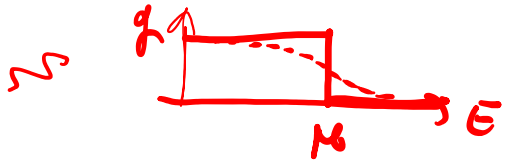
MSE 423 Fall 2025 – Week 12

Semi-conductors



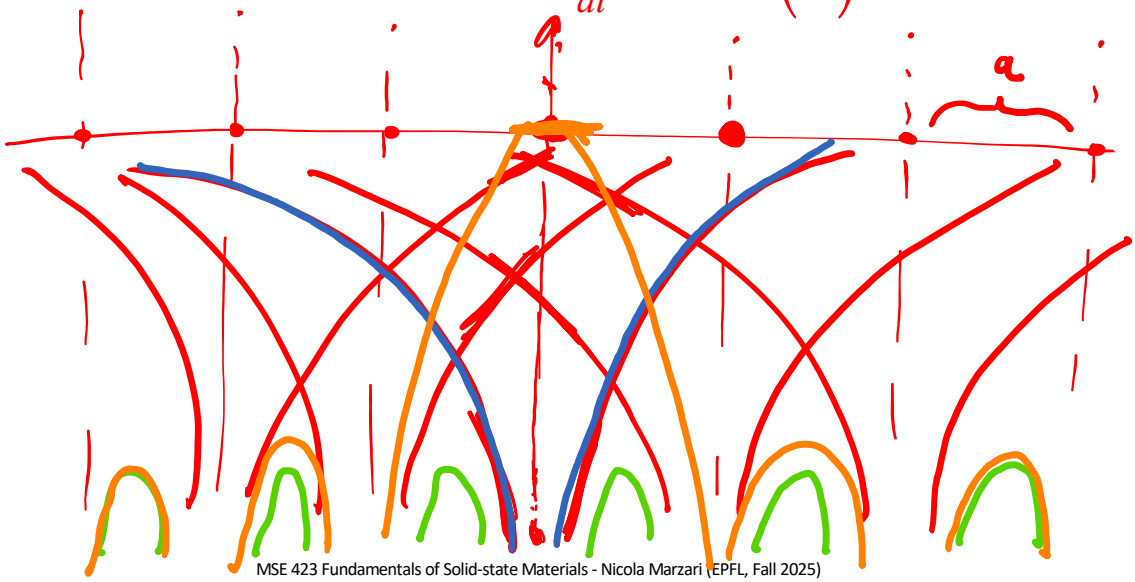
Last week

- Fermi surfaces
- The independent-electron gas: BvK boundary conditions and the counting of states
- Particles density and energy density
- Density of states; massive vs massless bands
- Statistics of classical and quantum particles
- Probability and partition function
- Chemical potential and Fermi-Dirac distribution



Tight-binding (LCAO for solids)

- Hamiltonian $\hat{H} = \hat{H}_{at} + \Delta\hat{U}(\vec{r})$



Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

$$\Psi_{i\vec{k}}(\vec{r}) = \sum_{\vec{R}'} \exp\left(i\vec{k}\cdot\vec{R}'\right)\varphi_i\left(\vec{r}-\vec{R}'\right)$$

(BLOCH SUM)

$$\Psi_{\vec{k}}(\vec{r}+\vec{R}) = \sum_{\vec{R}'} \exp\left(i\vec{k}\cdot\vec{R}'\right)\varphi\left((\vec{r}+\vec{R})-\vec{R}'\right)$$

$$= \sum_{\vec{R}'} \exp\left(i\vec{k}\cdot\vec{R}'\right) e^{i\vec{k}\cdot\vec{R}} \cdot e^{-i\vec{k}\cdot\vec{R}}\,\varphi\left(\vec{r}+\vec{R}-\vec{R}'\right)$$

$$= e^{i\vec{k}\cdot\vec{R}} \sum_{\vec{R}'} \exp\left(i\vec{k}\cdot(\vec{R}'-\vec{R})\right)\varphi\left(\vec{r}-(\vec{R}'-\vec{R})\right)$$

Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

BLOCH SUM OF WANN. FUNCTION.

