{\mathrm{d}S}{\mathrm{d}k} = 2 \cdot \frac{Na}{2\pi} = \frac{Na}{\pi}$$

$$\frac{\mathrm{d}E_k}{\mathrm{d}k} = 2a\gamma \sin ka$$

Density of states

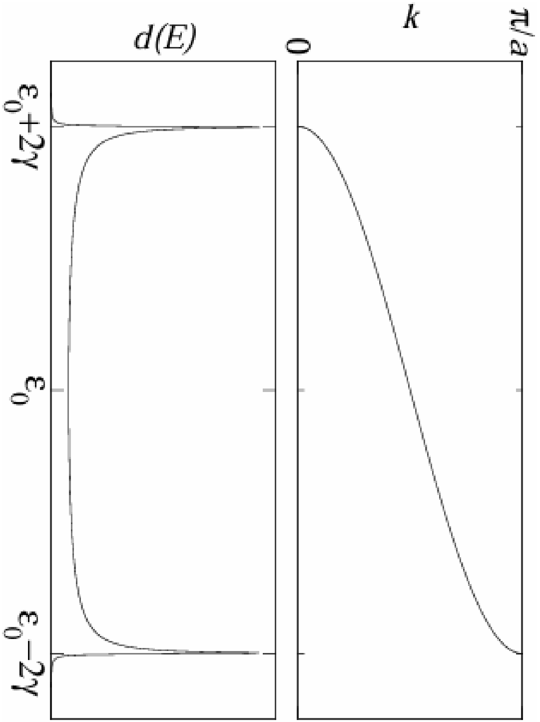
$$E_k = \epsilon_0 + 2\gamma \cos ka, \qquad k = \frac{2m\pi}{Na}$$

$$\frac{\mathrm{d}S}{\mathrm{d}k} = 2 \cdot \frac{Na}{2\pi} = \frac{Na}{\pi}$$

$$D(E) = \frac{Na}{\pi} \frac{1}{2a\gamma \sin ka} = \frac{N}{\pi} \frac{1}{[4\gamma^2 - (E - \epsilon_0)^2]^{1/2}}$$

$$\frac{\mathrm{d}E_k}{\mathrm{d}k} = 2a\gamma \sin ka$$

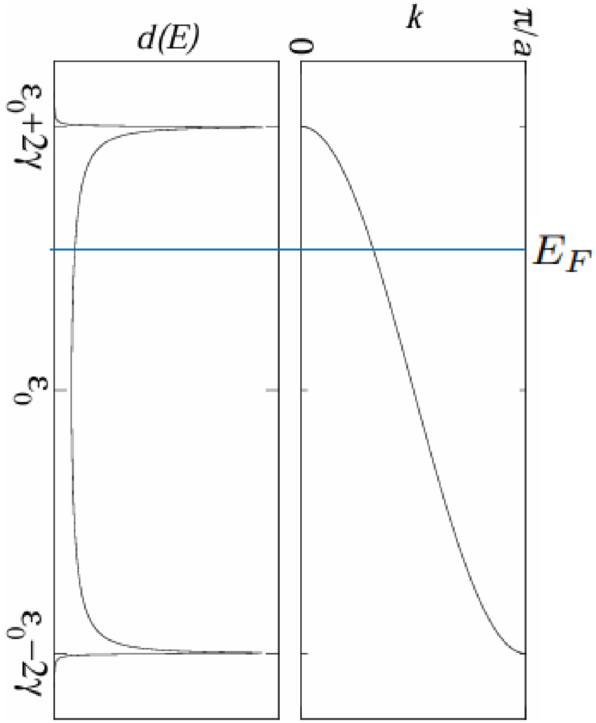
Density of states



Density of states

Number of electrons at zero temperature:

$$N = \int_{-\infty}^{E_F} dE\, D(E)$$



Bloch theorem

The eigenfunctions of a one-particle Hamiltonian with the translation periodicity of a lattice

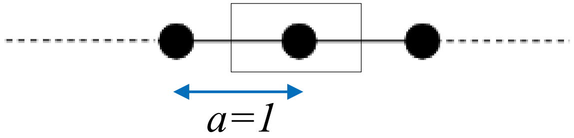
$$H(\vec{r}) = H(\vec{r}+\vec{T})$$

is periodic up to a phase:

$$\psi(\vec{r}+\vec{T}) = e^{i\vec{k}\vec{T}}\psi(\vec{r})$$

$\vec{T}$ translation vector defining a lattice

Bloch theorem



$$T = na$$

$$\psi(x) = \sum_j^N \psi_j \langle x | j \rangle$$

$$\boxed{\psi_j = A e^{iKj}}$$

Bloch theorem

$$H|\psi\rangle = E|\psi\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{j}^{N} \mathrm{e}^{iKj} |j\rangle$$

Bloch theorem

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{j}^{N} \mathrm{e}^{iKj} |j\rangle$$

$$\sum_{j}^{N} \mathrm{e}^{iKj} H |j\rangle = E \sum_{j}^{N} \mathrm{e}^{iKj} |j\rangle$$

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$$\sum_{j}^{N} \mathrm{e}^{iKj} H |j\rangle = E \sum_{j}^{N} \mathrm{e}^{iKj} |j\rangle$$

$$\sum_{j}^{N} \mathrm{e}^{iKj} \langle l | H | j\rangle = E \sum_{j}^{N} \mathrm{e}^{iKj} \langle l | j\rangle$$

Bloch theorem

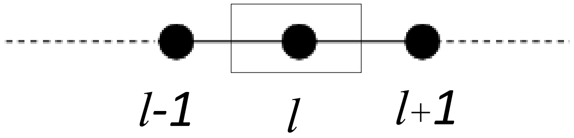
$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_j^N \mathrm{e}^{iKj} |j\rangle$$

$$\sum_j^N \mathrm{e}^{iKj} H|j\rangle = E \sum_j^N \mathrm{e}^{iKj} |j\rangle$$

$$\sum_j^N \mathrm{e}^{iKj} \langle l|H|j\rangle = E \sum_j^N \mathrm{e}^{iKj} \langle l|j\rangle$$

$$\boxed{E_K = \sum_j^N \mathrm{e}^{iK(j-l)} \langle l|H|j\rangle}$$

Bloch theorem: chain of H atoms



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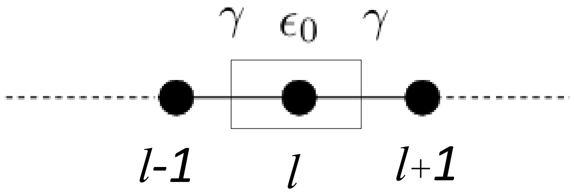

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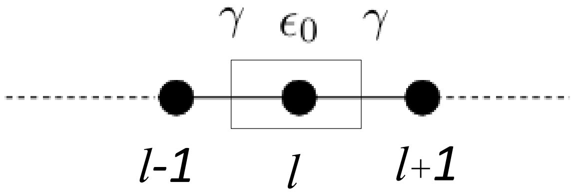
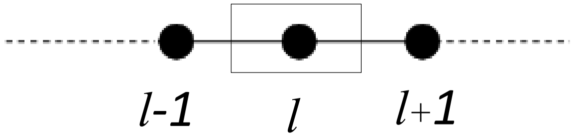


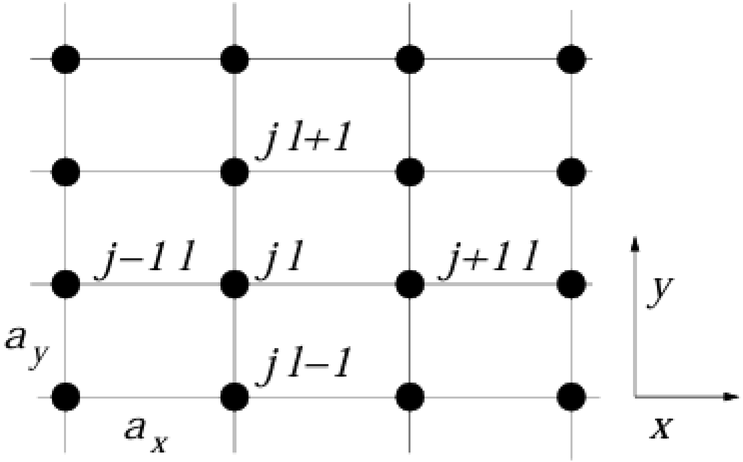
$$E_K = e^{-iK}\gamma + \epsilon_0 + e^{iK}\gamma$$

Bloch theorem: chain of H atoms



$$E_K = \epsilon_0 + 2\gamma \cos K$$

Bloch theorem: square H lattice

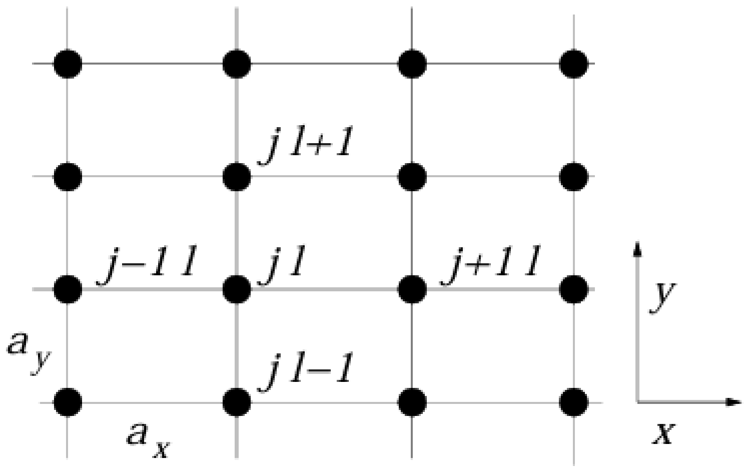


Bloch theorem: square lattice

$$|\psi_{\vec{k}}\rangle = \frac{1}{N^{1/2}} \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot\vec{R}} |\vec{R}\rangle$$

$$E(\vec{k}) = \sum_{\vec{R}} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} \langle \vec{R}' | H | \vec{R} \rangle$$

Bloch theorem: square lattice



$$\langle \vec{R}'|H|\vec{R}'\rangle = \epsilon_0$$

$$\langle \vec{R}'|H|\vec{R}' + (0, a_y)\rangle = \gamma_y$$

$$\langle \vec{R}'|H|\vec{R}' + (0, -a_y)\rangle = \gamma_y$$

$$\langle \vec{R}'|H|\vec{R}' + (a_x, 0)\rangle = \gamma_x$$

$$\langle \vec{R}'|H|\vec{R}' + (-a_x, 0)\rangle = \gamma_x$$

Bloch theorem: square lattice

$$(E - \epsilon_0) + \gamma_x(\mathrm{e}^{ik_x a_x} + \mathrm{e}^{-ik_x a_x}) + \gamma_y(\mathrm{e}^{ik_y a_y} + \mathrm{e}^{-ik_y a_y}) = 0$$

$$\boxed{E = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)}$$

Bloch theorem: square lattice

$$\boxed{E = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)}$$

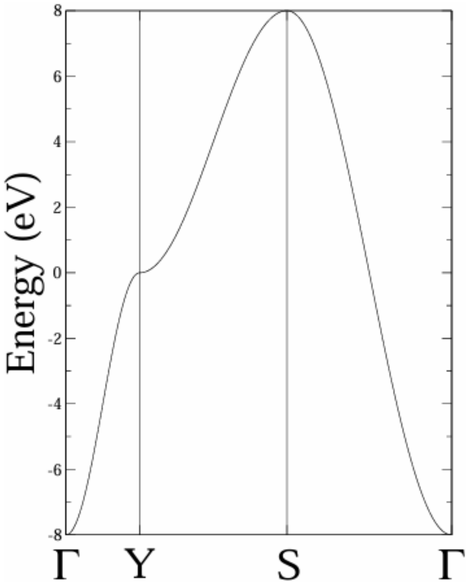
$$-\pi/a_x < k_x < \pi/a_x$$

$$-\pi/a_y < k_y < \pi/a_y$$

Bloch theorem: square H lattice

$$(k_x, k_y) = (0,0) \rightarrow (0, \pi/a_y) \rightarrow (\pi/a_x, \pi/a_y) \rightarrow (0,0)$$

$$(k_x, k_y) = \Gamma \rightarrow Y \rightarrow S \rightarrow \Gamma$$



$\epsilon_0 = 0$
$\gamma_x = -2$
$\gamma_y = -2$

Multi-orbital models

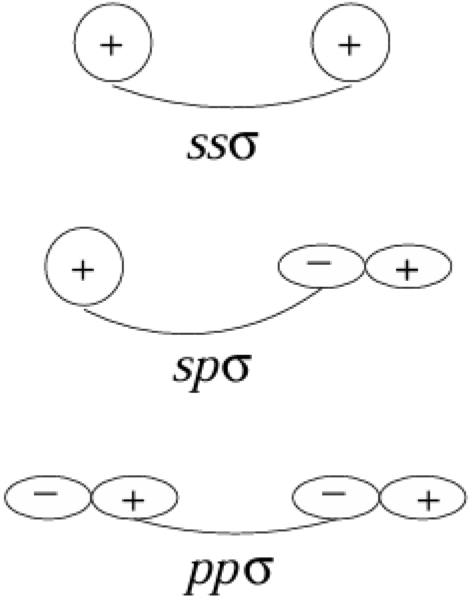
$$|\psi\rangle = \sum_j^N \sum_\alpha^{N_\alpha} \psi_{j\alpha} |j\alpha\rangle$$

$$\psi_{j\alpha} = A_\alpha \mathrm{e}^{iKj}$$

$$\sum_j^N \sum_\alpha^{N_\alpha} A_\alpha \mathrm{e}^{iKj} \langle l\beta | H | j\alpha\rangle = E \sum_j^N \sum_\alpha^{N_\alpha} A_\alpha \mathrm{e}^{iKj} \langle l\beta | j\alpha\rangle$$

sp model

1d atomic chain



Note that:

sp model

$$E\begin{pmatrix} A_s \\ A_p \end{pmatrix} = \left[\begin{pmatrix} \epsilon_s & 0 \\ 0 & \epsilon_p \end{pmatrix} + \right.$$

$$\left. + \begin{pmatrix} \gamma_{ss\sigma} & \gamma_{sp\sigma} \\ -\gamma_{sp\sigma} & \gamma_{pp\sigma} \end{pmatrix} \mathrm{e}^{iK} + \begin{pmatrix} \gamma_{ss\sigma} & -\gamma_{sp\sigma} \\ \gamma_{sp\sigma} & \gamma_{pp\sigma} \end{pmatrix} \mathrm{e}^{-iK}\right] \begin{pmatrix} A_s \\ A_p \end{pmatrix}$$

sp model

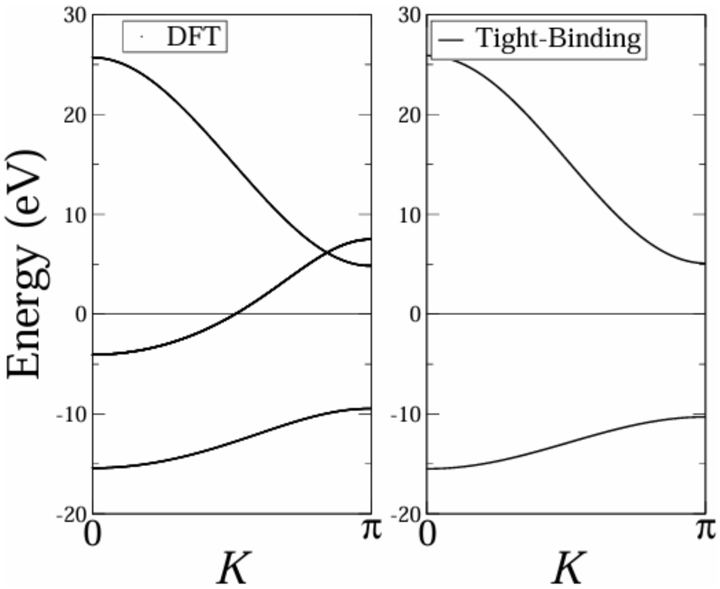
$$\left(\begin{array}{cc} \epsilon_s + 2\gamma_{ss\sigma}\cos K & 2i\gamma_{sp\sigma}\sin K \\ -2i\gamma_{sp\sigma}\sin K & \epsilon_p + 2\gamma_{pp\sigma}\cos K \end{array}\right)\left(\begin{array}{c} A_s \\ A_p \end{array}\right) = E\left(\begin{array}{c} A_s \\ A_p \end{array}\right)$$

sp model

$$E = \frac{1}{2}\left[\epsilon_s(K) + \epsilon_p(K) \pm \sqrt{[\epsilon_s(K) - \epsilon_p(K)]^2 + 16\gamma_{sp\sigma}\sin^2 K}\right]$$

