Electronic structure theory, some of the foundations and applications

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and
WISE-Wallenberg Initiative Materials Science

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Scopus on research

	Document title	Authors	Source	Year
1	Article • *Open access* **Topological metal-insulator transition within the ferromagnetic state** Show abstract · Uppsala UB · View at Publisher · Related documents	Forslund O.K.,Ong C.S., Hirschmann M.M., … Eriksson O.,Mansson M.	Nature Communications , 17(1), 2112	2026
2	Article • *Open access* **Morphology-modified contributions of electronic transitions to the optical response of plasmonic nanoporous gold metamaterial** Show abstract · Uppsala UB · View at Publisher · Related documents	Tapani T.,Pettersson J.M., Henriksson N.,… Garoli D., Maccaferri N.	Nature Communications , 17(1), 829	2026
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Article

16 **Electrolyte effects in proton–electron transfer reactions and implications for renewable fuels and chemicals synthesis**

Sebastian-Pascual P., Herzog A., Zhang Y., Shao-Horn Y., Escudero-Escribano M.

Nature Catalysis, 8(10) — 2025

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Zhang M., Ma X., Esguerra J.L.,... Li J., Gao F.

Nature Sustainability, 8(3), 5859 — 2025

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Xiao X., Xu N., Tian X., ... You F., Gao F.

Nature, 638(8051) — 2025

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19 **Equally high efficiencies of organic solar cells processed from different solvents reveal key factors for morphology control**

Zhang R., Chen H., Wang T., ... Li Y., Gao F.

Nature Energy, 10(1), 4949 — 2025

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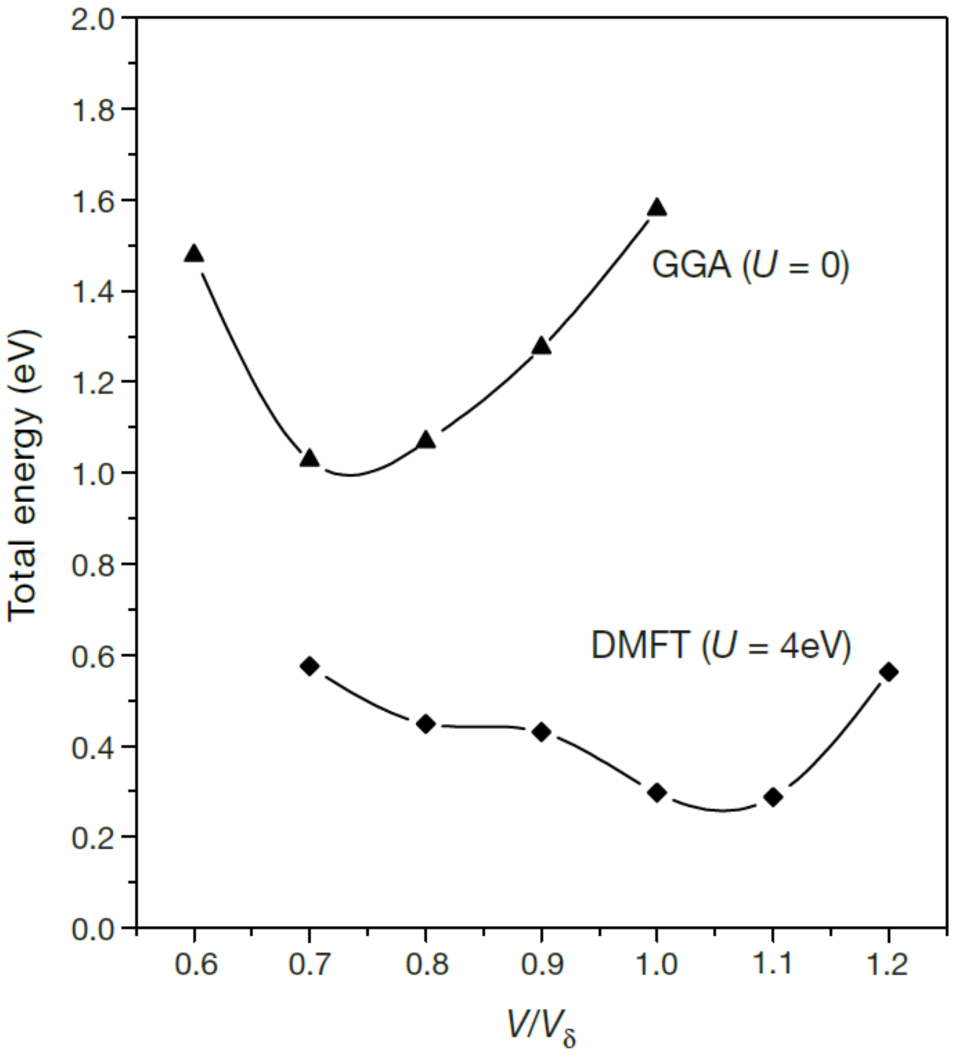
20 **Binding energy referencing in X-ray photoelectron spectroscopy**

Greczynski G., Hultman L.

Nature Reviews — 2025

The mysterious phase of δ-Pu

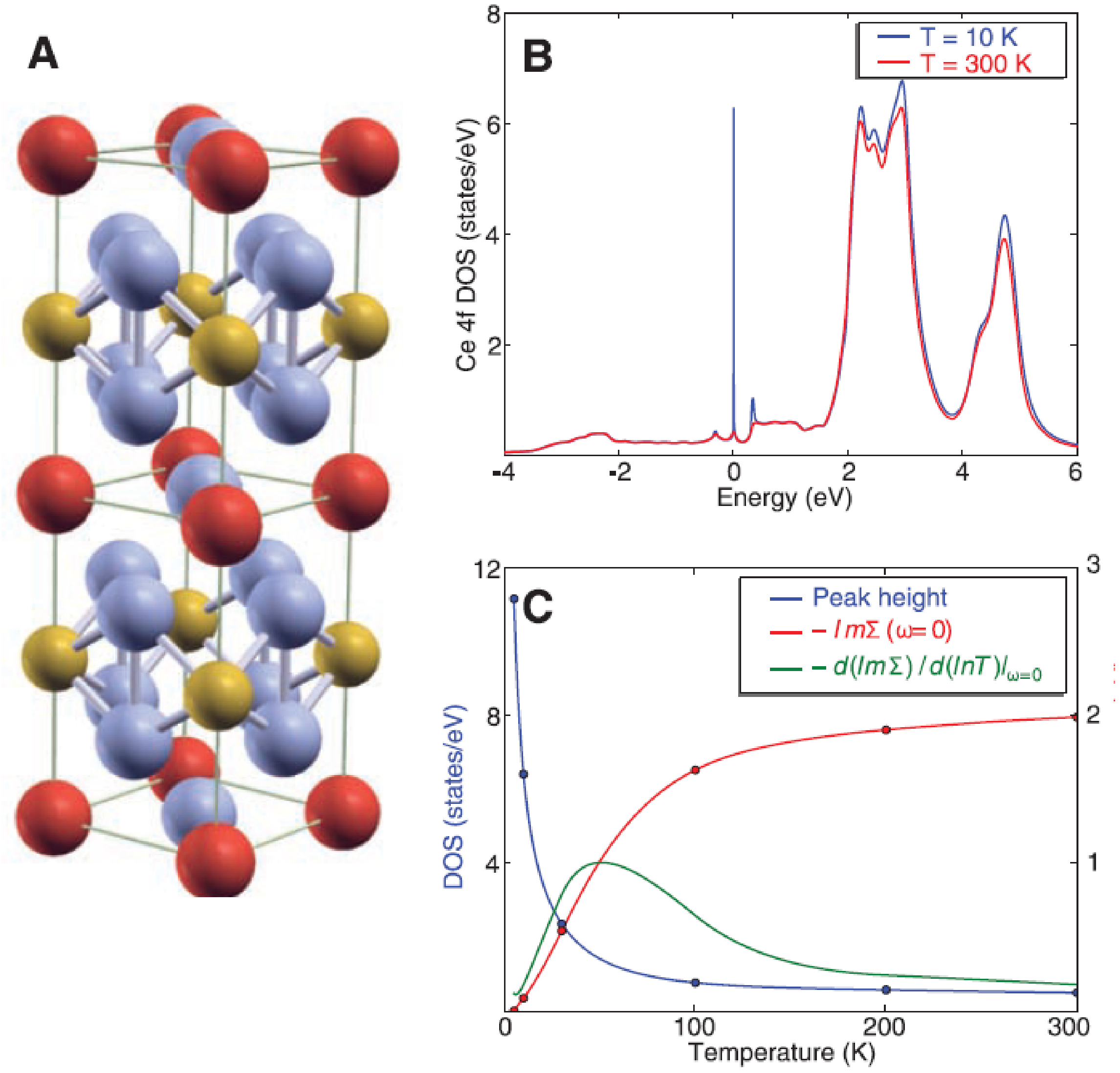


Correlated electrons in δ-plutonium within a dynamical mean-field picture

S. Y. Savrasov, G. Kotliar & E. Abrahams

Nature **410**, 793 (2001).