$$\Psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{R}} \exp\left(i\vec{k}\cdot\vec{R}\right)\phi_n\left(\vec{r}-\vec{R}\right)$$

$$\phi_n(\vec{r}) = \sum_m b_m \varphi_m(\vec{r})$$

"WANNIER FUNCTIONS"

$$E_{nk} = \langle \Psi_{nk} | \hat{H} | \Psi_{nk} \rangle$$

From levels to bands

$\langle \varphi | \hat{H}_{AT} | \varphi' \rangle$

$\gamma(\vec{R}) = -\int \varphi^*(\vec{r}) \Delta U \varphi(\vec{r}-\vec{R})$

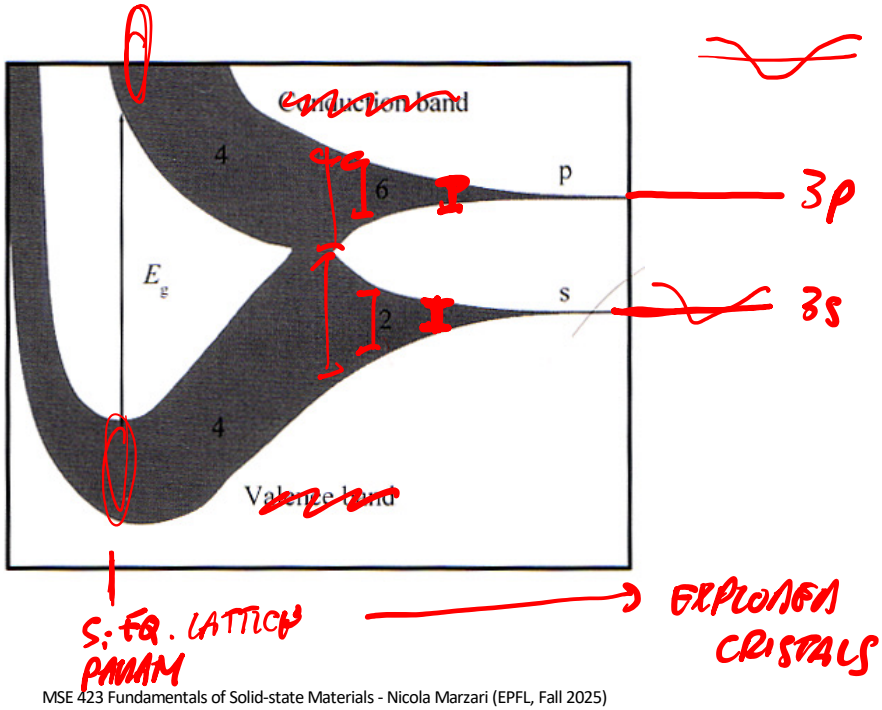
$$\varepsilon(\vec{k}) = E_m - \beta - \sum_{\substack{\text{nearest} \\ \text{neighb.}}} \gamma(\vec{R})\cos\left(\vec{k}\cdot\vec{r}\right)$$

$-|\gamma|$

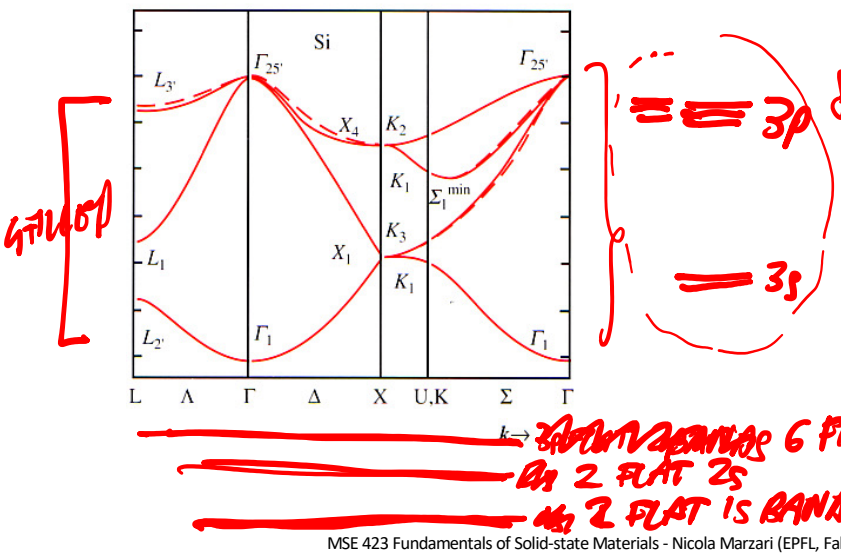
E_m

$\beta = -\int \varphi^*(\vec{r}) \Delta U \varphi(\vec{r})$ ΔU

From levels to bands



How many bands in silicon ?