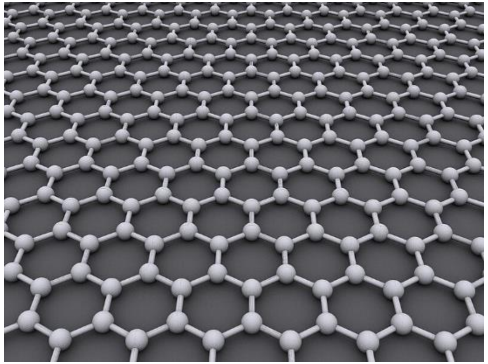
$$\epsilon_s(K) = \epsilon_s + 2\gamma_{ss\sigma}\cos K$$
$$\epsilon_p(K) = \epsilon_p + 2\gamma_{pp\sigma}\cos K$$

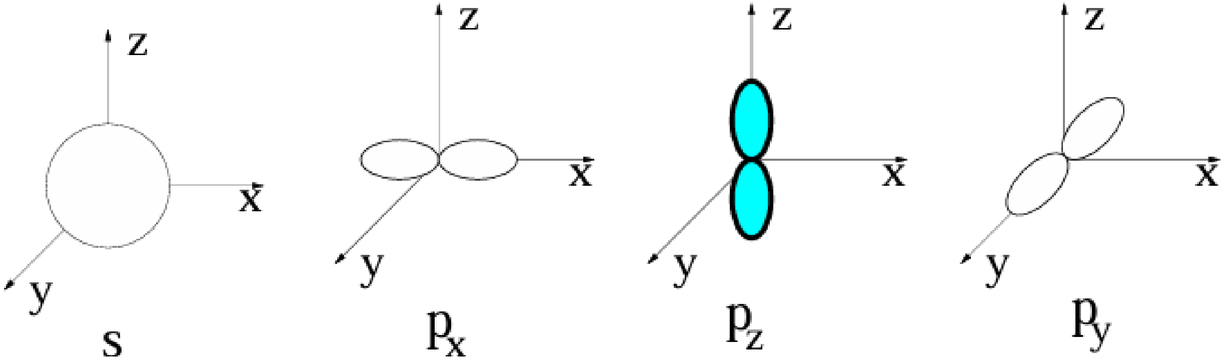
Graphene



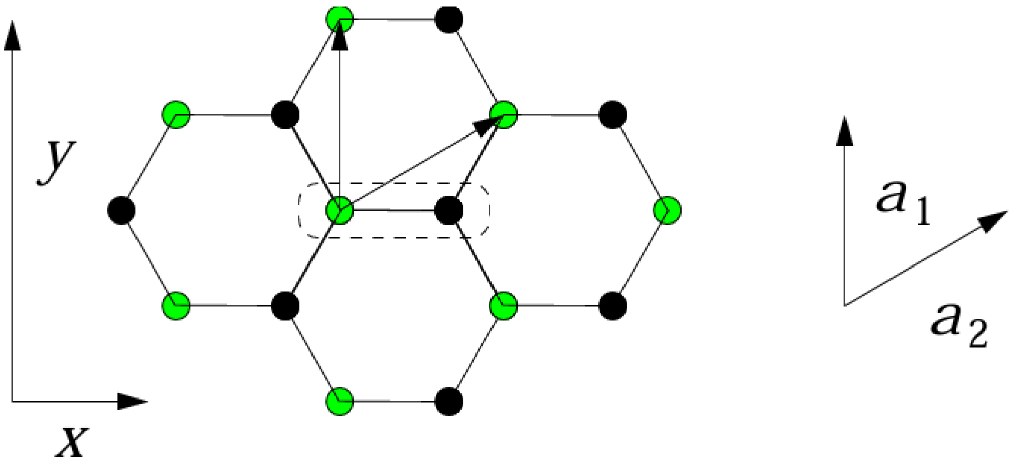
ϵ_s =-12.9 eV, ϵ_p =15.5 eV, $\gamma_{ss\sigma}$ =-1.3 eV, $\gamma_{pp\sigma}$ =5.2 eV, $\gamma_{sp\sigma}$ =0,5 eV

Graphene





Graphene



$$\begin{cases} \vec{a}_1 = a_0\,\hat{y} \\ \vec{a}_2 = a_0\,\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) \end{cases}$$

Graphene

Since we have two atoms in the cell a better choice of basis is $|\vec{R}\, n\rangle$:

$$|\psi_{\vec{k}}\rangle = \frac{1}{N^{1/2}} \sum_{\vec{R}} \sum_{n=1}^{2} \mathrm{e}^{i\vec{k}\cdot\vec{R}} A_n^{\vec{k}} |\vec{R}\, n\rangle$$

where $|\vec{R}\, n\rangle$ represents an atom n (n=1 for green atoms, n=2 for black atoms) belonging to the cell located at $\vec{R}$. We assume an orthogonal basis set.

Graphene

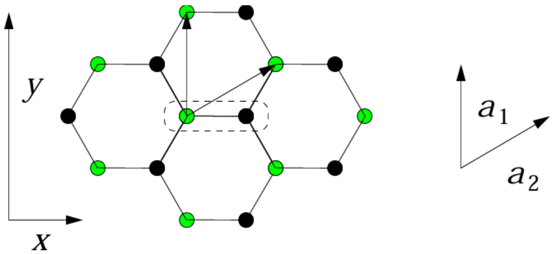
$$E(\vec{k})A^{\vec{k}}_{n'} = \sum_{\vec{R}} \sum_{n}^{2} \mathrm{e}^{i\vec{k}\cdot(\vec{R}-\vec{R}')} A^{\vec{k}}_{n} \langle \vec{R}'\, n' | H | \vec{R}\, n \rangle$$

Graphene

On-site energy: coupling with the primitive cell

$$\langle \vec{R}'\, n' | H | \vec{R}'\, n \rangle = \begin{pmatrix} \epsilon_p & \gamma_{pp\pi} \\ \gamma_{pp\pi} & \epsilon_p \end{pmatrix}$$

The phase factor is $e^{i\vec{k}\cdot(\vec{R}'-\vec{R}')} = 1$

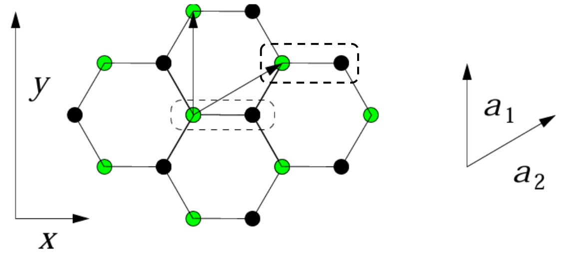


Graphene

1. Cell $\vec{a}_2$

$$\langle \vec{R}'\, n' | H | \vec{R}' + \vec{a}_2\, n \rangle = \begin{pmatrix} 0 & 0 \\ \gamma_{pp\pi} & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2-\vec{R}')} = \mathrm{e}^{i\vec{k}\cdot\vec{a}_2}$

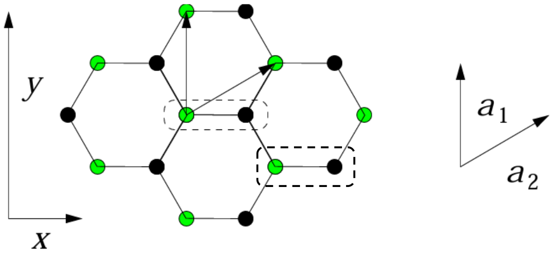


Graphene

2. Cell $\vec{a}_2 - \vec{a}_1$

$$\langle \vec{R}'\, n' | H | \vec{R}' + \vec{a}_2 - \vec{a}_1\, n \rangle = \begin{pmatrix} 0 & 0 \\ \gamma_{pp\pi} & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'+\vec{a}_2-\vec{a}_1-\vec{R}')} = \mathrm{e}^{i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)}$

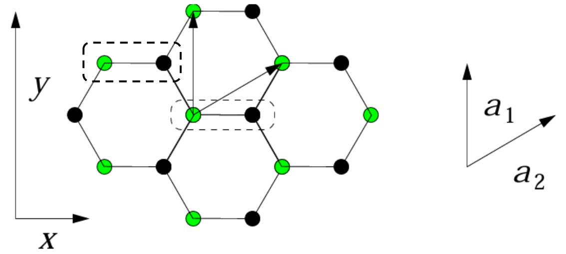


Graphene

3. Cell $-\vec{a}_2$

$$\langle \vec{R}'\, n' | H | \vec{R}' - \vec{a}_2\, n \rangle = \begin{pmatrix} 0 & \gamma_{pp\pi} \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2-\vec{R}')} = \mathrm{e}^{-i\vec{k}\cdot\vec{a}_2}$

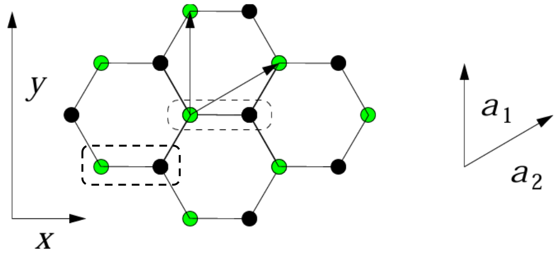


Graphene

4. Cell $-\vec{a}_2 + \vec{a}_1$

$$\langle \vec{R}'\, n' | H | \vec{R}' - \vec{a}_2 + \vec{a}_1\, n \rangle = \begin{pmatrix} 0 & \gamma_{pp\pi} \\ 0 & 0 \end{pmatrix}$$

The phase factor is $\mathrm{e}^{i\vec{k}\cdot(\vec{R}'-\vec{a}_2+\vec{a}_1-\vec{R}')} = \mathrm{e}^{-i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)}$



Graphene

$$E(\vec{k})\Psi_{\vec{k}} = \begin{pmatrix} \epsilon_p & \gamma_{pp\pi}\, f(\vec{k}) \\ \gamma_{pp\pi}\, f(\vec{k})^* & \epsilon_p \end{pmatrix} \Psi_{\vec{k}}$$

where:

$$\Psi_{\vec{k}} = \begin{pmatrix} A_1^{\vec{k}} \\ A_2^{\vec{k}} \end{pmatrix}$$

$$f(\vec{k}) = 1 + \mathrm{e}^{-i\vec{k}\cdot\vec{a}_2} + \mathrm{e}^{-i\vec{k}\cdot(\vec{a}_2-\vec{a}_1)} = 1 + 2\,\mathrm{e}^{-ik_x\frac{\sqrt{3}}{2}a_0}\cos(\frac{k_y}{2}a_0)$$

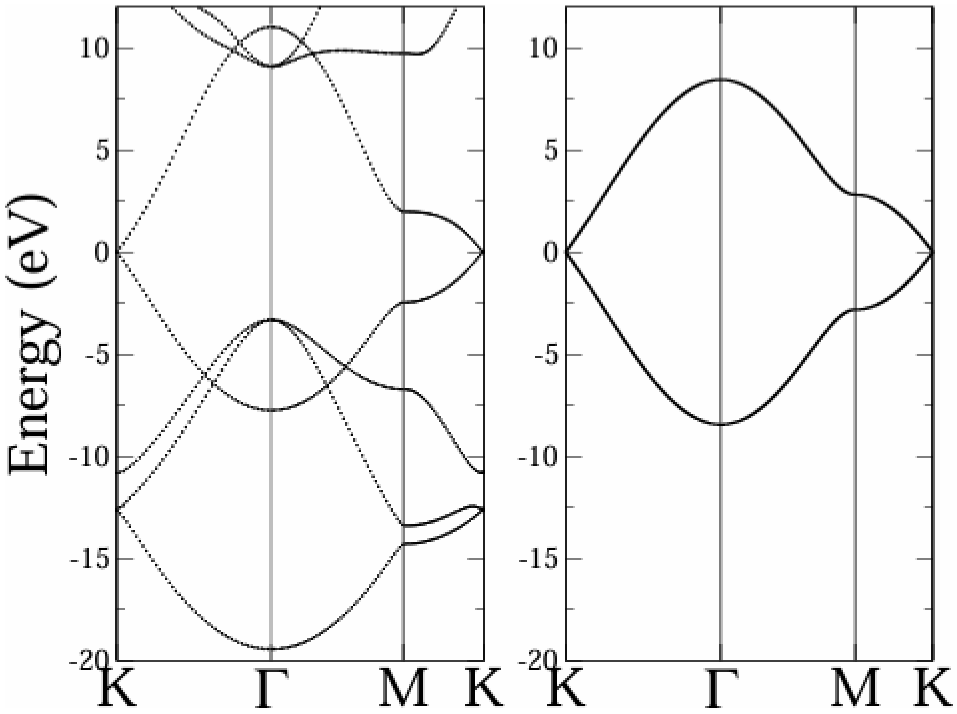
Graphene

$$\det \begin{pmatrix} \epsilon_p - E(\vec{k}) & \gamma_{pp\pi}\, f(\vec{k}) \\ \gamma_{pp\pi}\, f(\vec{k})^* & \epsilon_p - E(\vec{k}) \end{pmatrix} = 0$$

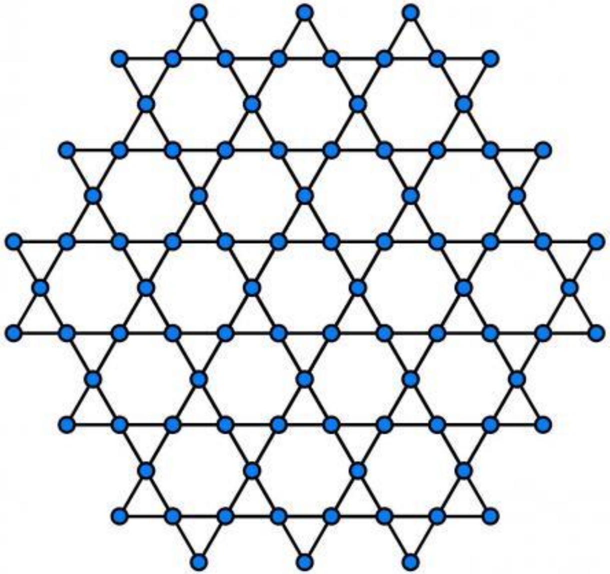
$$E(\vec{k}) = \epsilon_p \pm \gamma_{pp\pi} \sqrt{f(\vec{k}) f(\vec{k})^*}$$

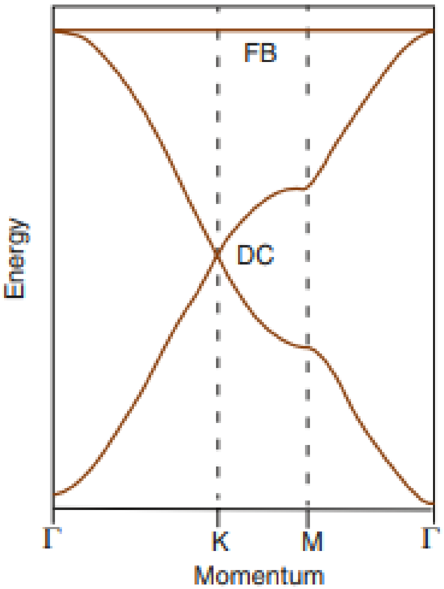
$$= \epsilon_p \pm \gamma_{pp\pi} \sqrt{1 + 4\cos^2\left(\frac{k_y a_0}{2}\right) + 4\cos\left(\frac{k_y a_0}{2}\right)\cos\left(\frac{\sqrt{3}}{2} k_x a_0\right)}$$