Heavy Fermions



CeIrIn5 – heay fermion system

Science **318**, 1615 (2007)

Electronic structure needed for:

Magnetism
Photovoltaics (solar cells)
LEDs
Batteries
Superconductors
Topological states

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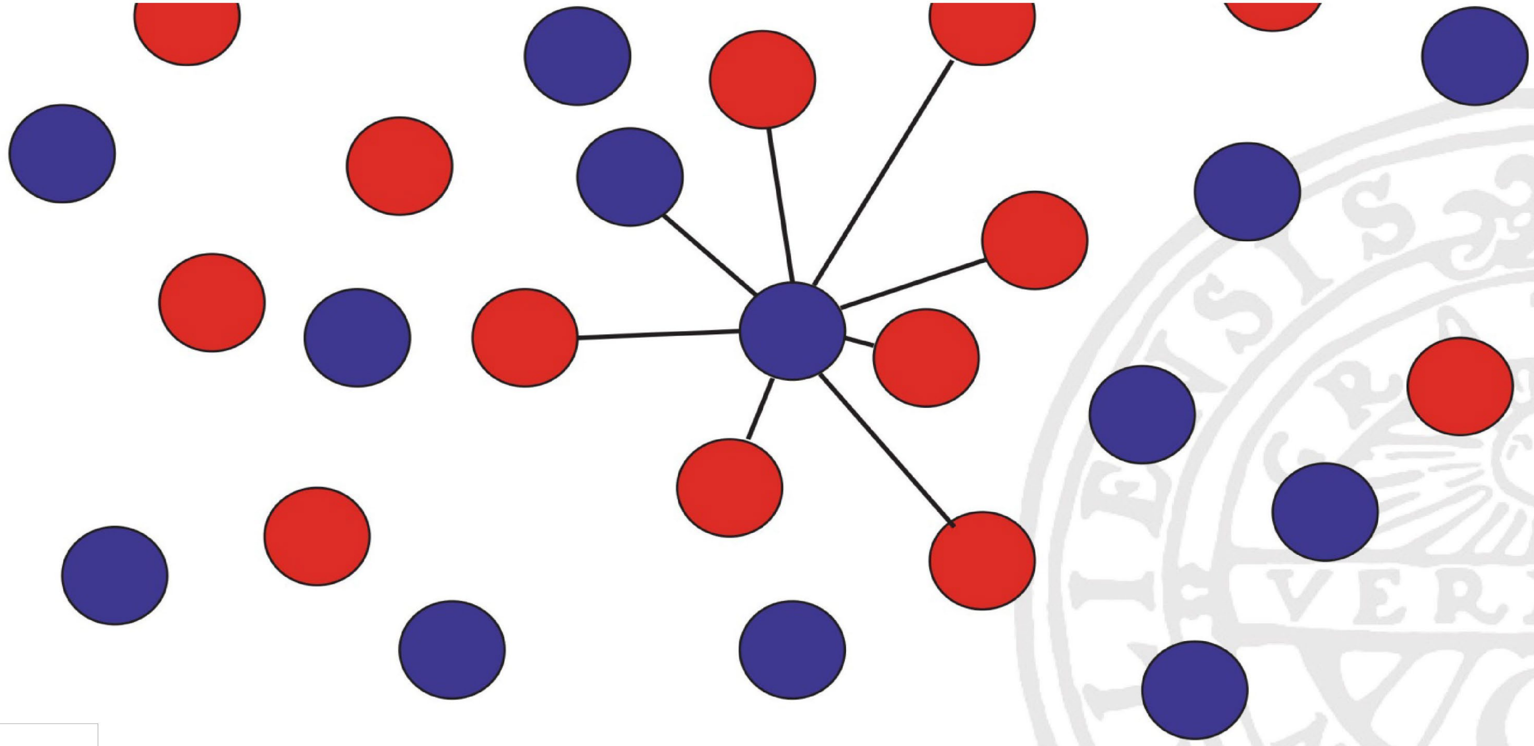
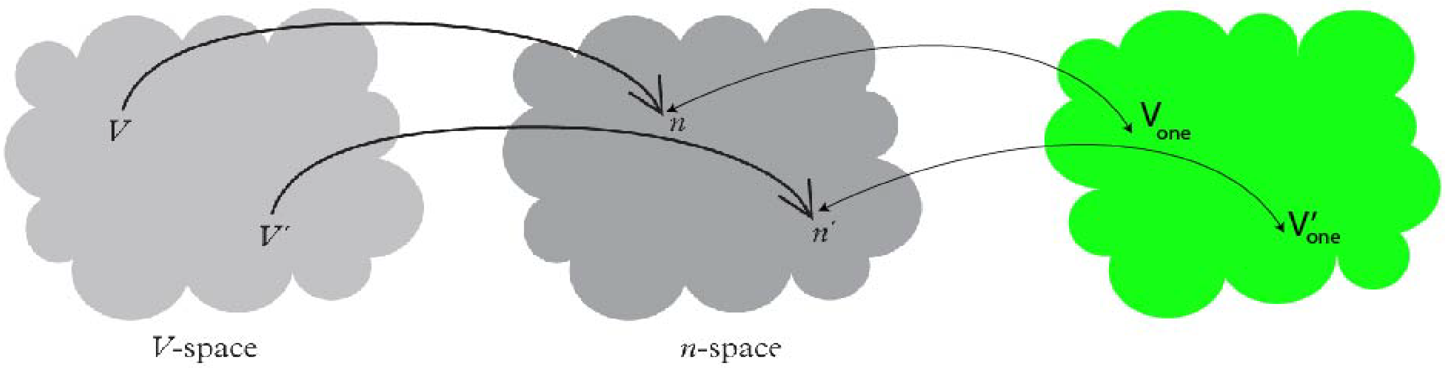
Full electron Hamiltonian

$$H = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i,I}\frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|}$$



Walter Kohns ideas



Hamiltonian of real systems

Hamiltonian of one-electron system

i) A functional exists that couples total energy to ground state electron density
ii) Find best approximation of E[n(r)] and minimize w.r.t. n(r)→ Dirac eller Schrödinger eqn. for one-electron system

Density Functional Theory

$$\hat{H}\Psi_{gs} = E_{gs}\Psi_{gs}$$

$$n_{gs}(\mathbf{r}) = \sum_{i=1}^{N} \int d^3r_i \;\; | \, \Psi_{gs}(\mathbf{r}_1, \mathbf{r}_2, \ldots . \mathbf{r}_N) \, |^2 \; \delta(\mathbf{r} - \mathbf{r}_i)$$ electron density

$$\hat{H}' \Psi'_{gs} = E'_{gs}\Psi'_{gs}$$

$$E_{gs} = \langle \Psi_{gs} \left| \hat{H} \right| \Psi_{gs} \rangle < \langle \Psi'_{gs} \left| \hat{H} \right| \Psi'_{gs} \rangle$$ variational principle

$$\langle \Psi'_{gs} \left| \hat{H} \right| \Psi'_{gs} \rangle = \langle \Psi'_{gs} \left| \hat{H} + V'_{ext} - V'_{ext} \right| \Psi'_{gs} \rangle = \langle \Psi'_{gs} \left| \hat{H}' + V_{ext} - V'_{ext} \right| \Psi'_{gs} \rangle$$