Tight-binding vs. empirical psp

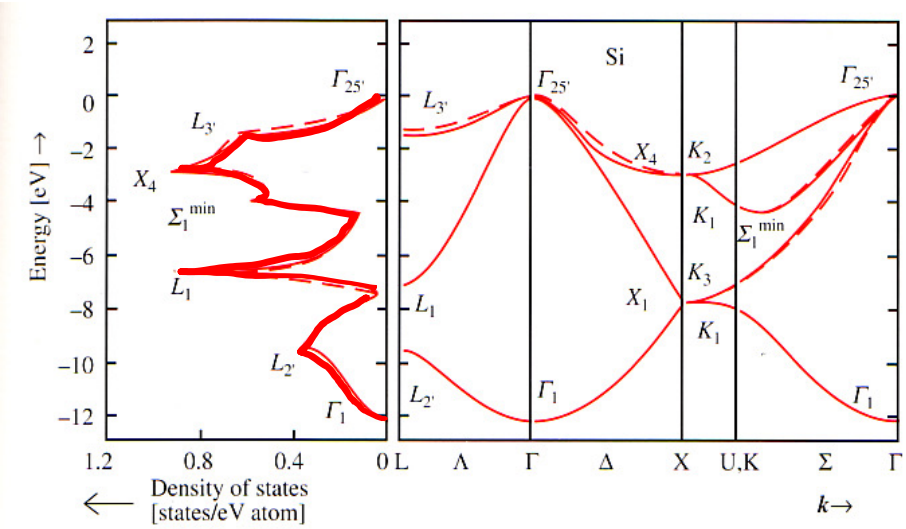


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

Tight-binding vs. empirical psp