Graphene

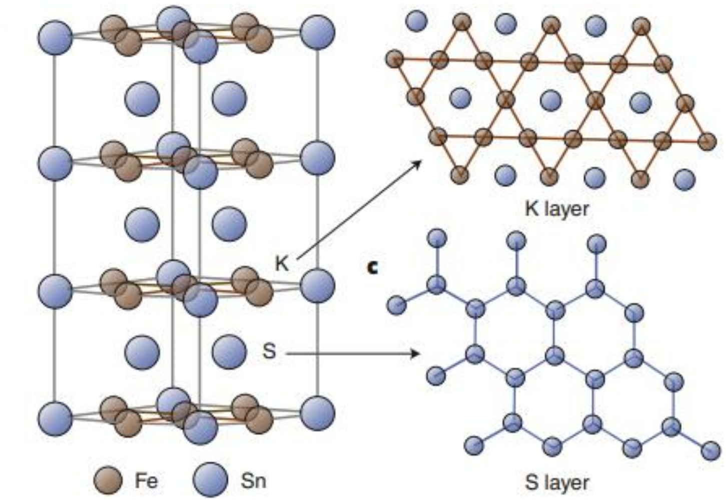


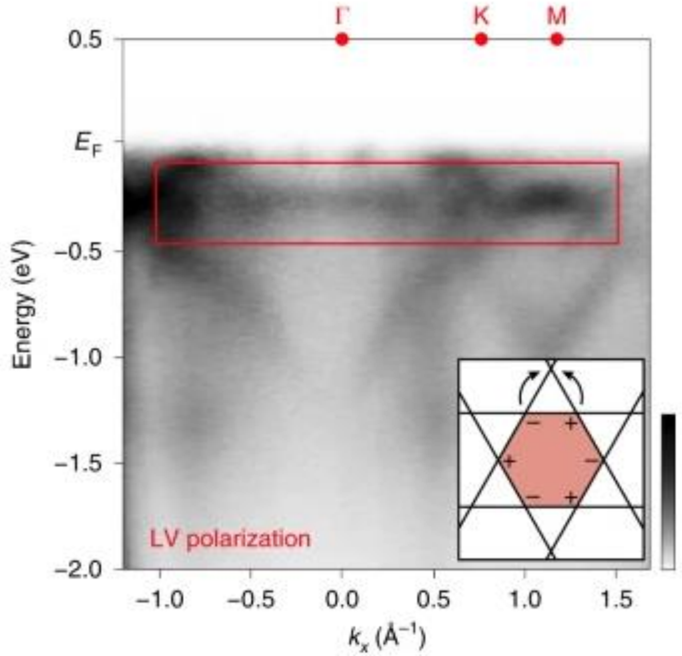
Kagome lattice





Kagome lattice





M. Kang, *et al.*, Nat. Mater. **19**, 163 (2020)

Magnetic systems

System in a magnetic field

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

magnetic field $\vec{B} = \vec{\nabla} \times \vec{A}(\vec{r})$

vector potential

System in a magnetic field

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Two changes to the Hamiltonian

1. $$T_e \rightarrow T_e = \frac{1}{2m_e}\left[\vec{p} - \frac{e}{c}\vec{A}(\vec{r})\right]^2$$

2. $$H_z = -g\mu_{\mathrm{B}}\vec{B}\vec{S} \qquad \mu_{\mathrm{B}} = \frac{e\hbar}{2m_e} \qquad \vec{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$$

System in a magnetic field

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Two changes to the Hamiltonian

1. $$T_e \rightarrow T_e = \frac{1}{2m_e}\left[\vec{p} - \frac{e}{c}\vec{A}(\vec{r})\right]^2$$

- Diamagnetism
- Zeeman coupling with the orbital angular momentum

neglected in the following

2. $$H_z = -g\mu_{\mathrm{B}}\vec{B}\vec{S} \qquad \mu_{\mathrm{B}} = \frac{e\hbar}{2m_e} \qquad \vec{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$$

System in a magnetic field

$$\left[\left(-\frac{\hbar^2}{2m_e}\nabla^2-\frac{1}{2}\sum_{I=1}^{M}\frac{e^2Z_I}{r_I}\right)\mathbb{1}_{2\times 2}-g\mu_{\mathrm{B}}\vec{B}\vec{S}\right]\begin{vmatrix}\psi^{\uparrow}(\vec{r})\\ \psi^{\downarrow}(\vec{r})\end{vmatrix}=E\begin{vmatrix}\psi^{\uparrow}(\vec{r})\\ \psi^{\downarrow}(\vec{r})\end{vmatrix}$$

System in a magnetic field

$$\left[\left(-\frac{\hbar^2}{2m_e}\nabla^2-\frac{1}{2}\sum_{I=1}^{M}\frac{e^2 Z_I}{r_I}\right)\mathbb{1}_{2\times 2}-g\mu_{\mathrm{B}}\vec{B}\vec{S}\right]\begin{vmatrix}\psi^{\uparrow}(\vec{r})\\ \psi^{\downarrow}(\vec{r})\end{vmatrix}=E\begin{vmatrix}\psi^{\uparrow}(\vec{r})\\ \psi^{\downarrow}(\vec{r})\end{vmatrix}$$

$$\psi^{\sigma}(\vec{r})=\langle\vec{r}|\psi^{\sigma}\rangle=\sum_{i=1}^{N}\langle\vec{r}|\phi_i\rangle\langle\phi_i|\psi^{\sigma}\rangle=\sum_{i=1}^{N}c_i^{\sigma}\phi_i(\vec{r})$$

System in a magnetic field

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{g\mu_{\mathrm{B}}}{2} B_z & -\frac{g\mu_{\mathrm{B}}}{2}(B_x - iB_y) \\ -\frac{g\mu_{\mathrm{B}}}{2}(B_x + iB_y) & h_{ij} + \frac{g\mu_{\mathrm{B}}}{2} B_z \end{vmatrix} \begin{vmatrix} c_j^{\uparrow} \\ c_j^{\downarrow} \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{vmatrix}$$

$$h_{ij} = \langle \phi_i | \left(-\frac{\hbar^2}{2m_e} \nabla^2 - \frac{1}{2} \sum_{I=1}^{M} \frac{e^2 Z_I}{r_I} \right) | \phi_j \rangle$$

System in a magnetic field

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{g\mu_{\mathrm{B}}}{2} B_z & -\frac{g\mu_{\mathrm{B}}}{2}(B_x - iB_y) \\ -\frac{g\mu_{\mathrm{B}}}{2}(B_x + iB_y) & h_{ij} + \frac{g\mu_{\mathrm{B}}}{2} B_z \end{vmatrix} \begin{vmatrix} c_j^{\uparrow} \\ c_j^{\downarrow} \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{vmatrix}$$

magnetic field along *z* (<u>collinear</u> system)

System in a magnetic field

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{g\mu_\mathrm{B}}{2} B_z & 0 \\ 0 & h_{ij} + \frac{g\mu_\mathrm{B}}{2} B_z \end{vmatrix} \begin{vmatrix} c_j^\uparrow \\ c_j^\downarrow \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^\uparrow \\ c_i^\downarrow \end{vmatrix}$$

(collinear system-> Hamiltonian matrix is block diagonal)

System in a magnetic field

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{g\mu_{\mathrm{B}}}{2} B_z & 0 \\ 0 & h_{ij} + \frac{g\mu_{\mathrm{B}}}{2} B_z \end{vmatrix} \begin{vmatrix} c_j^{\uparrow} \\ c_j^{\downarrow} \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{vmatrix}$$

H atomic chain

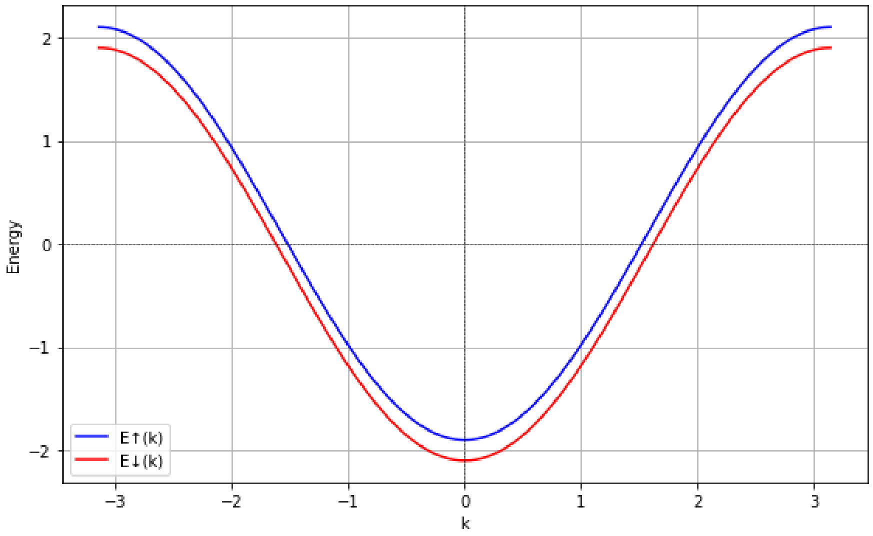
System in a magnetic field

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{g\mu_B}{2} B_z & 0 \\ 0 & h_{ij} + \frac{g\mu_B}{2} B_z \end{vmatrix} \begin{vmatrix} c_j^{\uparrow} \\ c_j^{\downarrow} \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{vmatrix}$$

$$E_K^{\uparrow} = \epsilon_0 + 2\gamma \cos(K) - \frac{g\mu_B}{2} B_z$$

$$E_K^{\downarrow} = \epsilon_0 + 2\gamma \cos(K) + \frac{g\mu_B}{2} B_z$$

System in a magnetic field



For B=1 T
Band splitting: 1.16 x 10^{-4} eV

$$E_K^{\uparrow} = \epsilon_0 + 2\gamma\cos(K) - \frac{g\mu_{\mathrm{B}}}{2}B_z$$

$$E_K^{\downarrow} = \epsilon_0 + 2\gamma\cos(K) + \frac{g\mu_{\mathrm{B}}}{2}B_z$$

Mean-field approximation

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Add electron-electron interaction V_{ee}

Mean-field approximation

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Add electron-electron interaction

$$V_{ee} \rightarrow v[n]$$

Mean-field approximation

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Add electron-electron interaction

$$V_{ee} \rightarrow v[n]$$

Single particle potential

Electrostatic potential on an electron due to the charge density of all other electrons

Mean-field approximation

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Add electron-electron interaction

$$V_{ee} \rightarrow v[n]$$

$$V_{ee} \rightarrow v[n] + \vec{B}_m[\vec{m}]\vec{S}$$

Mean-field approximation

$$[T_e + V_{Ne}]\psi(\vec{r}) = E\psi(\vec{r})$$

Add electron-electron interaction

$$V_{ee} \rightarrow v[n]$$

$$V_{ee} \rightarrow v[n] + \vec{B}_m[\vec{m}]\vec{S}$$

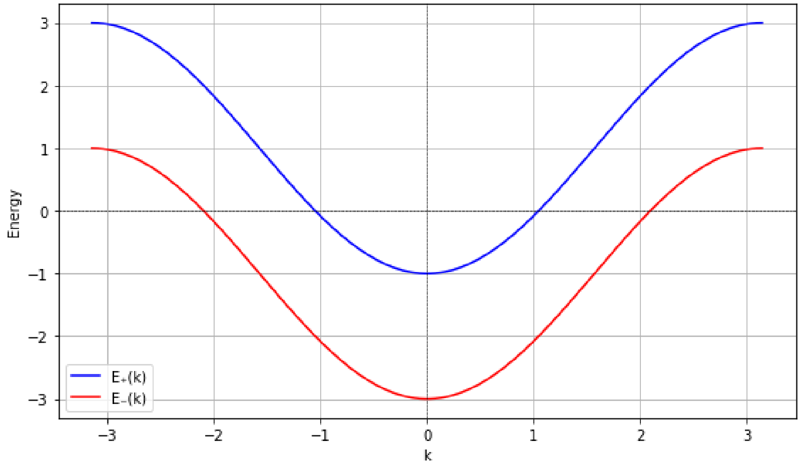
$$V_{ee} \rightarrow v[n] + B_{m,z}[m_z]S_z \qquad B_{m,z}[m_z] = -\frac{1}{2}Im_z$$

Mean-field approximation

$$\sum_{j=1}^{N} \begin{vmatrix} h_{ij} - \frac{1}{2} I m_z & 0 \\ 0 & h_{ij} + \frac{1}{2} I m_z \end{vmatrix} \begin{vmatrix} c_j^{\uparrow} \\ c_j^{\downarrow} \end{vmatrix} = E \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \begin{vmatrix} c_i^{\uparrow} \\ c_i^{\downarrow} \end{vmatrix}$$

Mean-field approximation

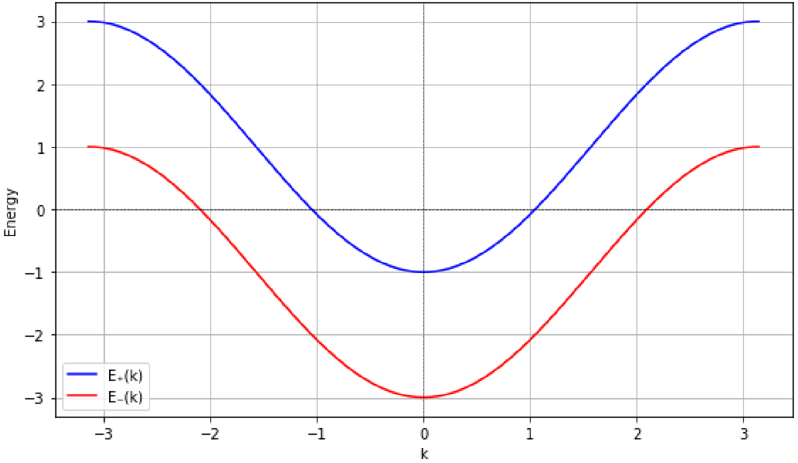
Example: 1d chain studied previously



Im_z

Mean-field approximation

Example: 1d chain studied previously



$$Im_z$$

$$m_z = N^{\uparrow} - N^{\downarrow}$$

Number of electrons that occupy the lower band minus the number of electrons that occupy that highest band

Stoner model

$$m_z = N^{\uparrow} - N^{\downarrow}$$

$$N^{\uparrow} = \int_{-\infty}^{E_F} dE\, D(E + \frac{1}{2} I m_z)$$

$$N^{\downarrow} = \int_{-\infty}^{E_F} dE\, D(E - \frac{1}{2} I m_z)$$

Stoner model

$$m_z = \int_{-\infty}^{E_F} dE \left[D(E + \frac{1}{2}Im_z) - D(E - \frac{1}{2}Im_z)\right]$$

For small m_z $$m_z \approx Im_z D(E_F)$$

1. trivial solution:

$$m_z = 0$$

2. non-trivial solution:

$$m_z \neq 0 \qquad ID(E_F) = 1$$

Stoner model

1. trivial solution:

$$m_z = 0$$

Stoner's picture

2. non-trivial solution:

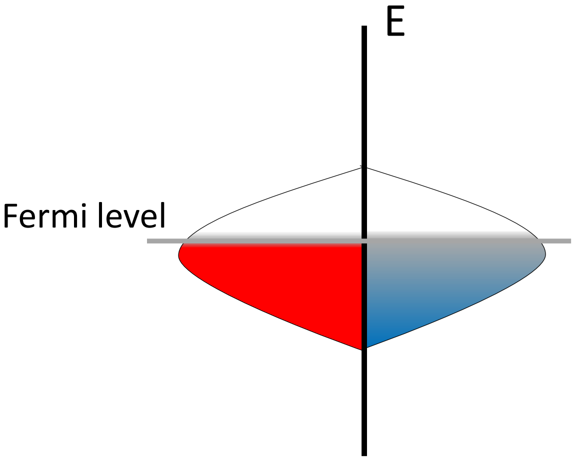
$$m_z \neq 0 \qquad ID(E_F) \geq 1$$

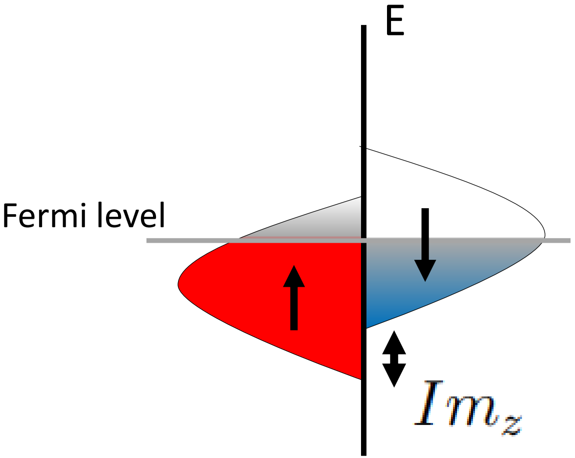
Stoner criterion

Stoner model

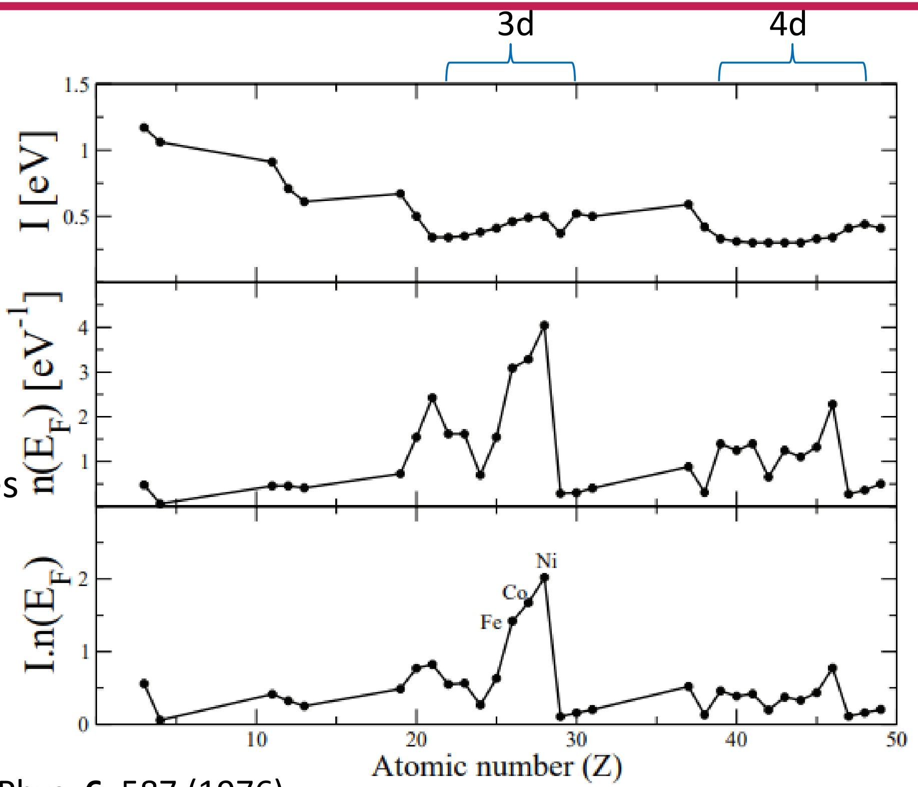
$$ID(E_F) \geq 1$$ **Stoner criterion**

Stoner's picture





Stoner criterion



Note energy scale: eV!!!

Density of states

O. Gunnarsson, J. Phys. F: Met. Phys. **6**, 587 (1976)
J.F. Janak, Phys. Rev. B **16**, 255 (1977)

Stoner criterion

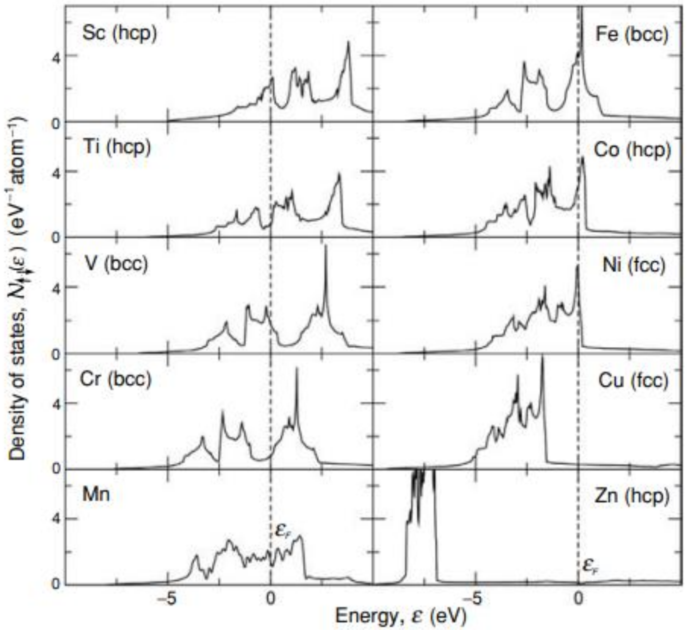
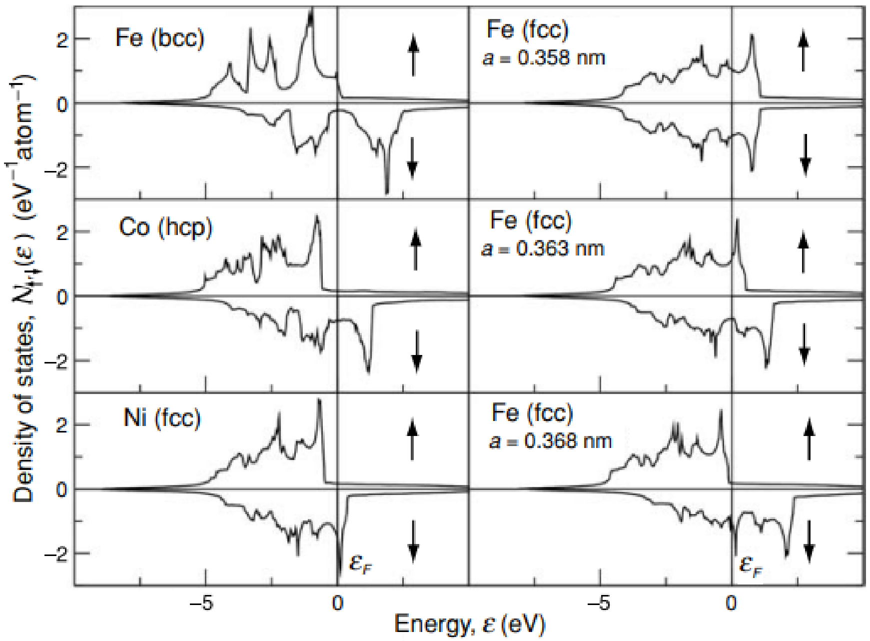


Figure by C.D. Pemmaraju in J.M.D. Coey, *Magnetism and Magnetic Materials* (Cambridge University Press; 2010)

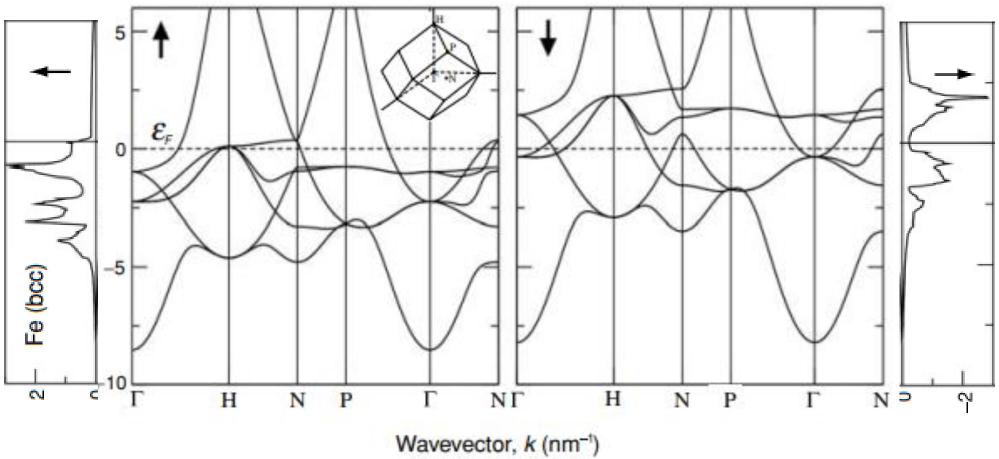
Stoner criterion



metal	$M_{LSDA}[\mu_B/atom]$
Fe	2.15
Co	1.56
Ni	0.59

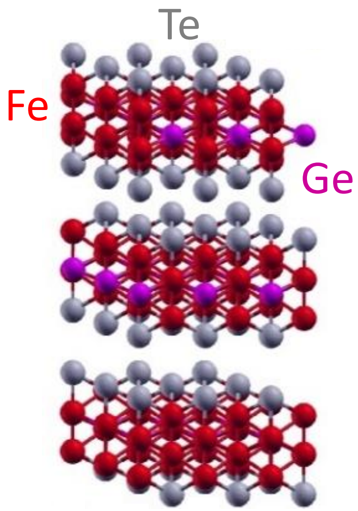
Figure by C.D. Pemmaraju in J.M.D. Coey, *Magnetism and Magnetic Materials* (Cambridge University Press; 2010)

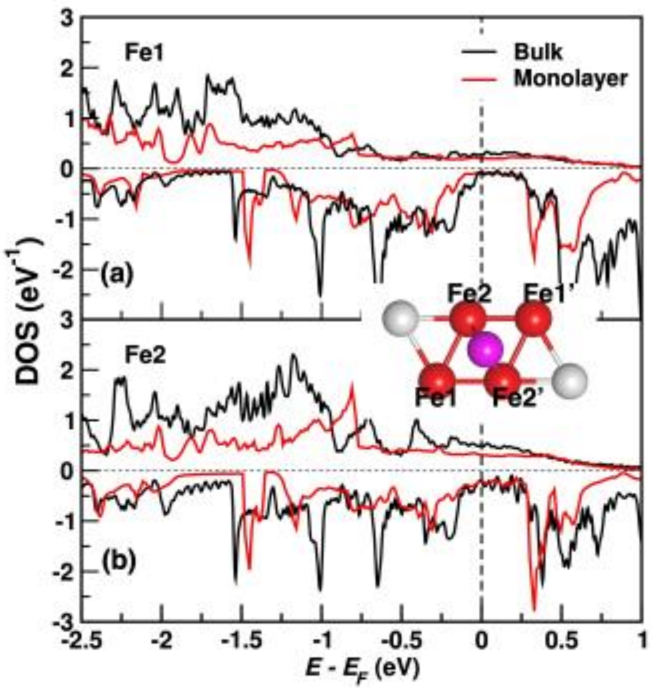
Iron



Band structure and DOS of bcc Fe

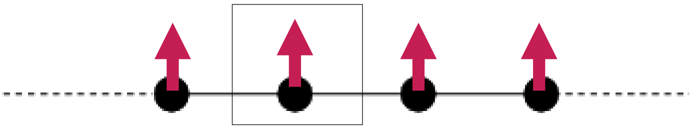
Fe_4GeTe_2



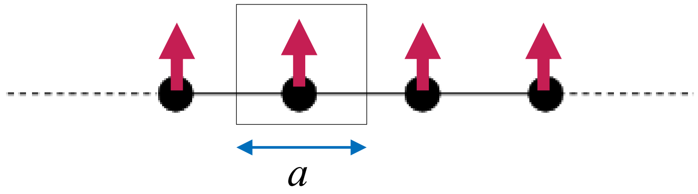


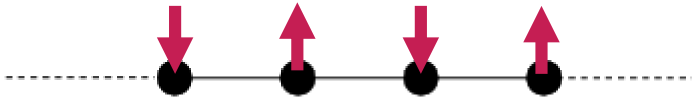
A. Halder, …,and A. Droghetti, *Nano Lett.* **24**, 9221 (2024)

Ferro vs Antiferromagnetism

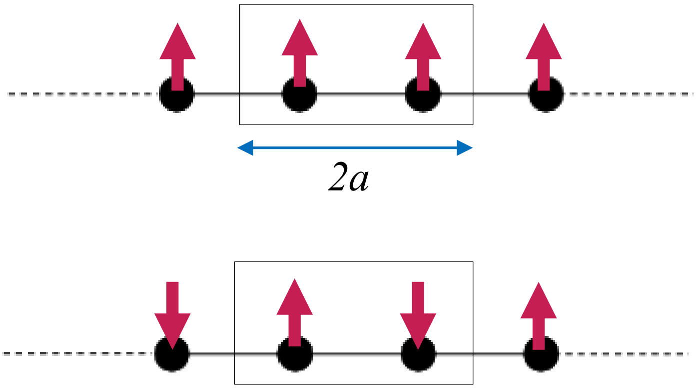


Ferro vs Antiferromagnetism

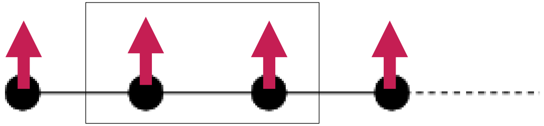




Ferro vs Antiferromagnetism



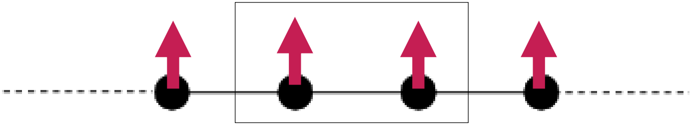
Ferro vs Antiferromagnetism

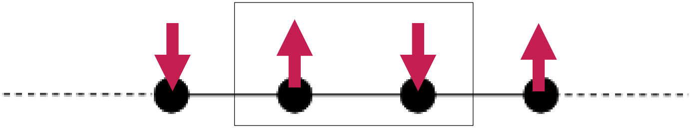


$$H^{\uparrow} = \begin{vmatrix} Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & Im_z \end{vmatrix}$$

$$H^{\downarrow} = \begin{vmatrix} -Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & -Im_z \end{vmatrix}$$

Ferro vs Antiferromagnetism





$$H^{\uparrow} = \begin{vmatrix} Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & Im_z \end{vmatrix}$$

$$H^{\downarrow} = \begin{vmatrix} -Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & -Im_z \end{vmatrix}$$

$$E_k^{\uparrow} = Im_z \pm 2t\cos(ka)$$

$$E_k^{\downarrow} = -Im_z \pm 2t\cos(ka)$$

$$H^{\uparrow} = \begin{vmatrix} Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & -Im_z \end{vmatrix}$$

$$H^{\downarrow} = \begin{vmatrix} -Im_z & t(1+e^{2ika}) \\ t(1+e^{-2ika}) & Im_z \end{vmatrix}$$

$$E_k^{\uparrow} = \pm\sqrt{(Im_z)^2 + 4t^2\cos^2(ka)}$$

$$E_k^{\downarrow} = \pm\sqrt{(Im_z)^2 + 4t^2\cos^2(ka)}$$

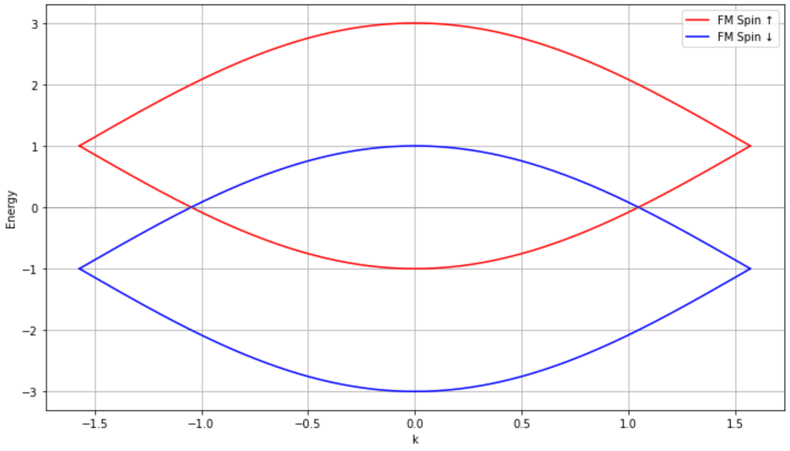
Ferro vs Antiferromagnetism

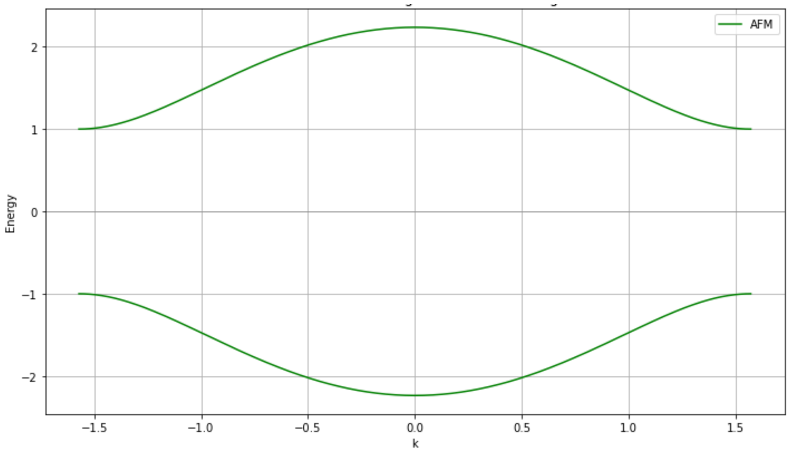
$$E_k^{\uparrow} = Im_z \pm 2t\cos(ka)$$