Density Functional Theory

$$\langle \Psi'_{gs} | \hat{H} | \Psi'_{gs} \rangle = E'_{gs} + \int n'_{gs} (V_{ext} - V'_{ext})\, d^3 r$$

$$E_{gs} < E'_{gs} + \int n'_{gs} (V_{ext} - V'_{ext})\, d^3 r$$

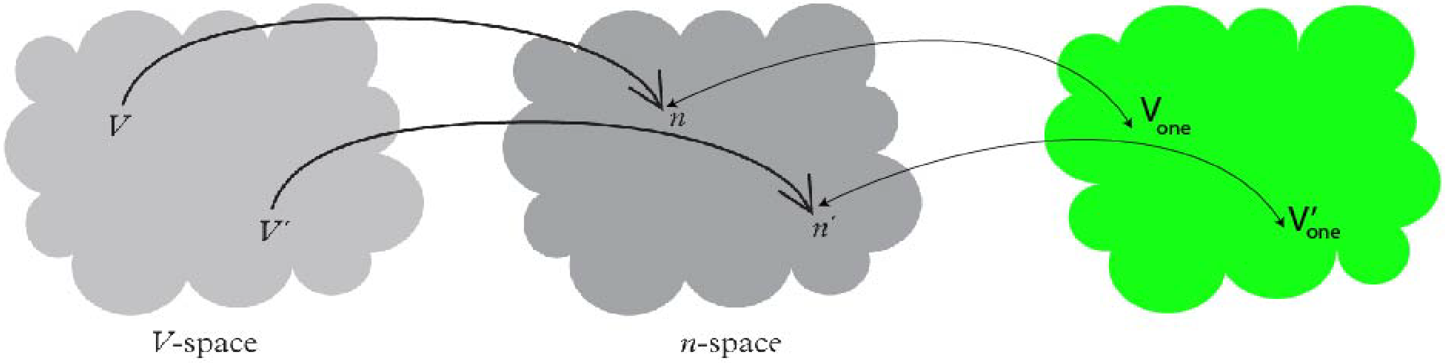
$$E'_{gs} < E_{gs} + \int n_{gs} (V'_{ext} - V_{ext})\, d^3 r$$

Assume densities are the same

$$E_{gs} + E'_{gs} < E'_{gs} + E_{gs} + \int n_{gs} (V_{ext} - V'_{ext})\, d^3 r + \int n_{gs} (V'_{ext} - V_{ext})\, d^3 r,$$

$$E_{gs} + E'_{gs} < E'_{gs} + E_{gs}$$

Walter Kohns ideas



Hamiltonian of real systems

Hamiltonian of one-electron system

i) A functional exists that couples total energy to ground state electron density

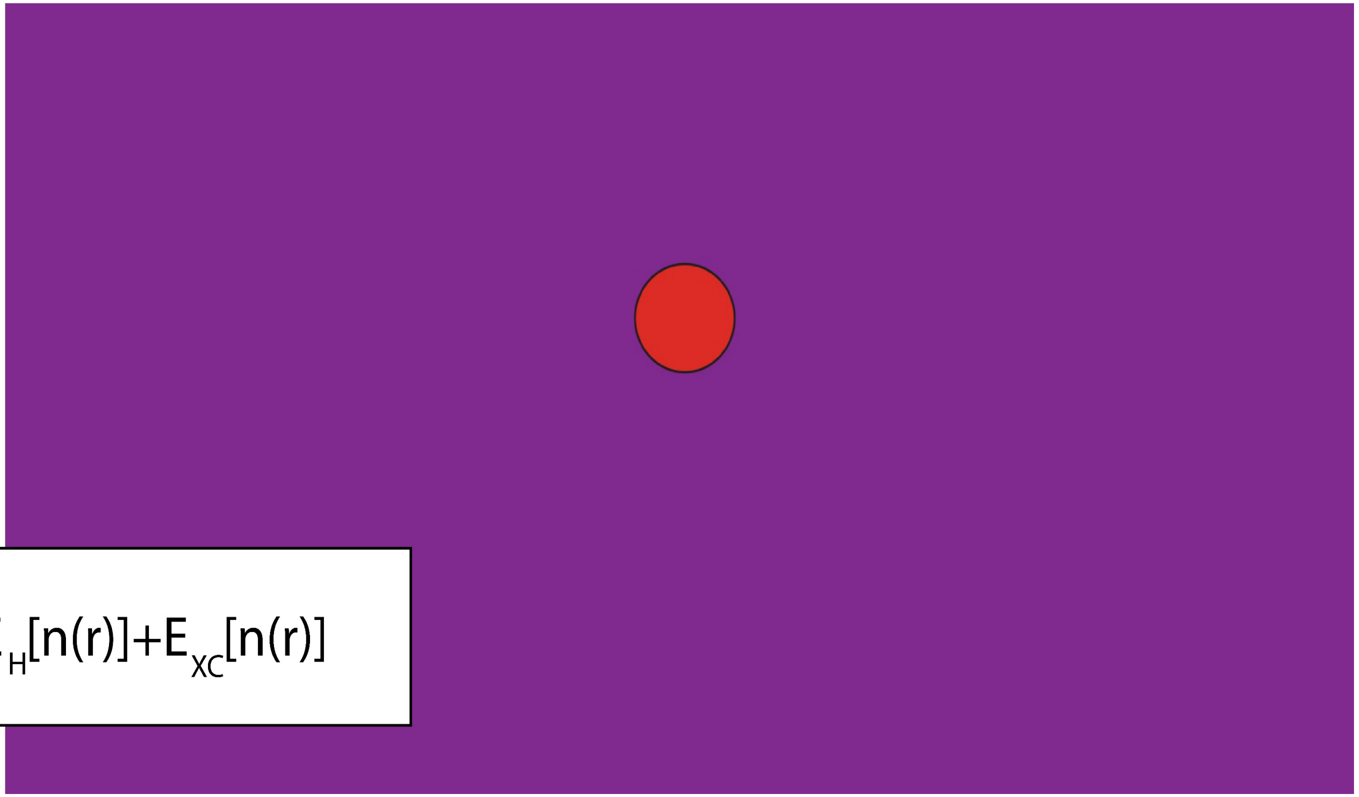
ii) Find best approximation of E[n(r)] and minimize w.r.t. n(r)→ Dirac eller Schrödinger eqn. for one-electron system

One-electron Hamiltonian

$$\left(-\frac{\nabla^2}{2} + V_{eff}\right)\psi = \varepsilon\psi$$

$$V_{eff}(n(r))$$

$$n(r) = \sum |\psi(r)|^2$$



$dE[n(r)]/dn=0$

$E[n(r)]=E_{kin}[n(r)]+E_H[n(r)]+E_{XC}[n(r)]$

The density functional

$$E[n_{op}(\mathbf{r})] = T_{op}[n_{op}(\mathbf{r})] + \int n_{op}(\mathbf{r}) V_{ext}(\mathbf{r})\, d^3r + \iint \frac{n_{op}(\mathbf{r}) \cdot n_{op}(\mathbf{r}')}{\mathbf{r} - \mathbf{r}'} d^3r\, d^3r' + E_{xc}[n_{op}(\mathbf{r})]$$

$$E_{xc}[n_{op}(\mathbf{r})] = \int \epsilon_{xc}[n_{op}(\mathbf{r})] n_{op}(\mathbf{r})\, d^3r$$

$$V_{eff}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int \frac{n_{op}(\mathbf{r}')}{|\,\mathbf{r} - \mathbf{r}'\,|} d^3r' + \mu_{xc}[n_{op}(\mathbf{r})]$$

$$\mu_{xc}[n_{op}(\mathbf{r})] = \frac{\partial \{\epsilon_{xc}[n_{op}(\mathbf{r})] n_{op}(\mathbf{r})\}}{\partial n_{op}(\mathbf{r})} = \epsilon_{xc}[n_{op}(\mathbf{r})] + n_{op}(\mathbf{r}) \frac{\partial \{\epsilon_{xc}[n_{op}(\mathbf{r})]\}}{\partial n_{op}(\mathbf{r})}$$