TIGHT BINDING → TRUE ← FREE

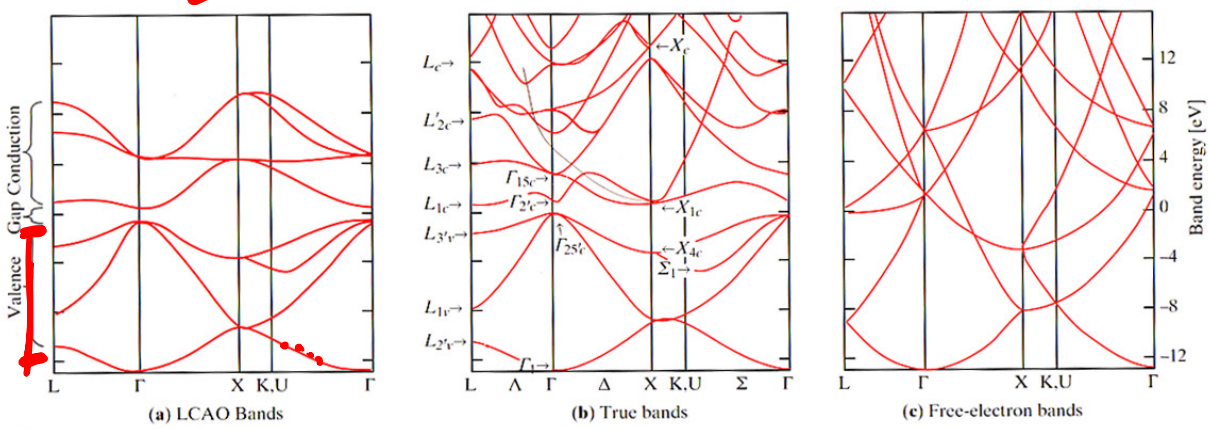
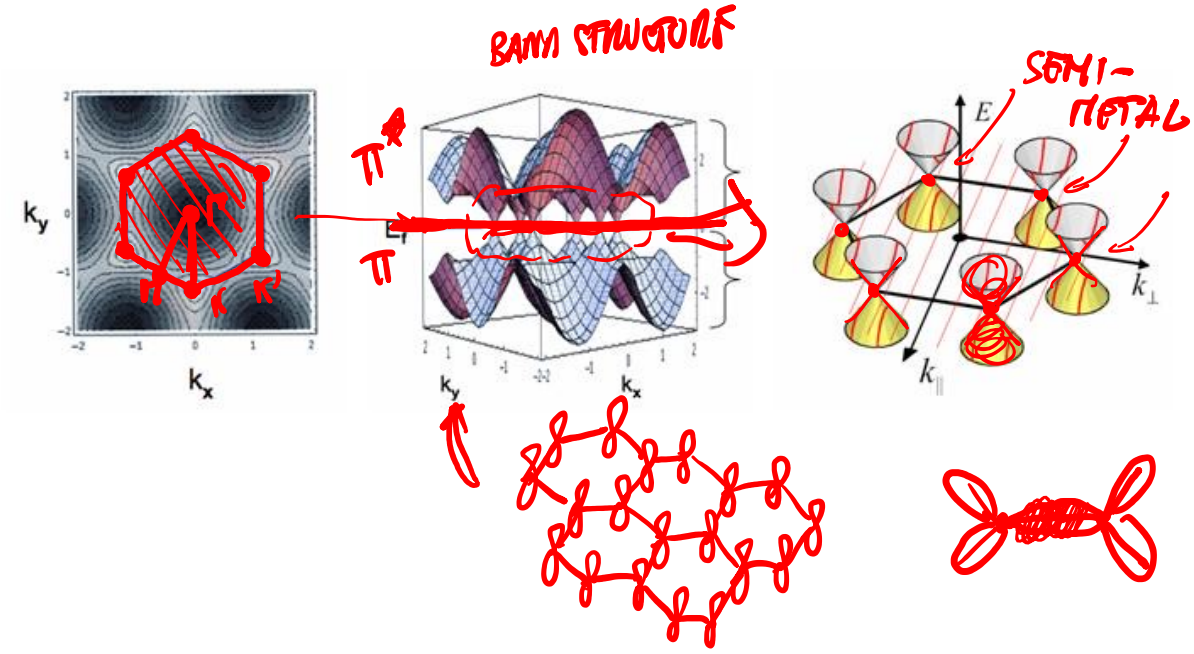
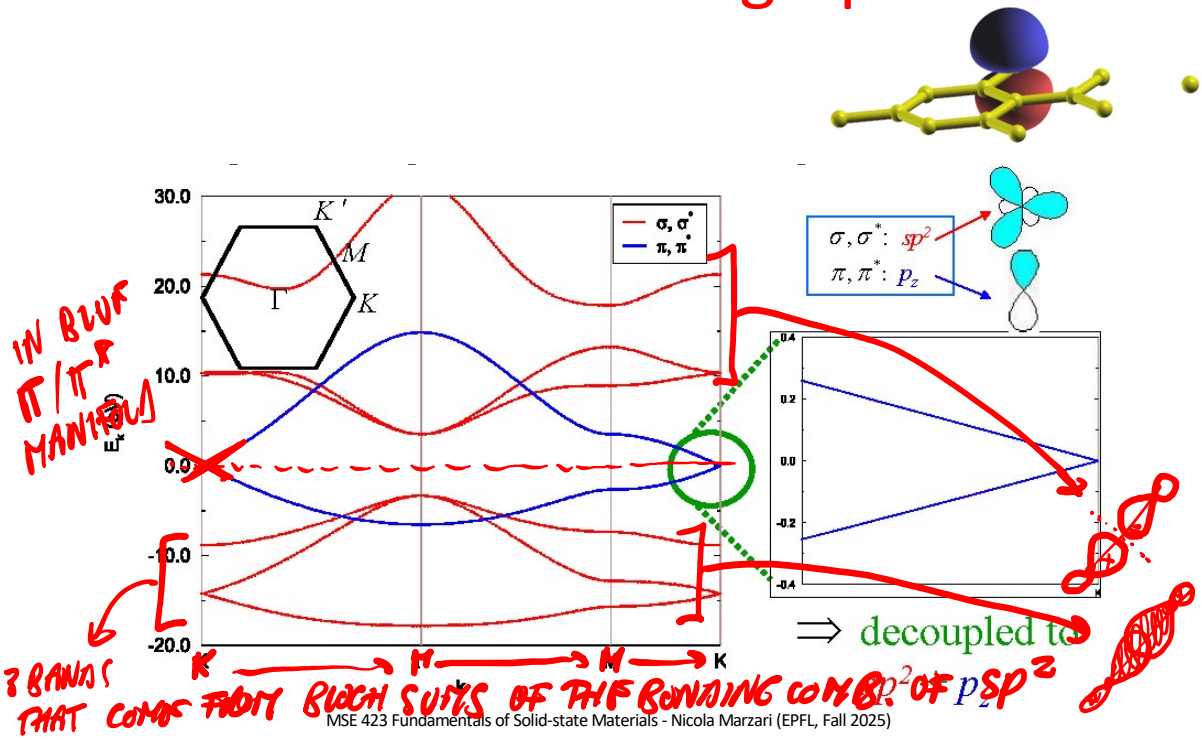