$$E_k^{\downarrow} = -Im_z \pm 2t\cos(ka)$$

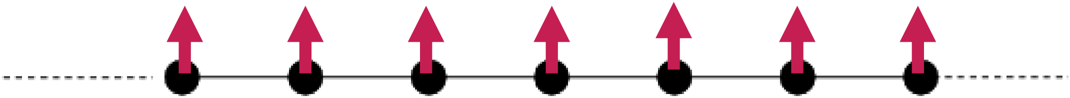
$$E_k^{\uparrow} = \pm\sqrt{(Im_z)^2 + 4t^2\cos^2(ka)}$$

$$E_k^{\downarrow} = \pm\sqrt{(Im_z)^2 + 4t^2\cos^2(ka)}$$

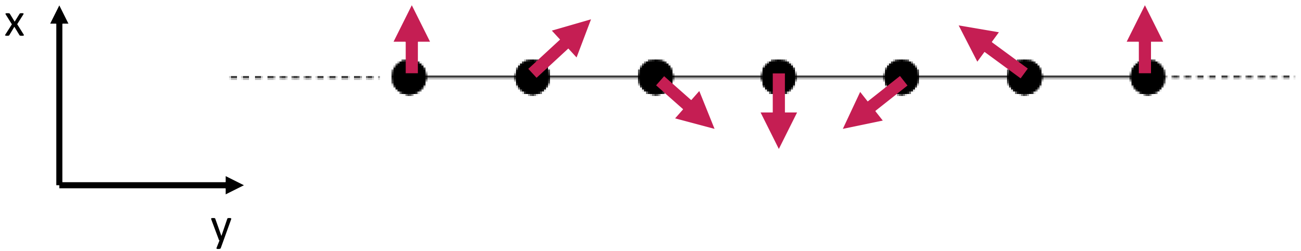




Generalized Bloch theorem



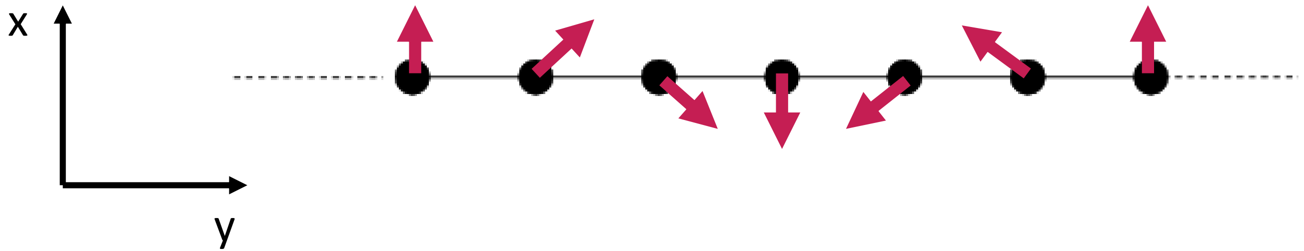
Generalized Bloch theorem



$$\vec{M}_j = M[\cos(qj), \sin(qj), 0]$$

$q \cdot j$ angle of rotation of the spin at lattice site j

Generalized Bloch theorem



$q = \pi/6$

$$\vec{M}_j = M[\cos(qj), \sin(qj), 0]$$

The generalized Bloch theorem combines the **spatial translation** by a lattice vector with a **spin rotation** by an angle $q \cdot j$

L.M. Sandratskii. J. Phys.: Condens. Matter **3**, 8565 (1991)

Generalized Bloch theorem

Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj} |j\rangle$$

Generalized Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj} e^{iqj\sigma^z/2} |j\rangle$$

Generalized Bloch theorem

Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj}|j\rangle$$

$$H_{jl} = h_{jl}$$

Generalized Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj} e^{iqj\sigma^z/2}|j\rangle$$

$$H_{jl} = h_{jl}\,\mathbb{1}_{2\times 2} + I\vec{M}_j\vec{\sigma}\delta_{jl}$$

Generalized Bloch theorem

Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj}|j\rangle$$

$$H_{jl} = h_{jl}$$

$$E_k = \sum_j e^{ik(l-j)} H_{jl}$$

Generalized Bloch theorem

$$|\psi_k\rangle = \sum_{j=1}^{N} e^{ikj} e^{iqj\sigma^z/2}|j\rangle$$

$$H_{jl} = h_{jl}\,\mathbb{1}_{2\times 2} + I\vec{M}_j\vec{\sigma}\delta_{jl}$$

$$E_k\mathbb{1} = \sum_j e^{ik(l-j)} e^{-iqj\sigma^z/2} H_{jl} e^{iql\sigma^z/2}$$

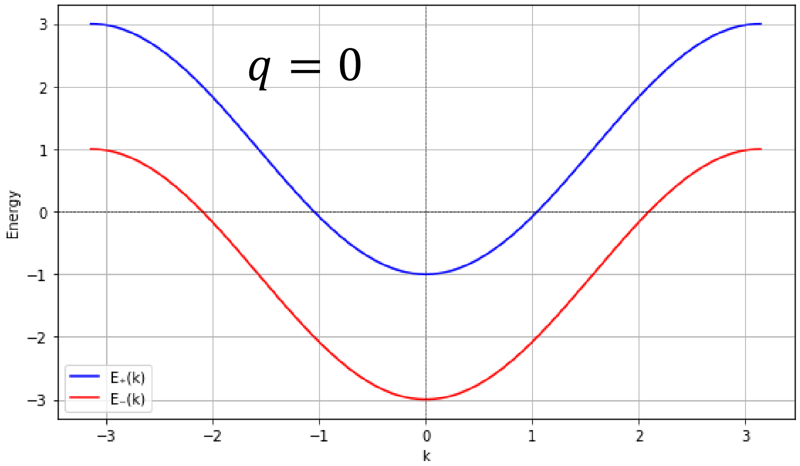
Generalized Bloch theorem

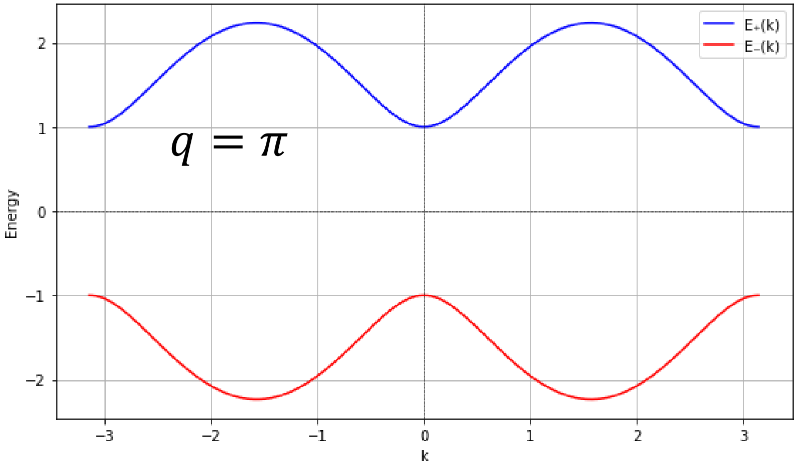
$$E_k\mathbb{1} = \sum_j e^{ik(l-j)} e^{-iqj\sigma^z/2} H_{jl} e^{iql\sigma^z/2}$$

$$E(k)\mathbb{1} = 2\gamma\cos k\cos(q/2)\mathbb{1} - 2\gamma\sin k\sin(q/2)\sigma^z + IM\sigma^x$$

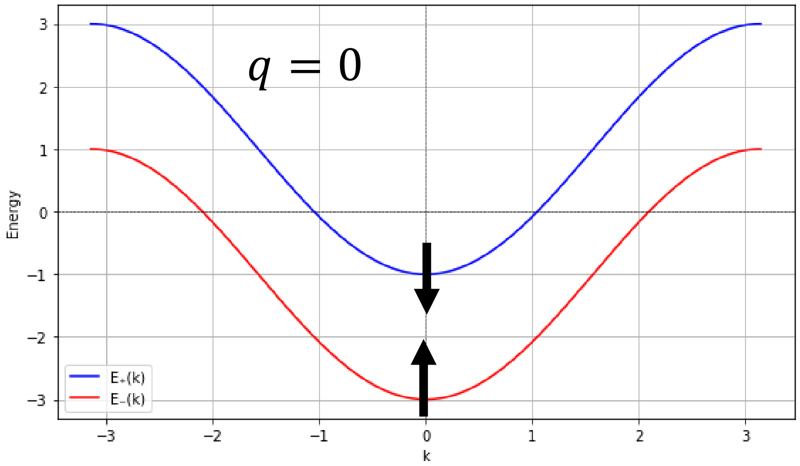
$$E_k = 2\gamma\cos k\cos(q/2) \pm \sqrt{(IM)^2 + [2\gamma\sin k\sin(q/2)]^2}$$