For a crystalline material

$$H_{one} = \frac{-\nabla^2}{2} + V_{eff}$$

$$H_{one}\psi(\mathbf{r}) = \epsilon\psi(\mathbf{r})$$

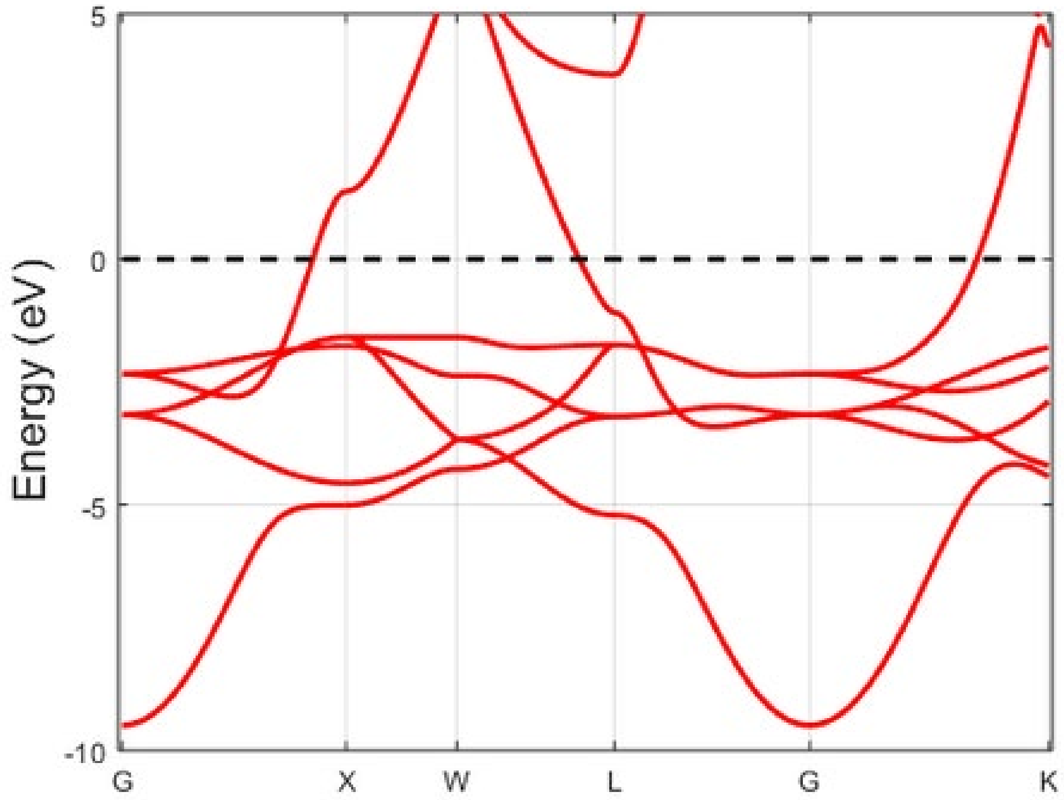
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

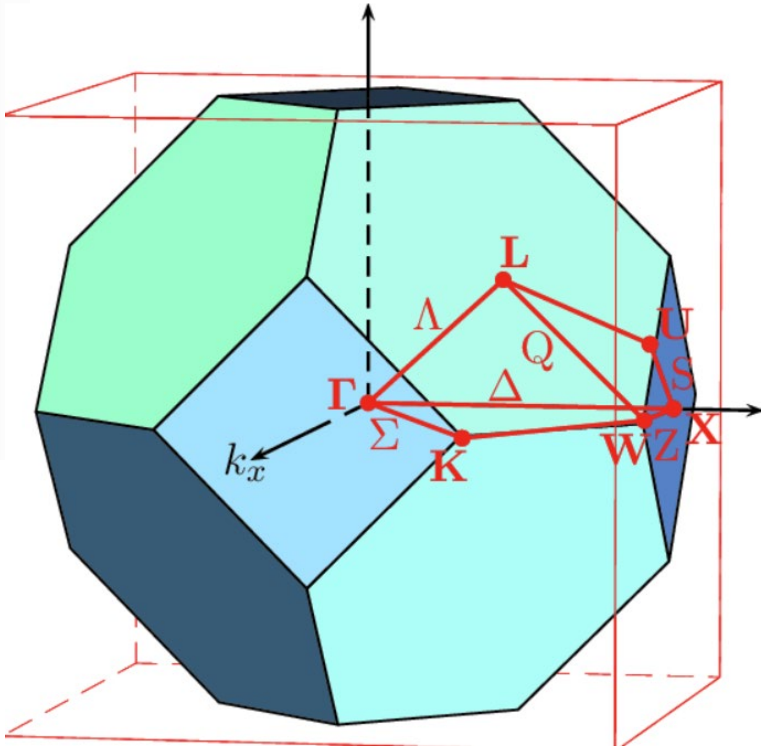
with $u(\mathbf{r})$ having the same periodicity as the lattice

$$\psi(\mathbf{r}) \rightarrow \psi_{\mathbf{k}}(\mathbf{r})$$

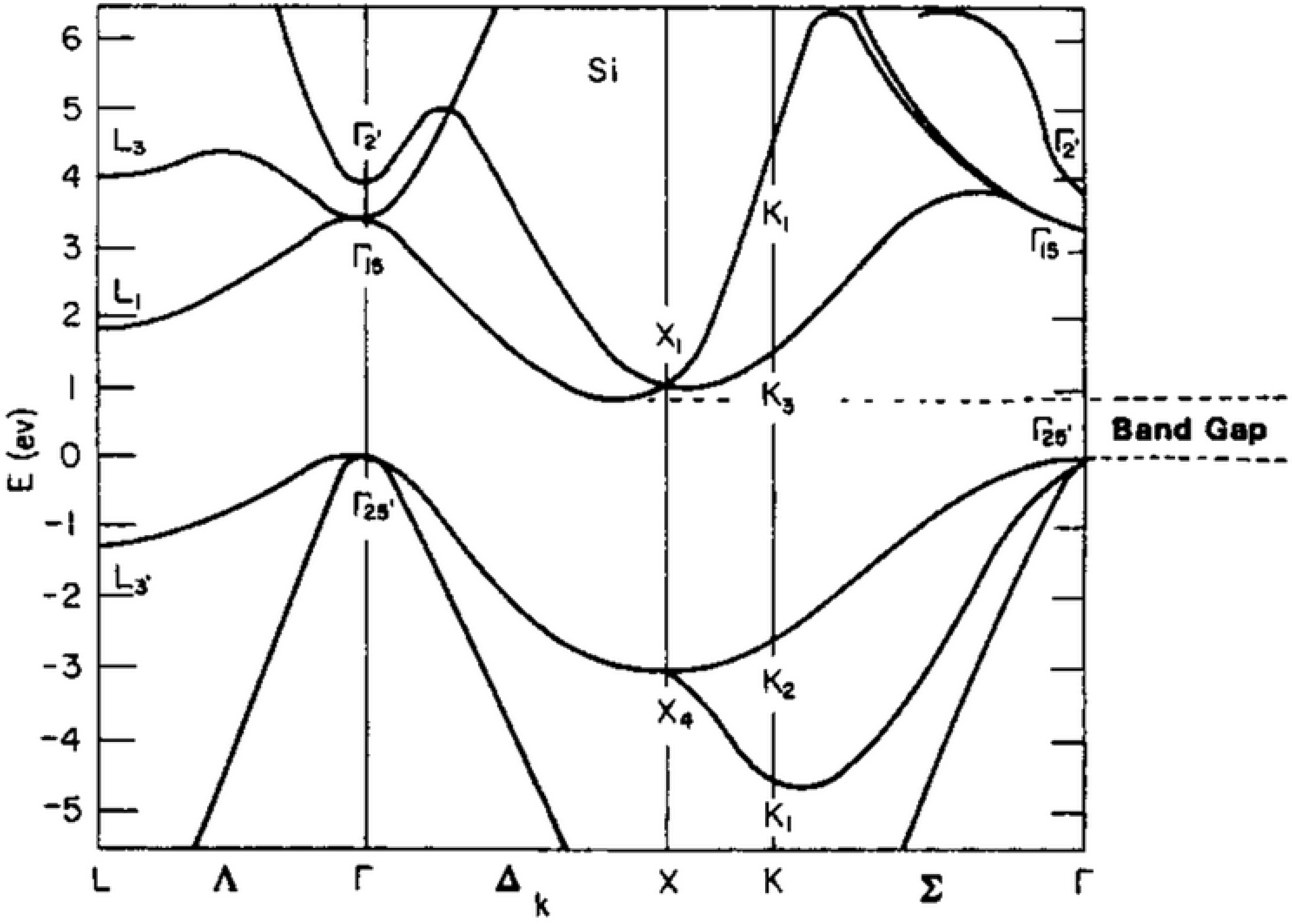
$$\epsilon \rightarrow \epsilon_{\mathbf{k}}$$