Fig. 2.25. A comparison between the band structure of Ge calculated by **(a)** the tight-binding method, **(b)** the empirical pseudopotential method, and **(c)** the nearly free electron model [Ref. 2.18, p. 79]

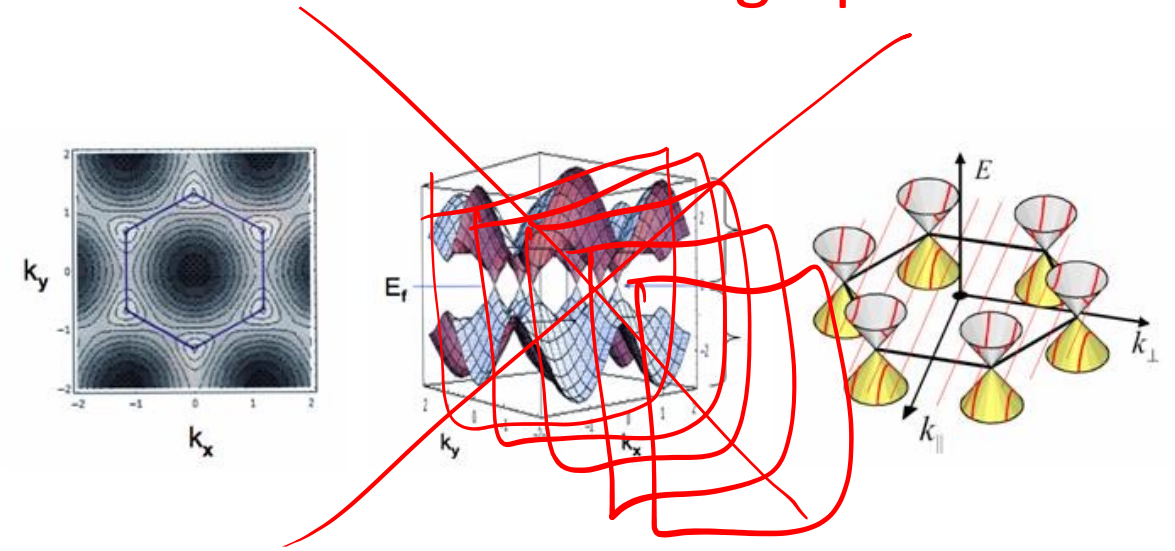
Band structure of graphene