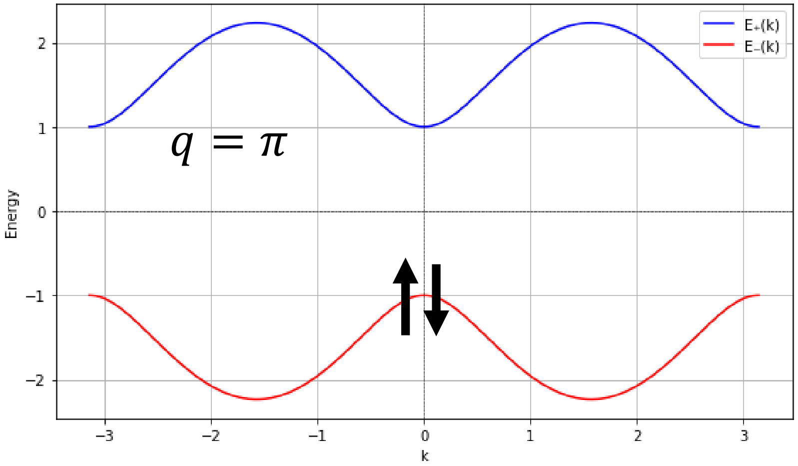
Generalized Bloch theorem





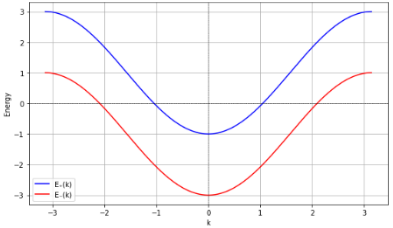
Generalized Bloch theorem



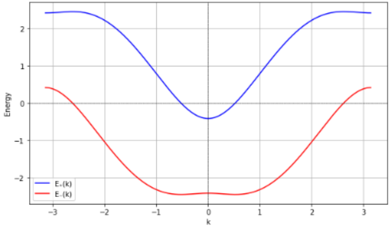


Generalized Bloch theorem

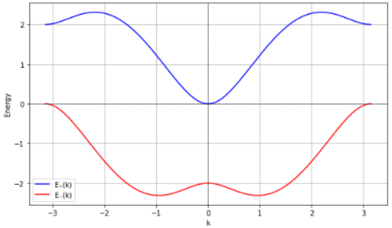
$q = 0$



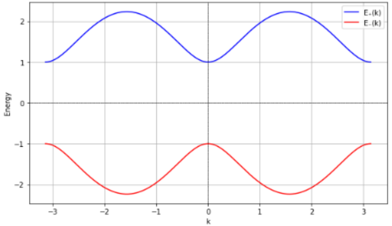
$q = \pi/2$



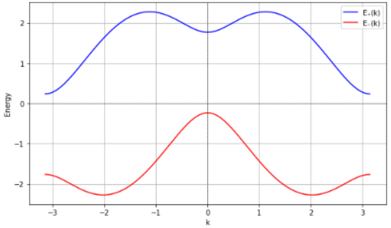
$q = 2\pi/3$



$q = \pi$

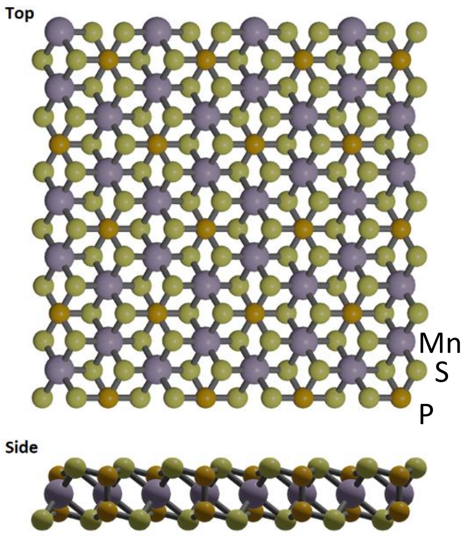


$q = 5\pi/4$



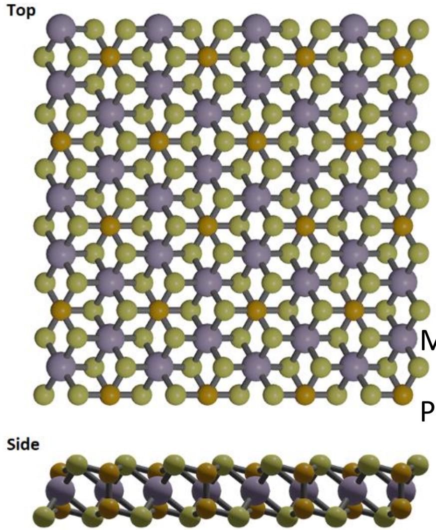
Band structure of selected 2d materials

$MnPS_3$

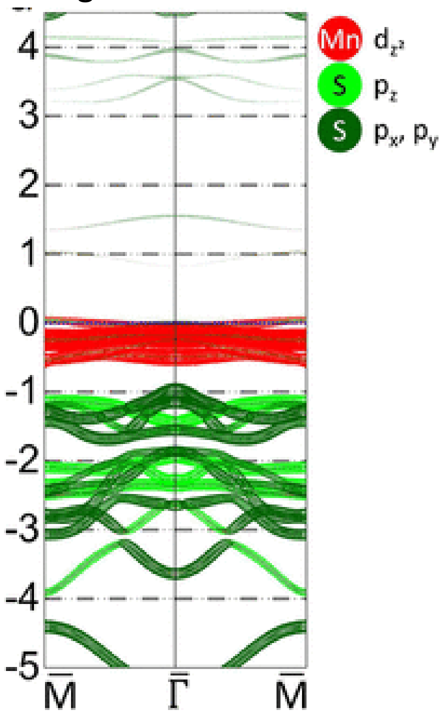


$MnPS_3$

$MnPS_3$



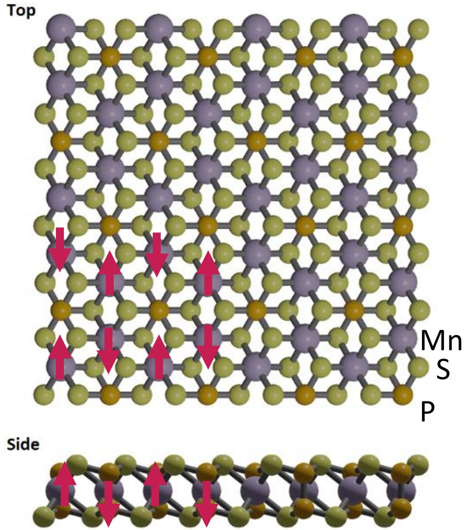
Non-magnetic band structure

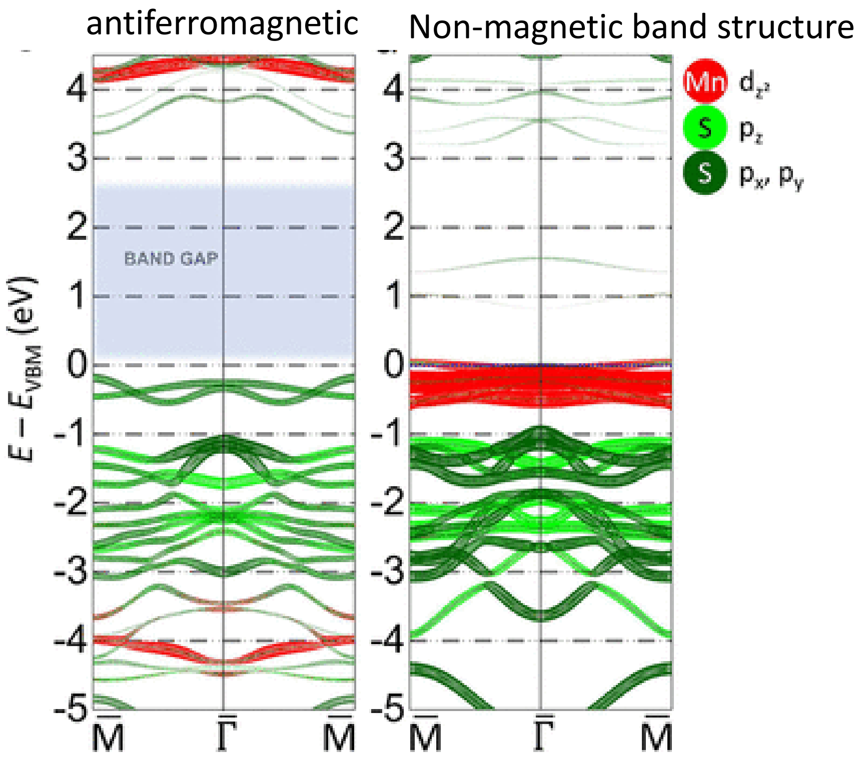


J. Strasdas et al., Nano Lett. **23**, 10342 (2023)

$MnPS_3$

$MnPS_3$

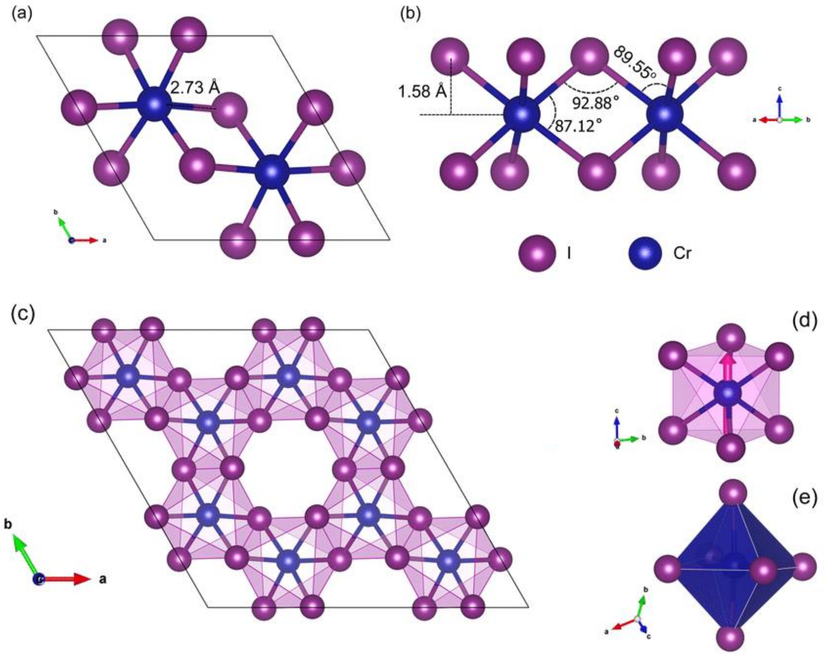




J. Strasdas et al., Nano Lett. **23**, 10342 (2023)

CrI_3

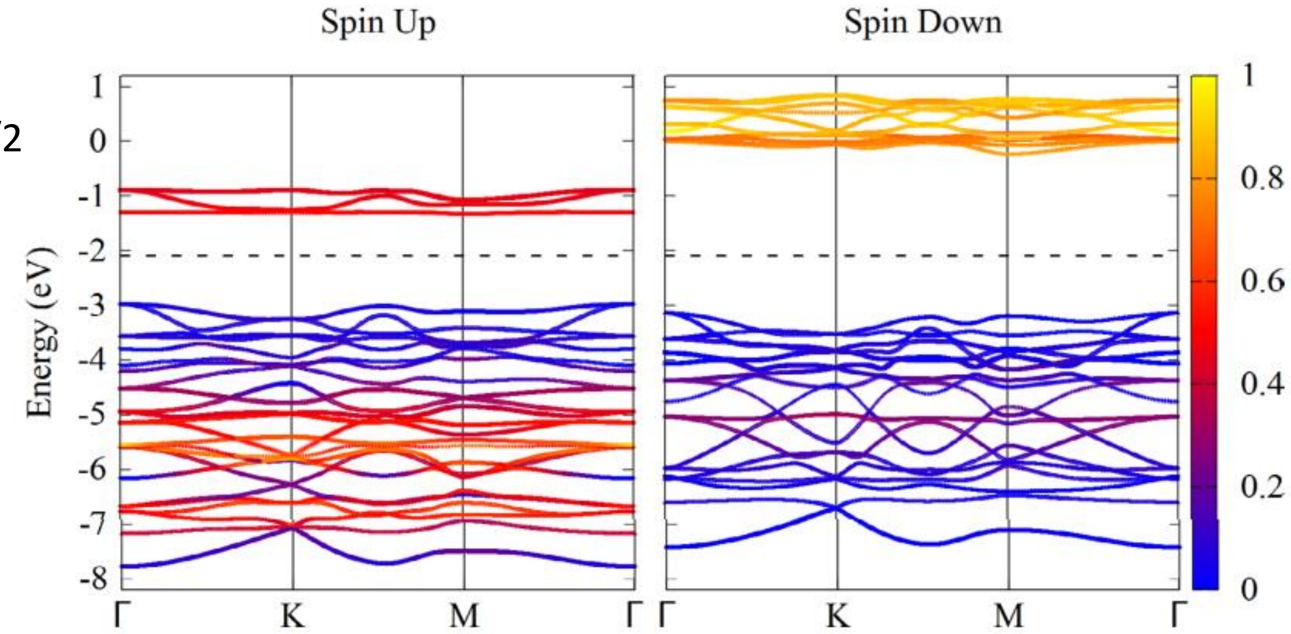
monolayer CrI_3
ferromagnetic



CrI_3

ferromagnetic

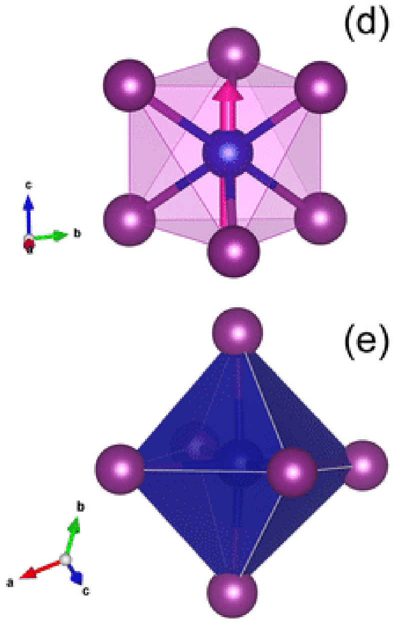
each Cr atom S=3/2



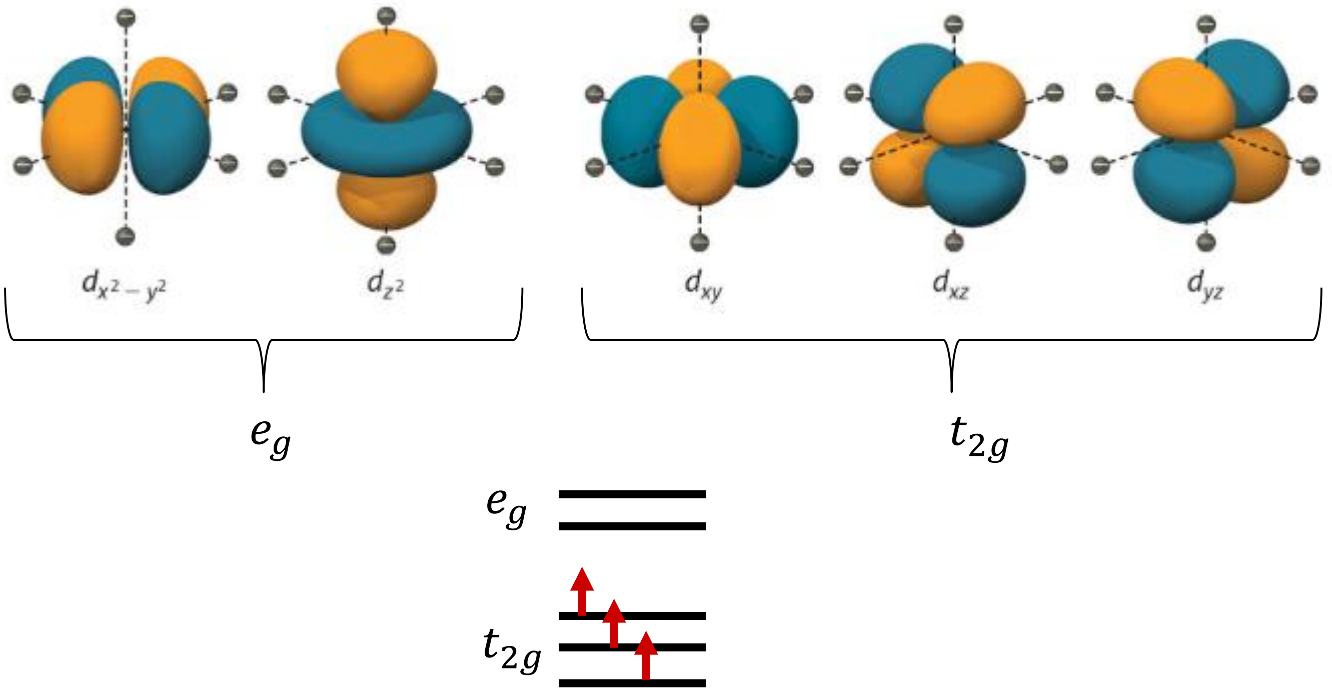
I.V. Kashin et al. 2D Mater. **7**, 025036 (2020)

J.L. Lado and J. Fernández-Rossier, *2D Mater.* **4** 035002 (2017)

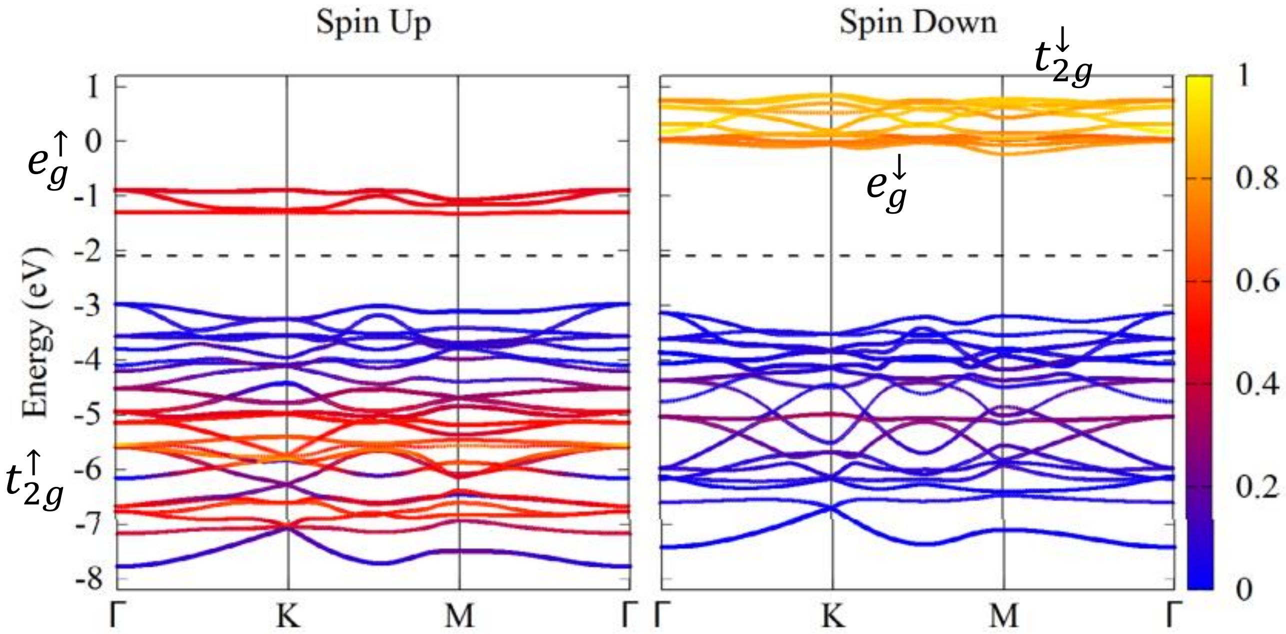
CrI_3



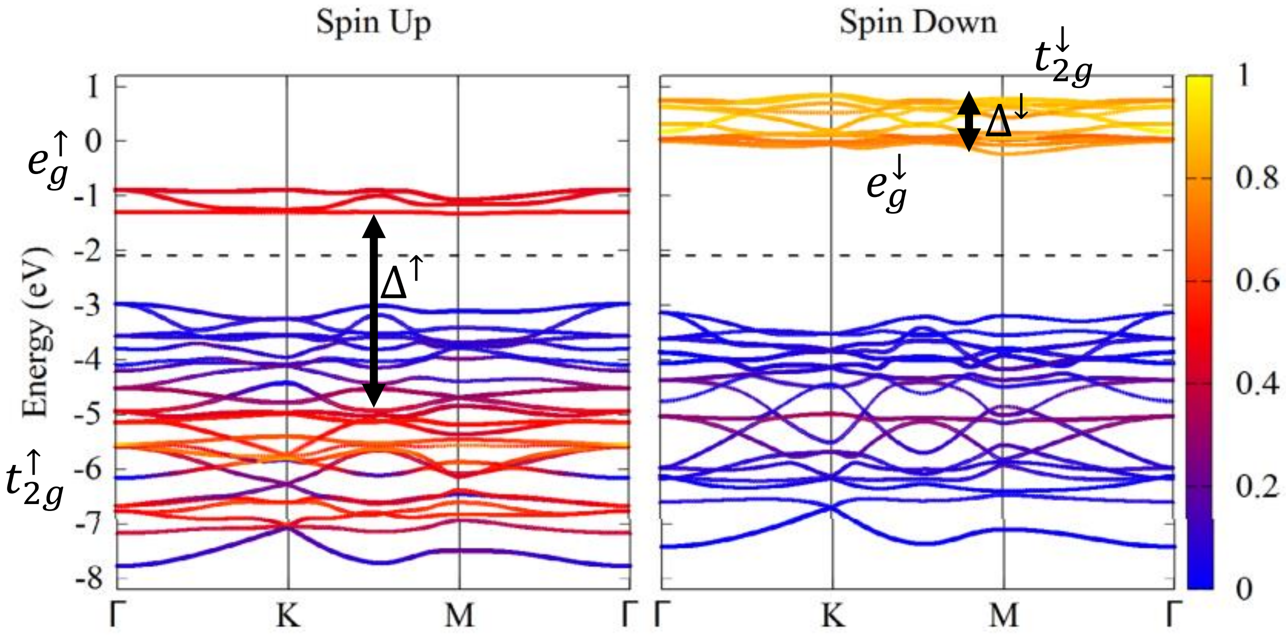
CrI_3



CrI_3


Spin Up
Spin Down
$e_g^{\uparrow}$
$t_{2g}^{\uparrow}$
$t_{2g}^{\downarrow}$
$e_g^{\downarrow}$
Energy (eV)
1
0
-1
-2
-3
-4
-5
-6
-7
-8
Γ
K
M
Γ
Γ
K
M
Γ
1
0.8
0.6
0.4
0.2
0