Bands of fcc Cu



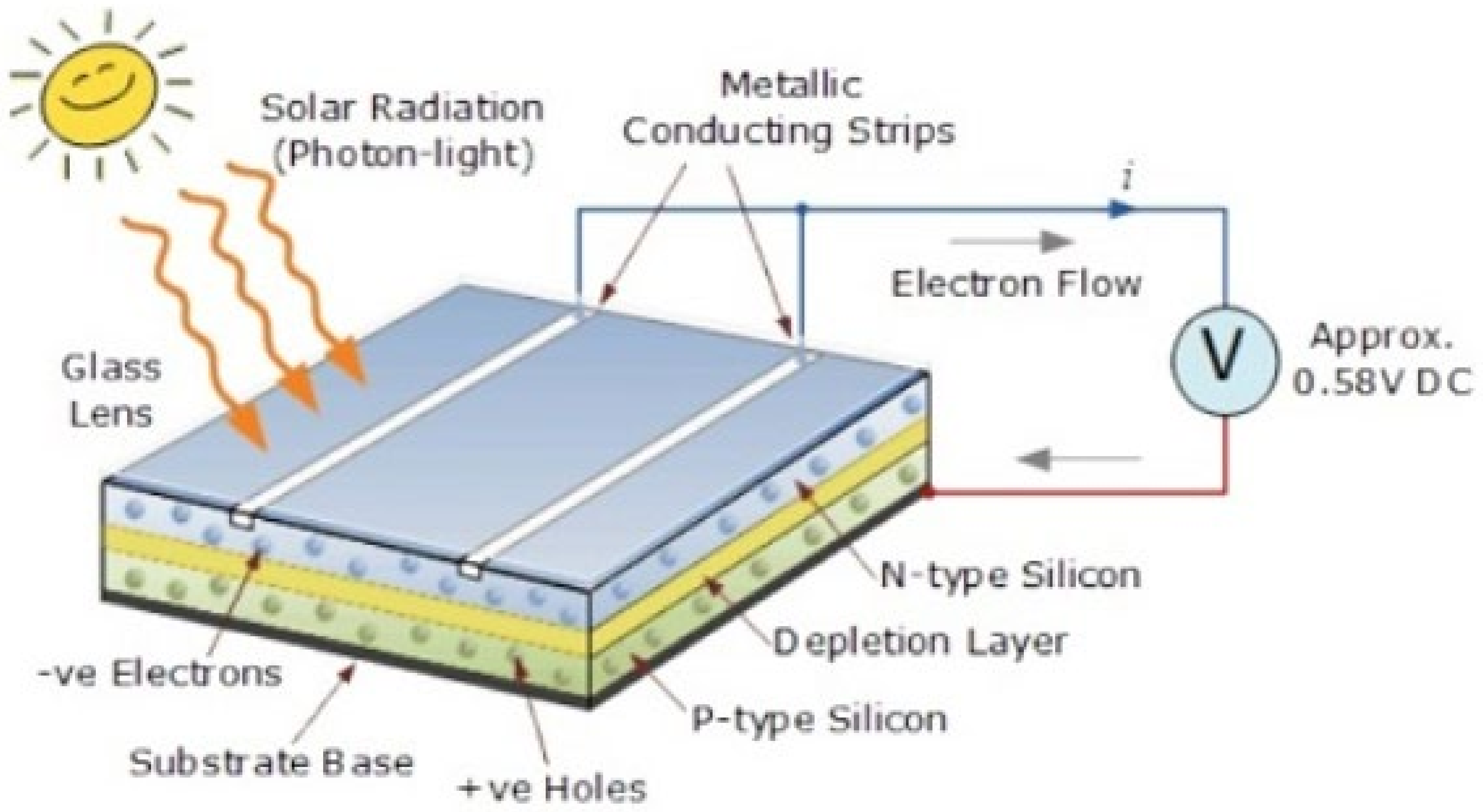


Bands of Si

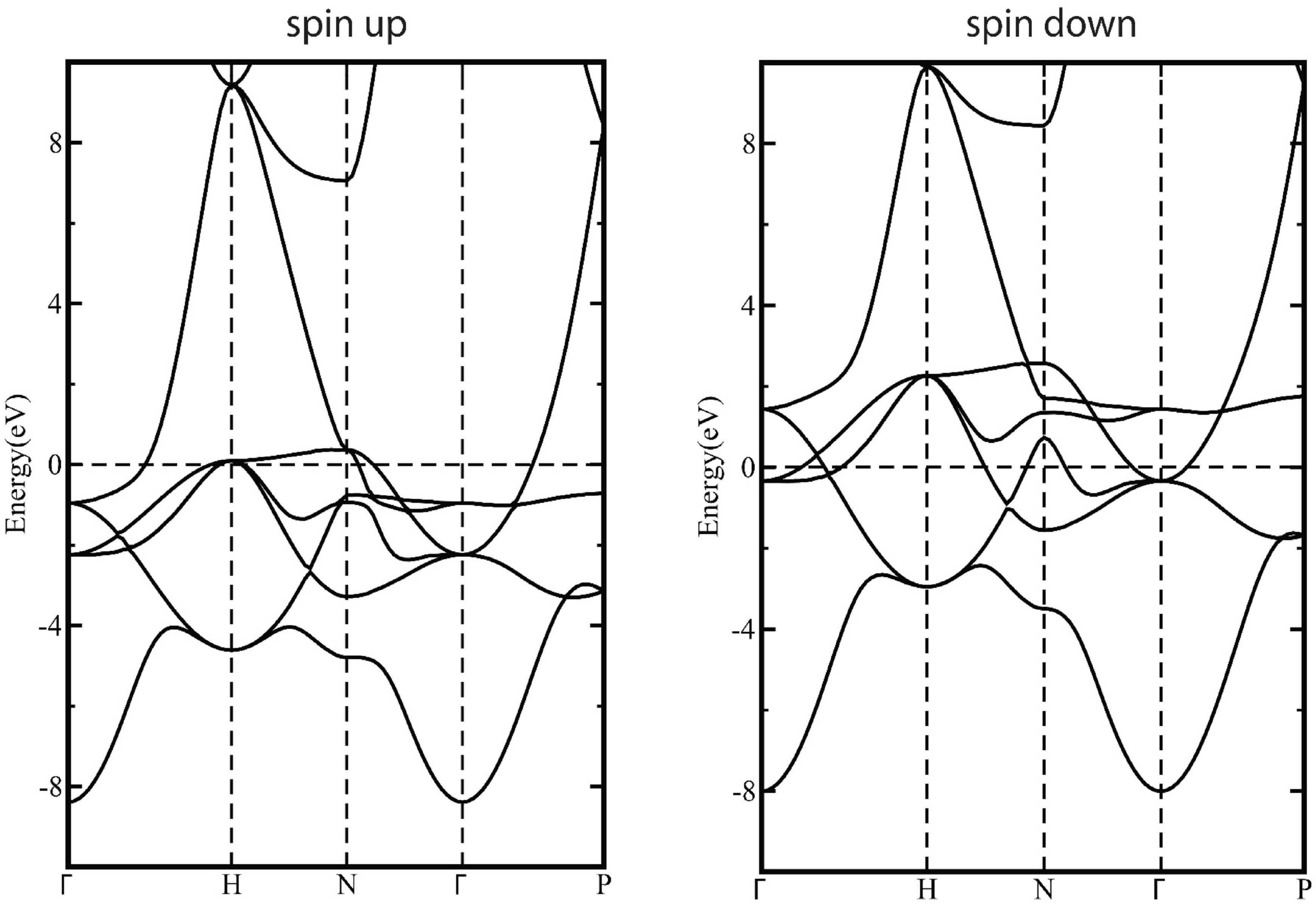


Si
E (ev)
6
5
4
3
2
1
0
-1
-2
-3
-4
-5
L₃
L₁
L₃'
Γ₂'
Γ₁₅
Γ₂₅'
X₁
X₄
K₁
K₃
K₂
K₁
Γ₂'
Γ₁₅
Γ₂₅'
Band Gap
L
Λ
Γ
Δ
k
X
K
Σ
Γ

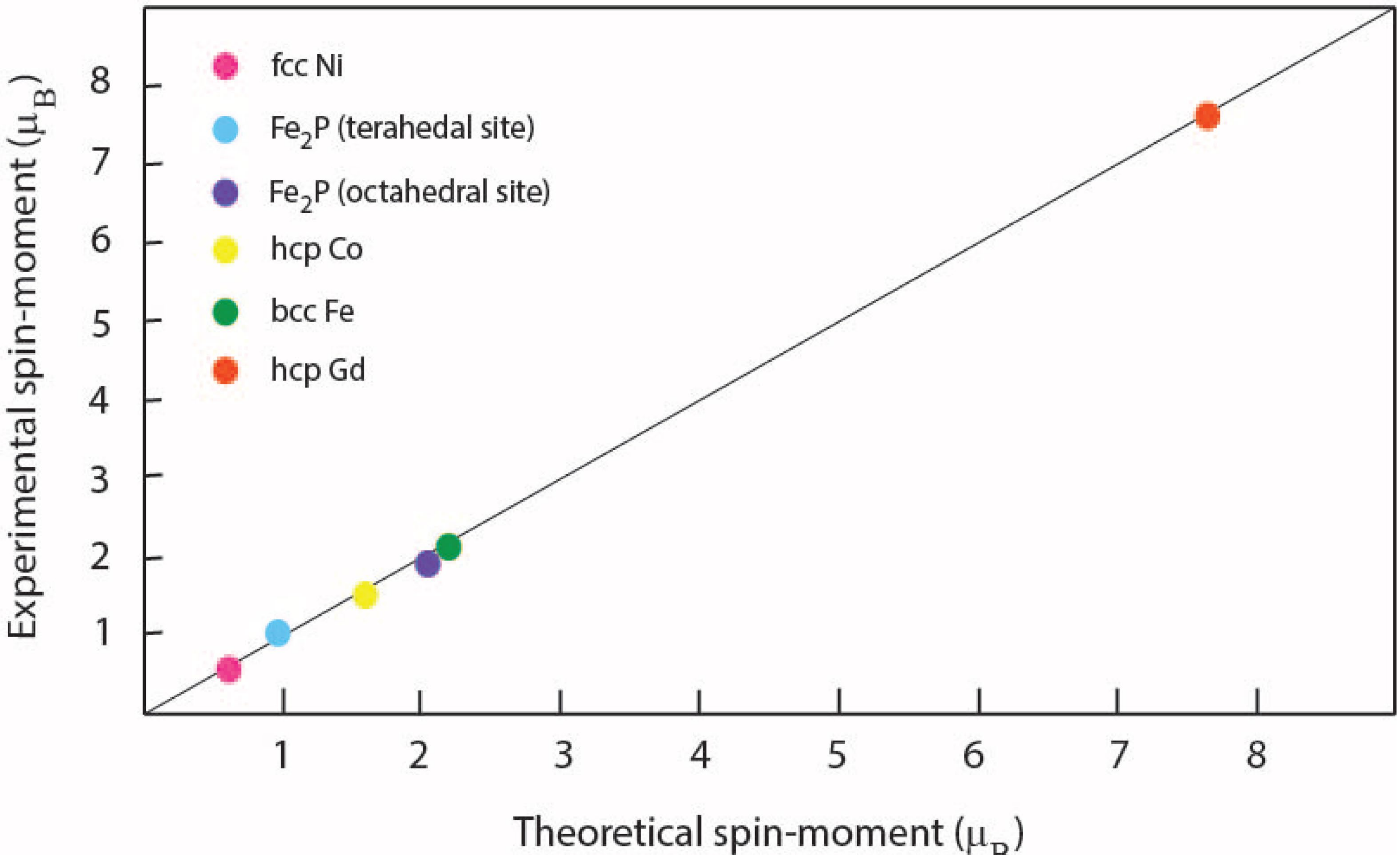
Si solar cells/Light emitting diodes



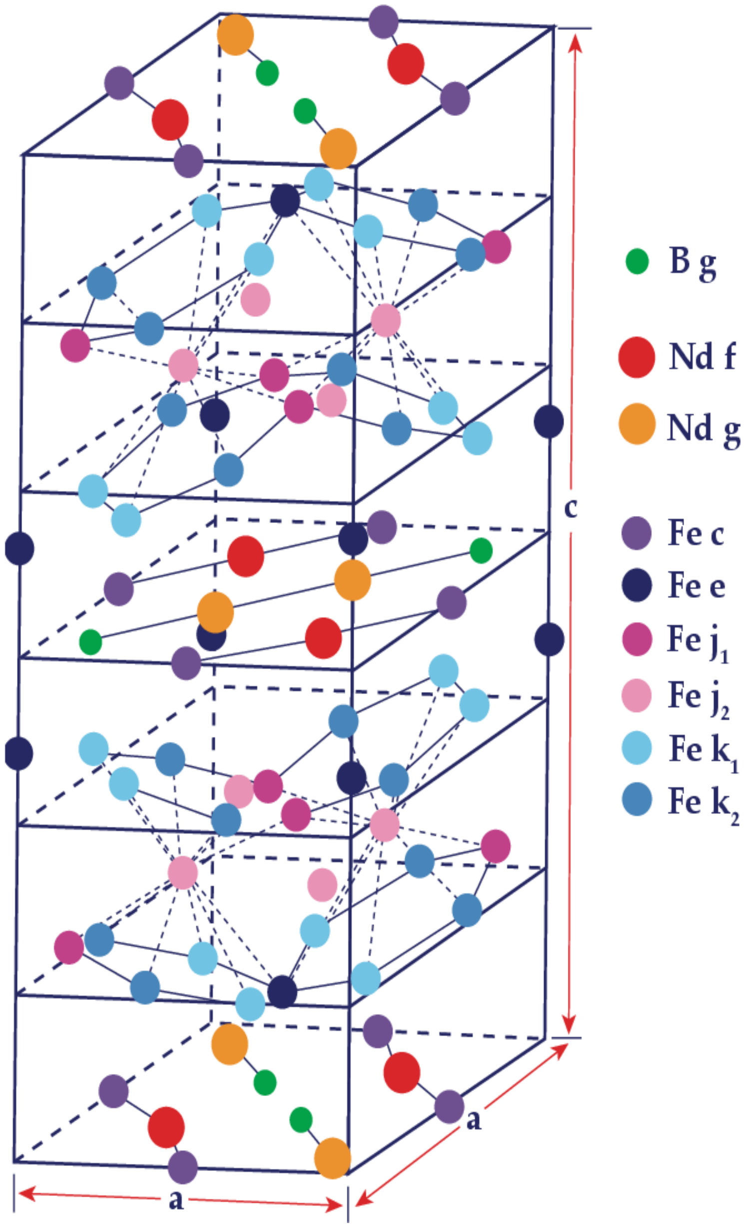
Bands of bcc Fe



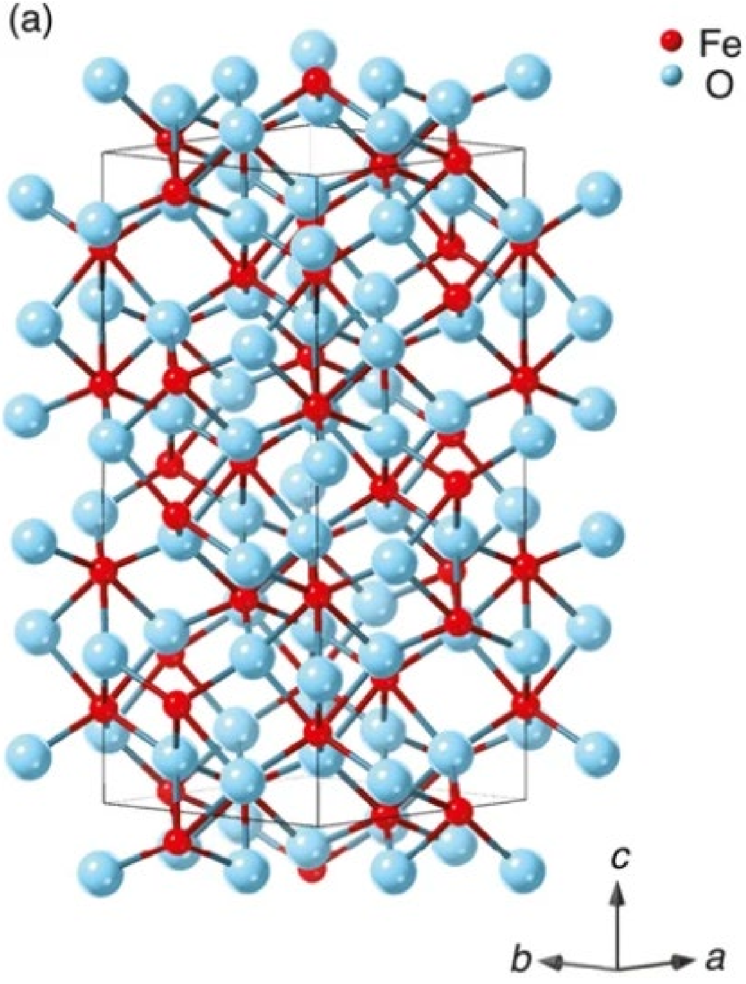
Calculations of magnetic moments