CrI_3



$\gamma_{t_{2g}t_{2g}}, \gamma_{t_{2g}e_g}, \gamma_{t_{2g}p}, \gamma_{e_g p}$

Altermagnets

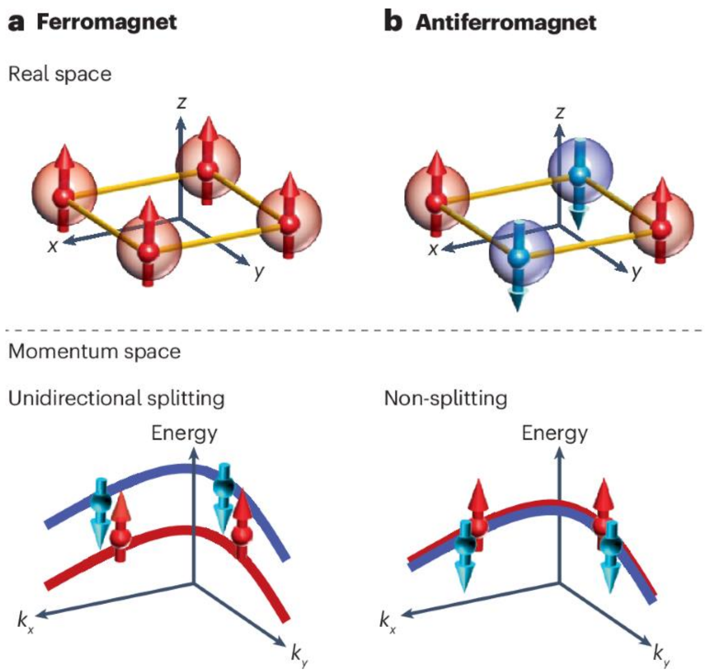


Figure from Nat. Rev. Mater. **10**, 473 (2025)

Altermagnets

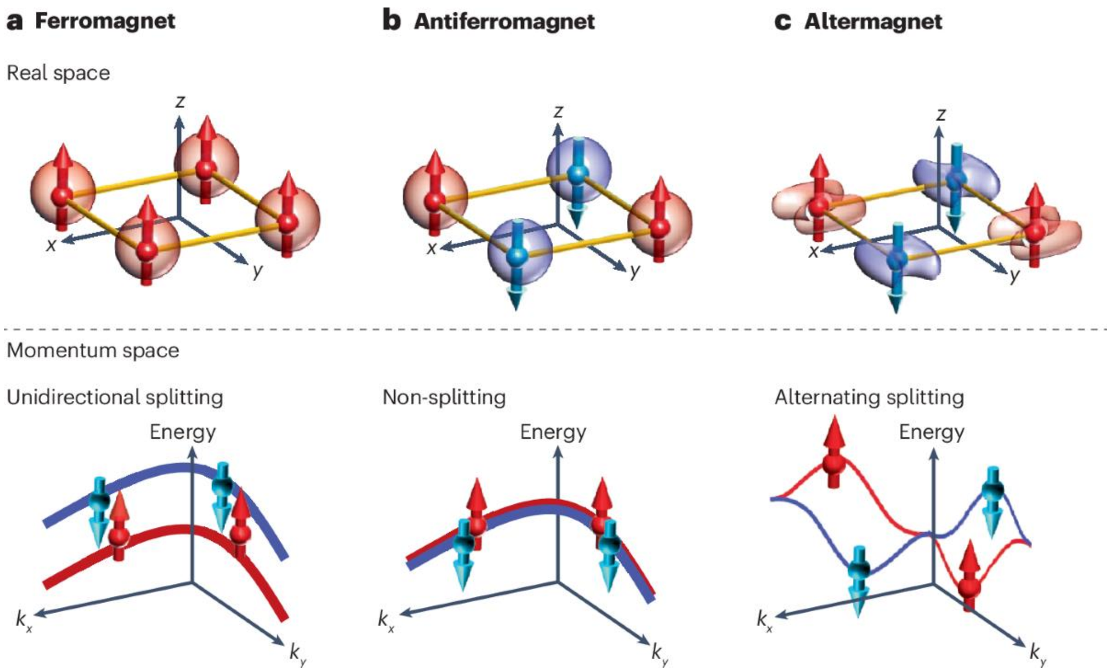
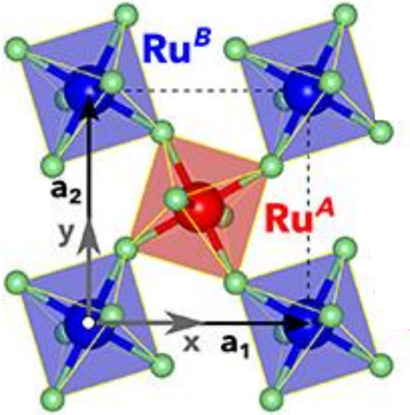


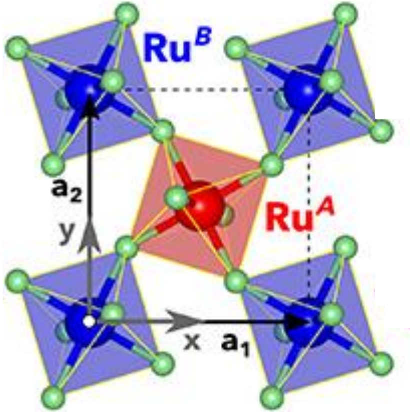
Figure from Nat. Rev. Mater. **10**, 473 (2025)

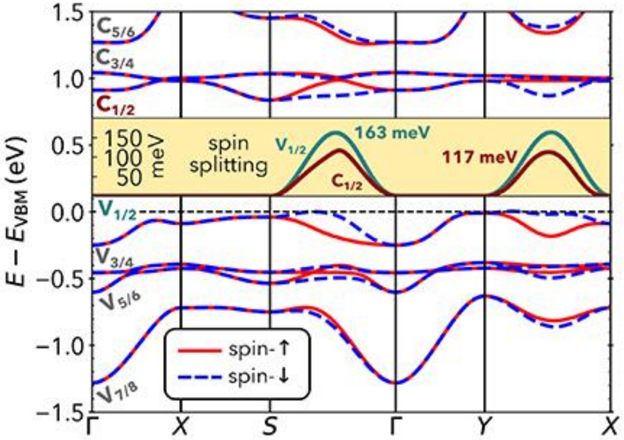
L. Šmejkal, J. Sinova, T. Jungwirth, *Phys. Rev. X* **12**, 040501 (2022)

RuF_4



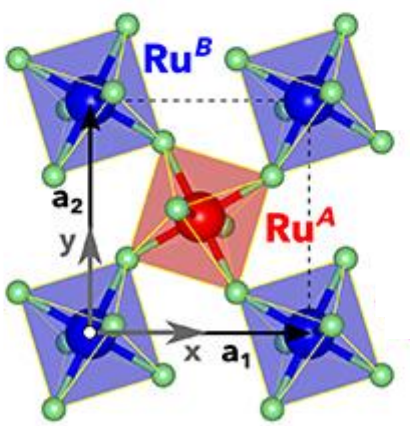
RuF_4

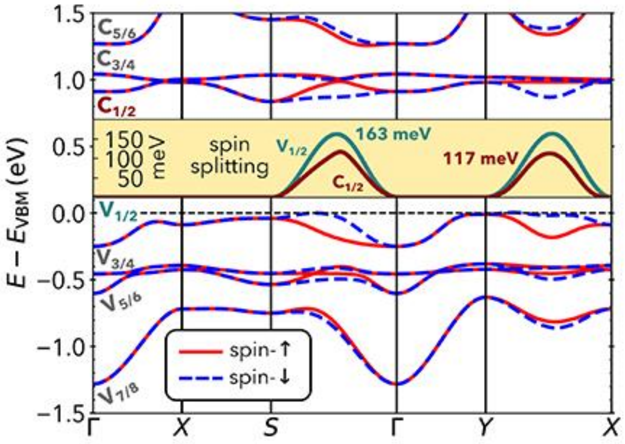


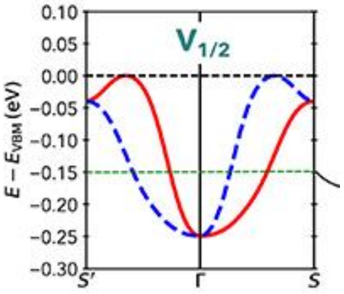


M. Milivojević *et al.*, 2D Mater. **11**, 035025 (2024)

RuF_4

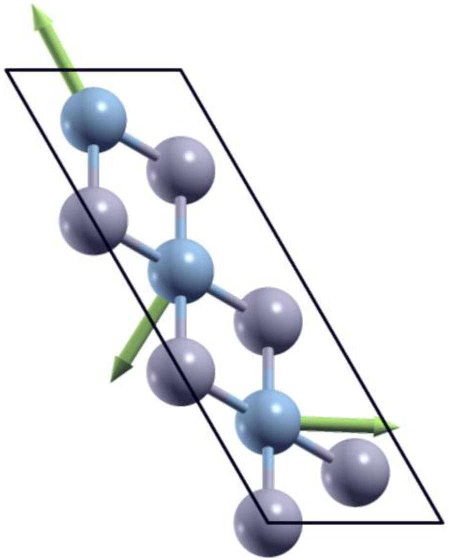


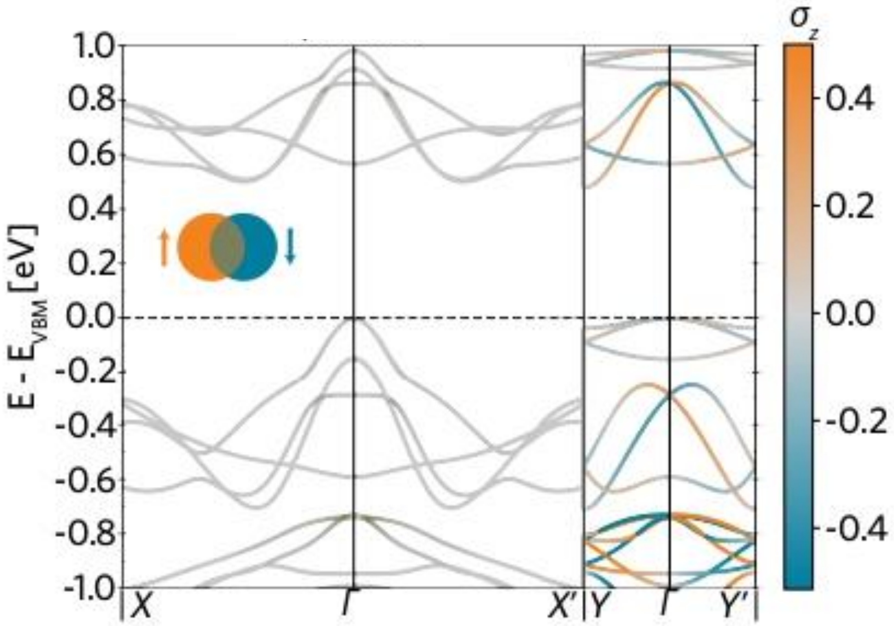




M. Milivojević *et al.*, 2D Mater. **11**, 035025 (2024)

NiI_2

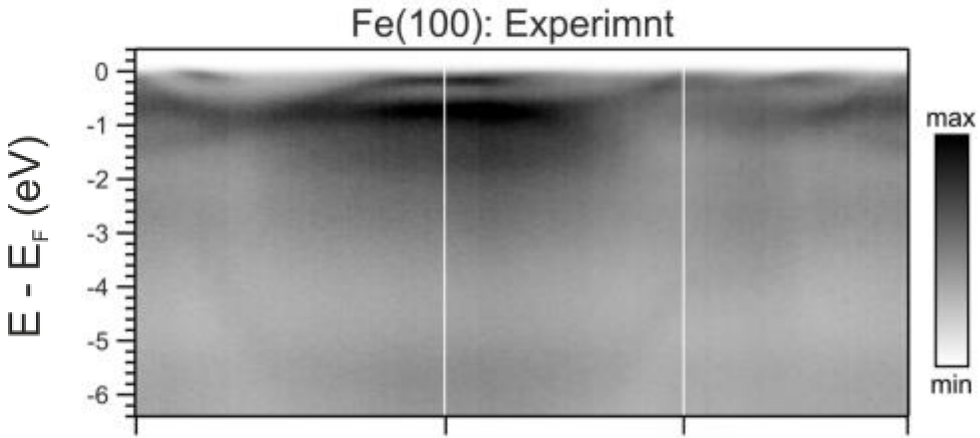




Q. Song, …, A. Droghetti, *et al.,* Nature **642**, 64 (2025)

Electronic structure of ferromagnets beyond the Stoner picture

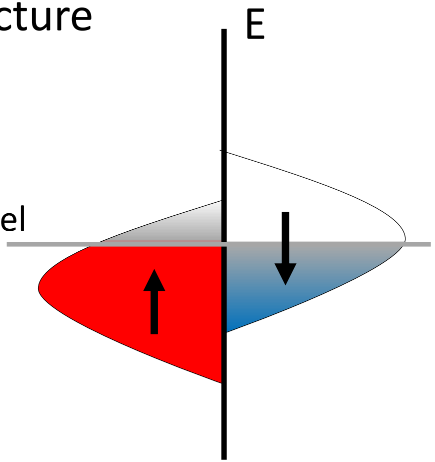
Electronic structure beyond Stoner



Experiment: Mirko Cinchetti's group (TU Dortmund, Germany)

Electronic structure beyond Stoner

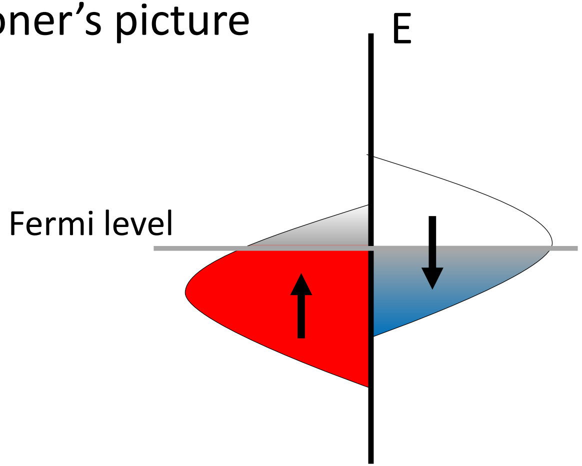
Stoner's picture



$$H_\sigma = \mp I \langle n_{-\sigma} \rangle n_\sigma = \mp B_s n_\sigma$$

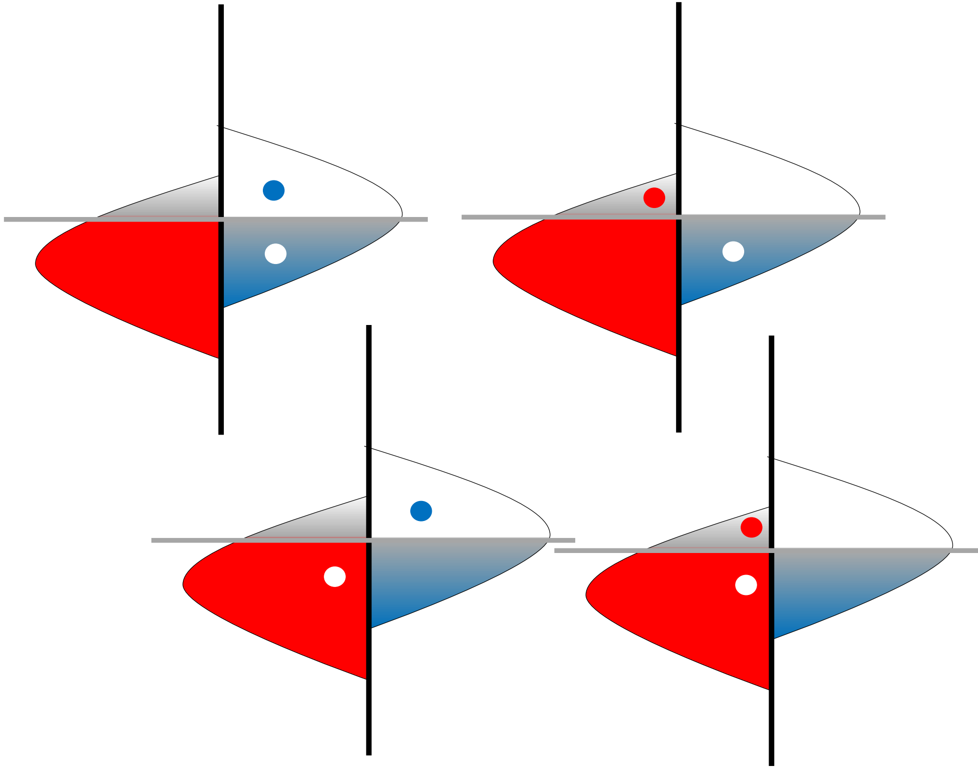
Electronic structure beyond Stoner

Stoner's picture



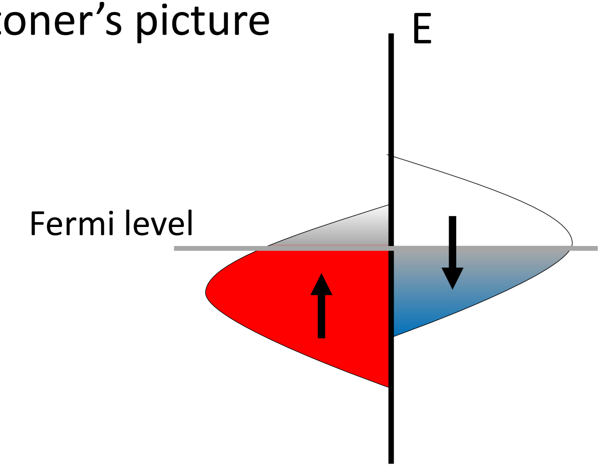
$$H_\sigma = \mp I\langle n_{-\sigma}\rangle n_\sigma = \mp B_s n_\sigma$$