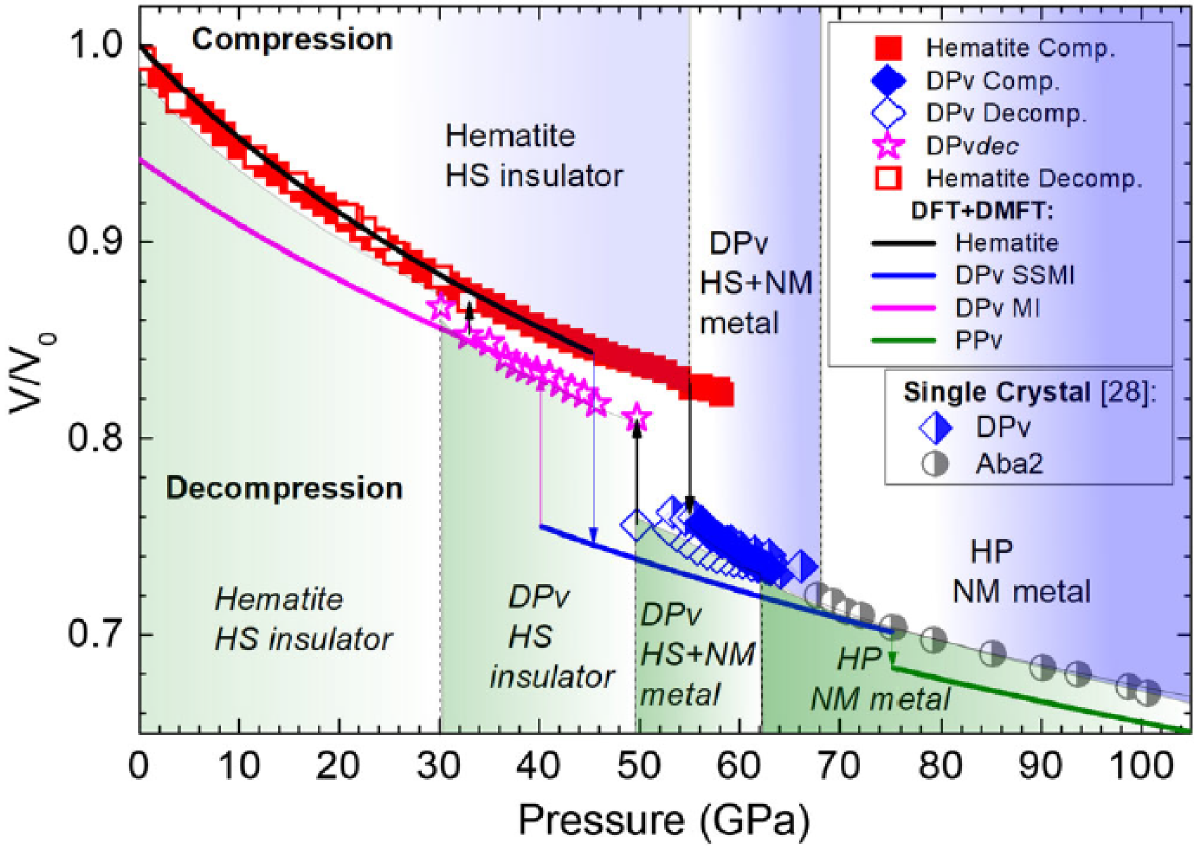


Permanent magnet applications



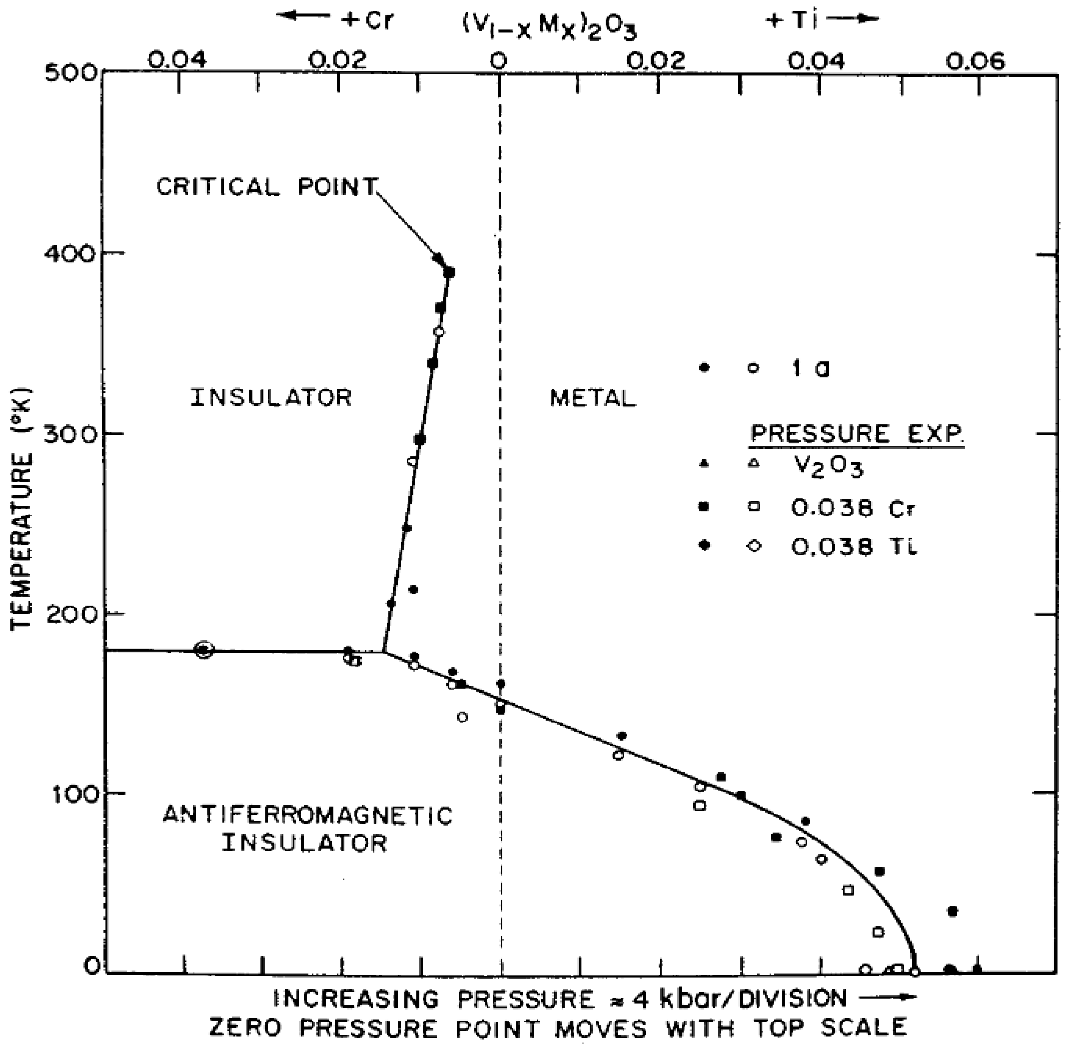
ESS (European Spallation Source) and Fe_2O_3

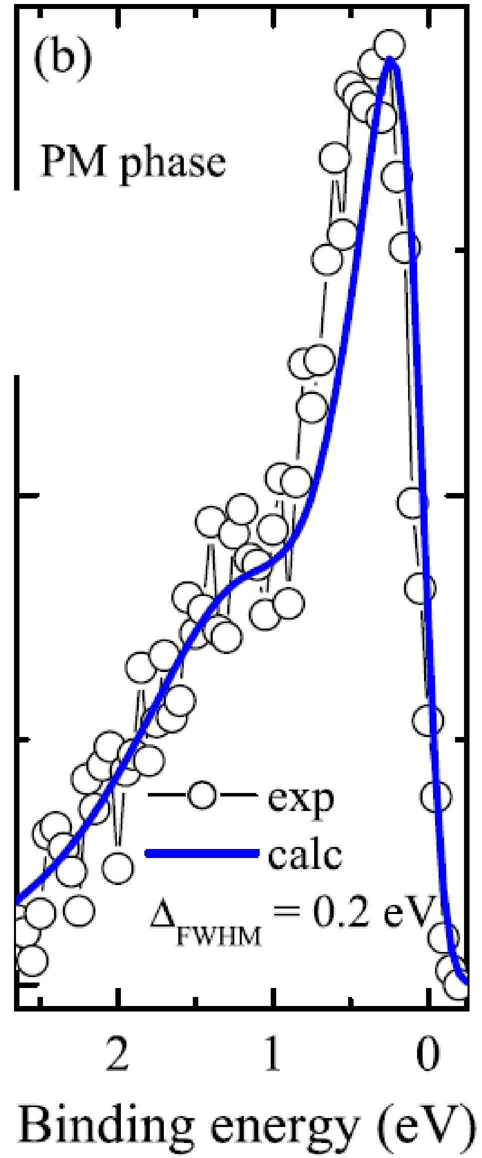




PRX **8**, 031059 (2018)