Stoner picture + scattering with particle-hole pairs



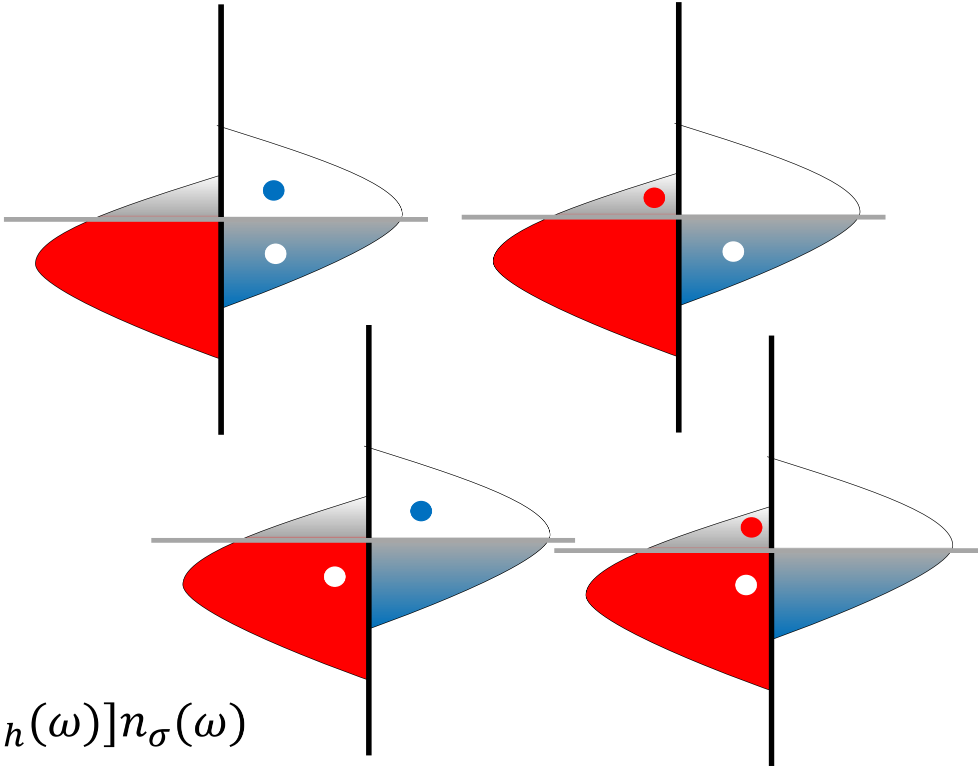
Electronic structure beyond Stoner

Stoner's picture



$$H_\sigma = \mp I\langle n_{-\sigma}\rangle n_\sigma = \mp B_s n_\sigma$$

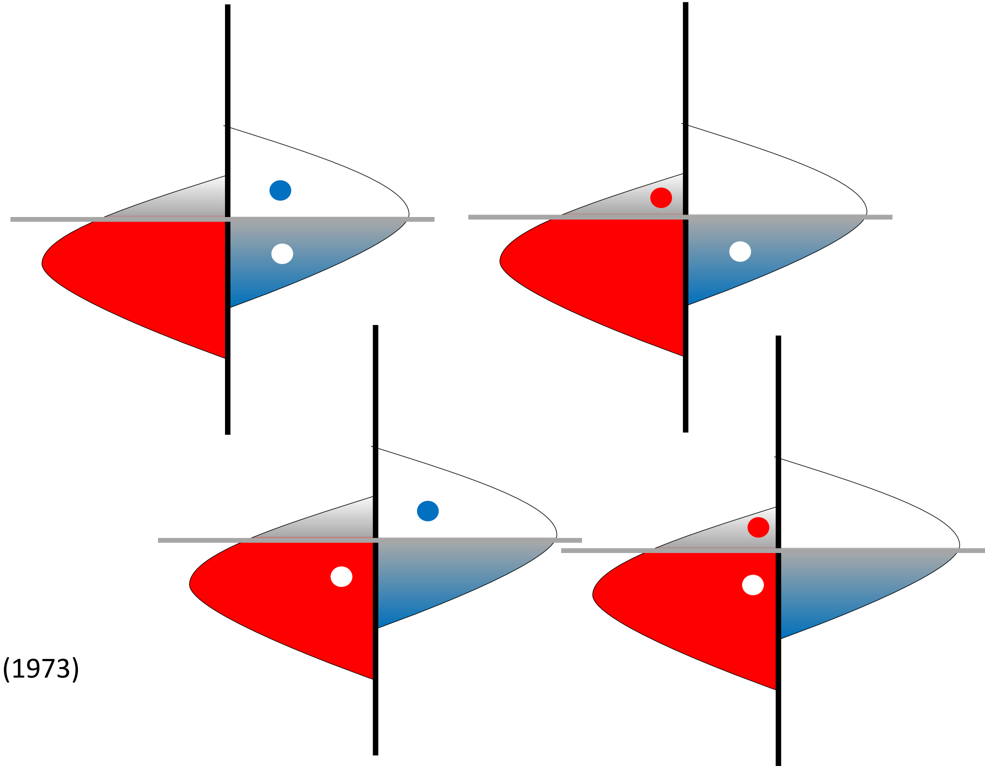
Stoner picture + scattering with particle-hole pairs



$$[B_s + B_{p-h}(\omega)]n_\sigma(\omega)$$

Electronic structure beyond Stoner

Stoner picture + scattering with particle-hole pairs



$$B_{p-h}(\omega)n_\sigma(\omega)$$

$$\Sigma^\sigma(\omega) \approx I \int d\omega' \, G^\sigma(\omega')\chi^{+-}(\omega-\omega')$$

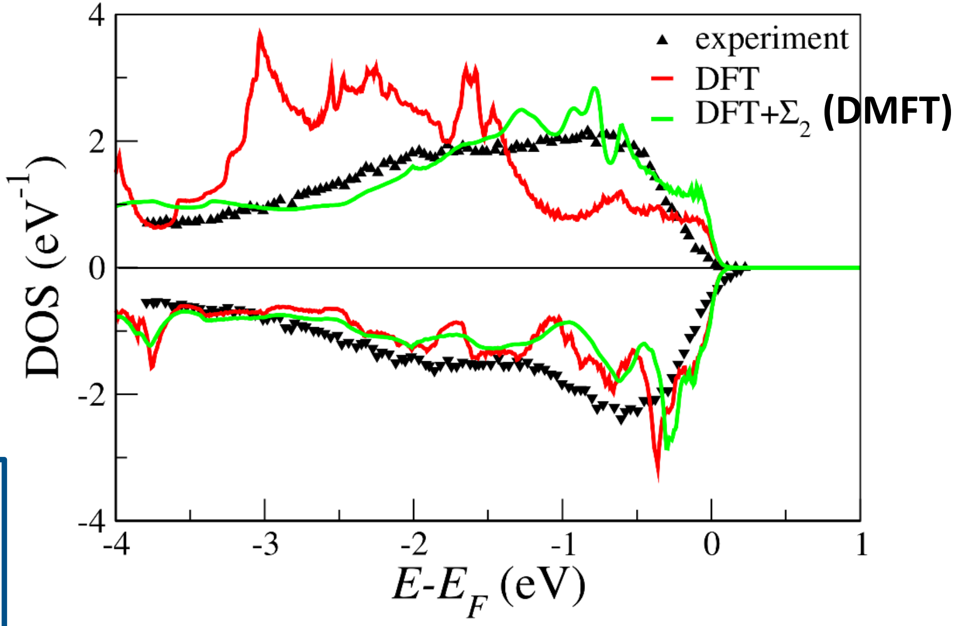
For example: D. M. Edwards and J. A. Hertz, J. Phys. F: Met. Phys. **3**, 2191 (1973)

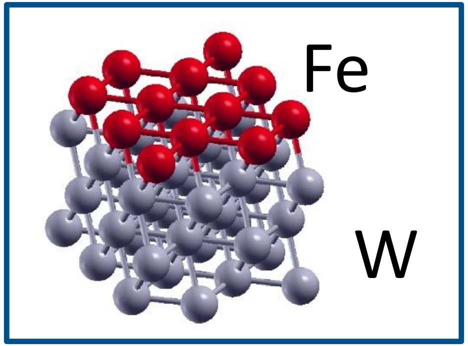
Electronic structure beyond Stoner

$$\Sigma^{\sigma}(\omega) = Re\Sigma^{\sigma}(\omega) + iIm\Sigma^{\sigma}(\omega)$$

Shift of the bands   Broadening of the bands

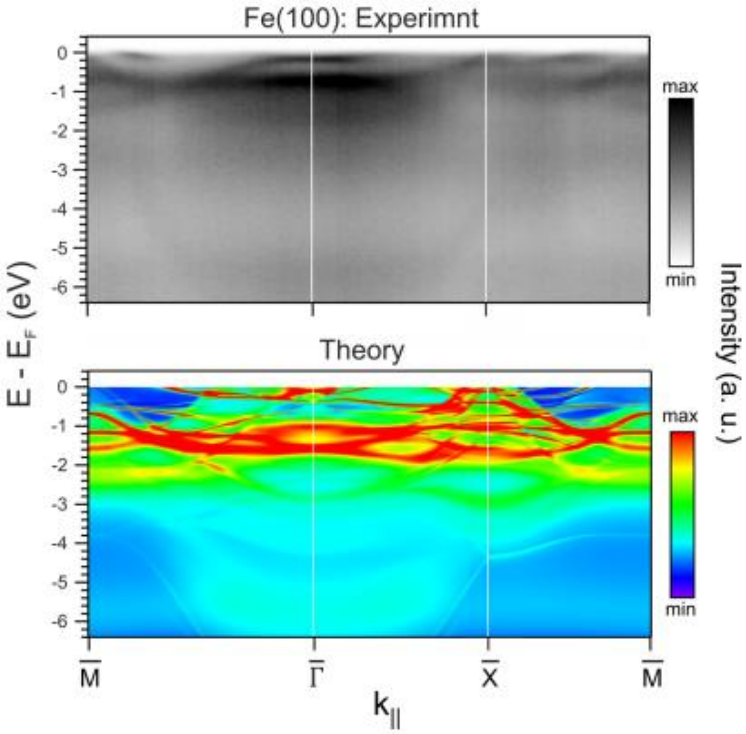
Fe surface layer





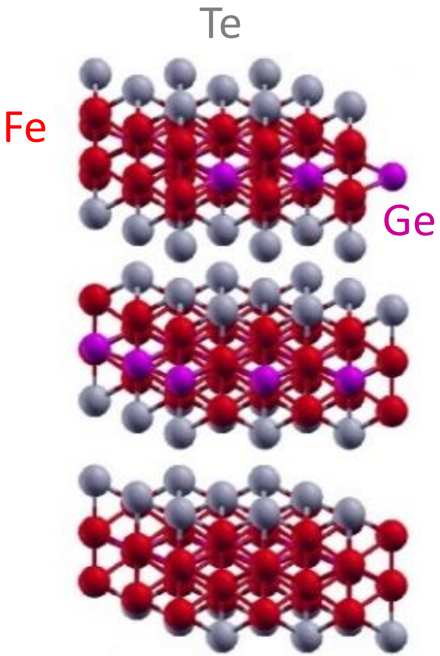
A. Droghetti *et al.* Phys. Rev. B **105**, 115129 (2022) – editors' suggestion

Fe surface

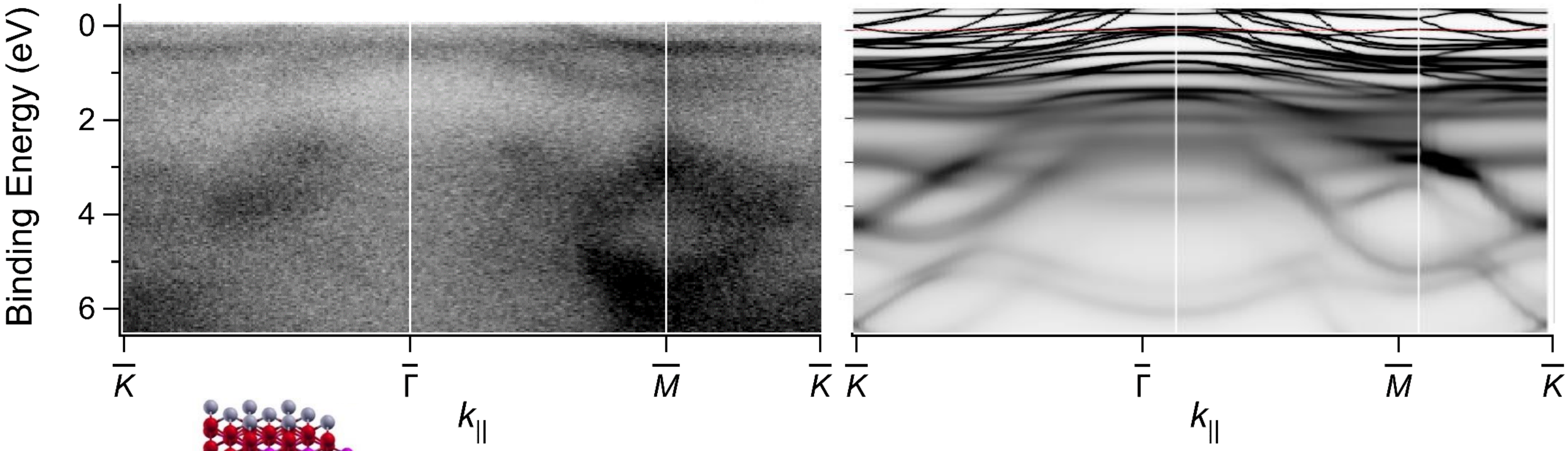


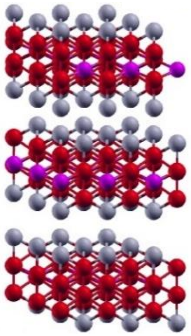
D. Janas, A. Droghetti, *et al.*, Adv. Mater., **35**, 2205698 (2023)

Fe_4GeTe_2



Fe_4GeTe_2





Experiment: Mirko Cinchetti's group (TU Dortmund, Germany)

Calculations: Antik Sihi, Anita Halder, and Declan Nell (Trinity College Dublin)

Thank you!