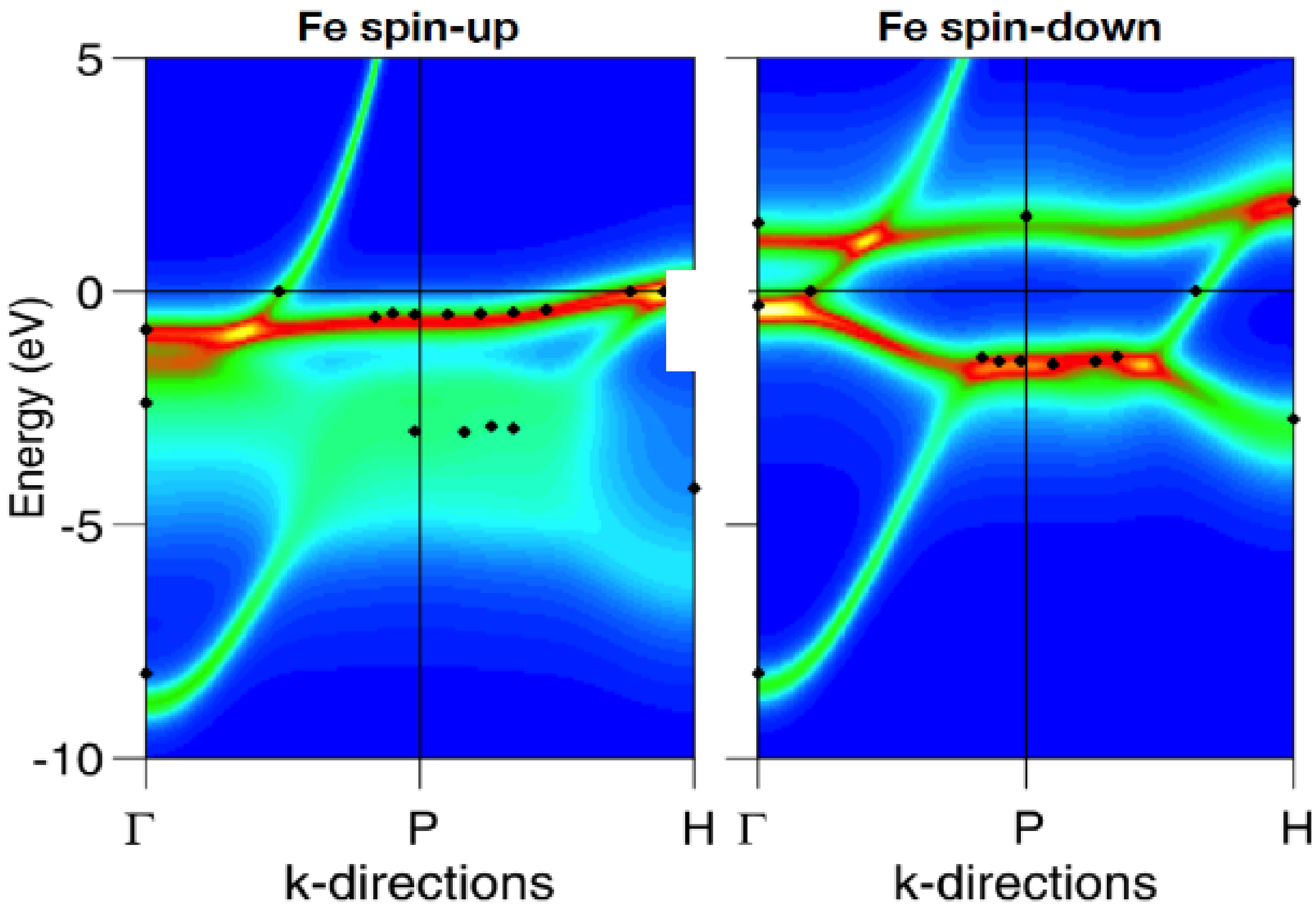
MAX IV, photoelectron spectroscopy





PRL **97**, 116401 (2006)

MAX IV, Bloch beam line for ARPES



Lichtenstein och Katsnelson,
J.Phys. Cond. Matt. ***11****, 1037 (1999)*

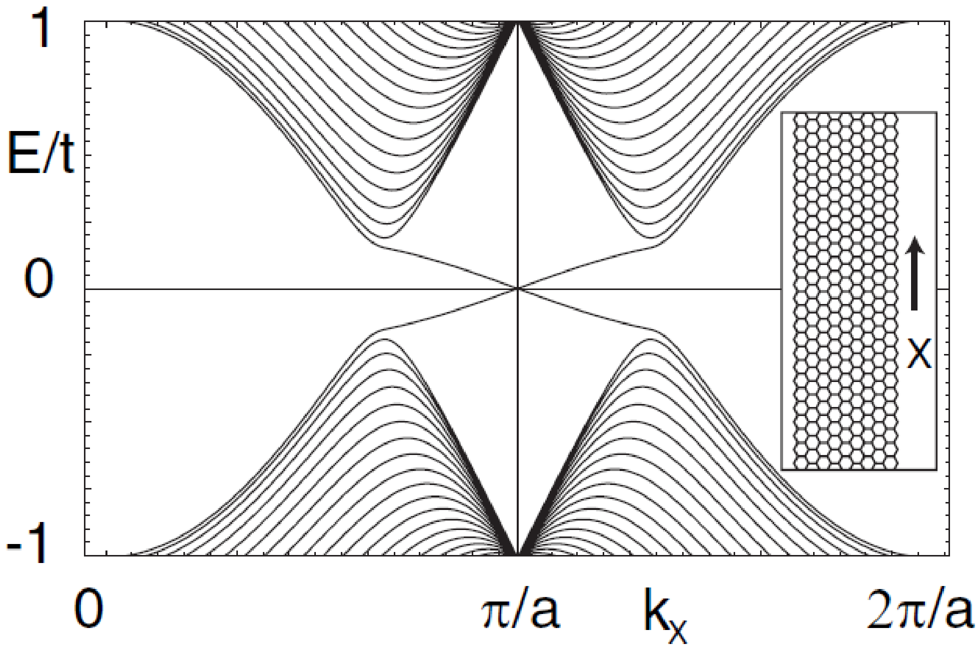
MAX IV, Topological edge states

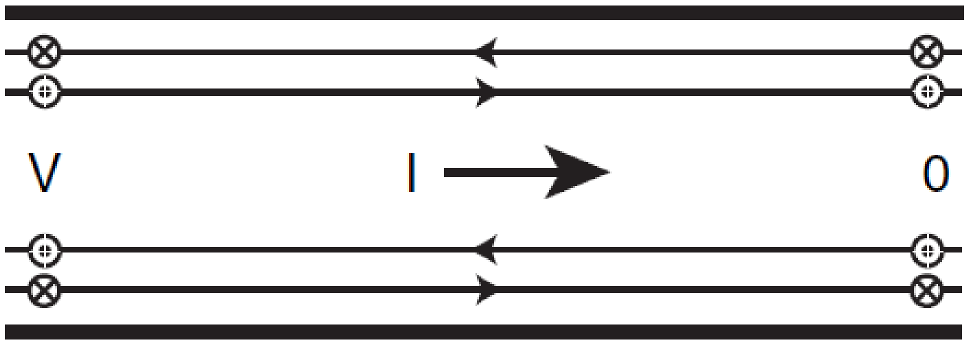
$$\sigma^s_{xy} = \frac{e}{2\pi}$$

$$\sigma_0^{xy} = \nu e^2/(2\pi\hbar)$$

$$\nu_n(\mu) = \frac{1}{2\pi}\int d^2\boldsymbol{k}\,\mathcal{F}_n^{xy}(\boldsymbol{k})P_{\mathrm{BZ}}(\boldsymbol{k})n_n(\boldsymbol{k},\mu)$$

$$\mathcal{A}_n^a(\boldsymbol{k}) = -i\langle\psi_n(\boldsymbol{k})|\nabla_k^a\psi_n(\boldsymbol{k})\rangle,$$
$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = \nabla_k^a\mathcal{A}_n^b(\boldsymbol{k}) - \nabla_k^b\mathcal{A}_n^a(\boldsymbol{k})$$





Kane & Mele, Phys. Rev. Lett. 95, 226802 (2005)
Haldane, Phys. Rev. Lett. 93, 206602 (2004)