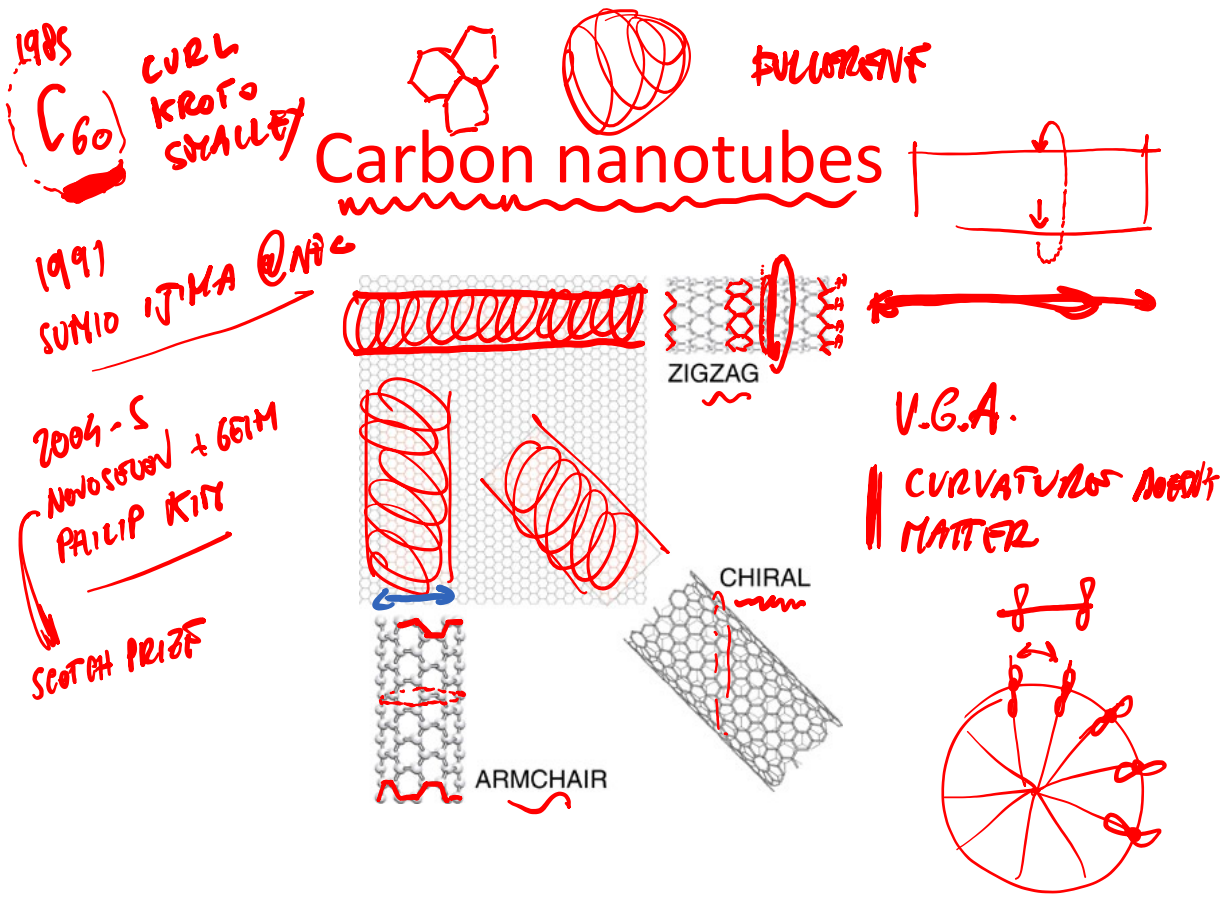
Band structure of graphene



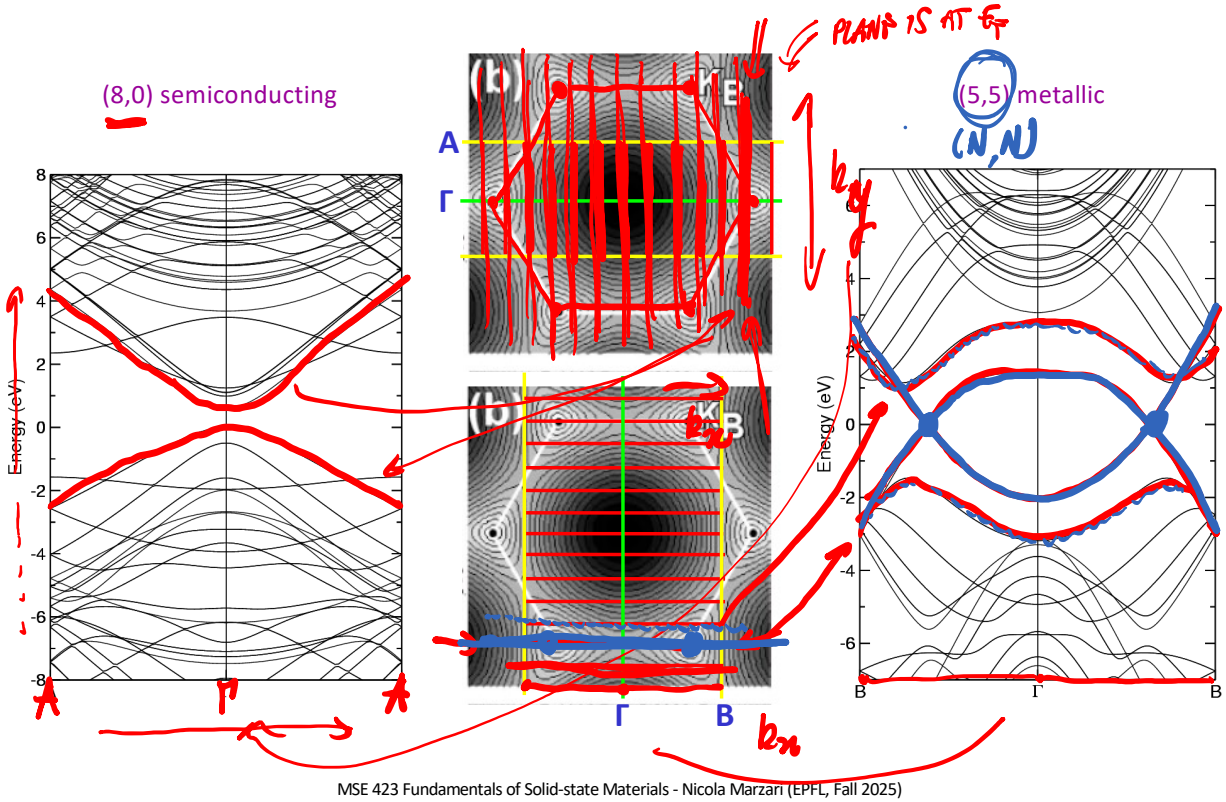
Band structure of graphene



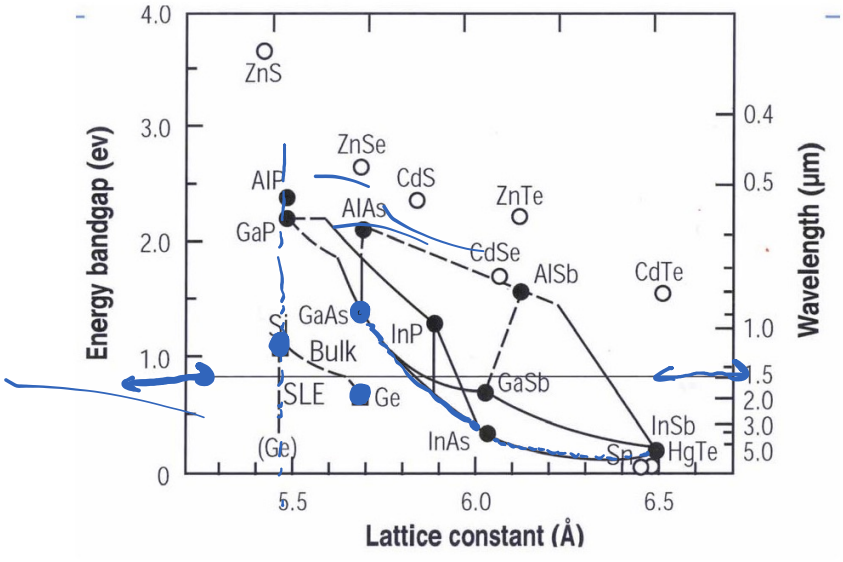
Carbon nanotubes



Zone folding: Band structure of nanotubes



Semiconductors



Sb-doped Germanium

~ 10^{23} Ge atoms

Specimen	Donor concentration (cm^{-3})
1	5.3×10^{14}
2	9.3×10^{14}
5	1.6×10^{15}
7	2.3×10^{15}
8	3.0×10^{15}
10	5.2×10^{15}
12	8.5×10^{15}
15	1.3×10^{16}
17	2.4×10^{16}
18	3.5×10^{16}
20	4.5×10^{16}
21	5.5×10^{16}
22	6.4×10^{16}
23	7.4×10^{16}
24	8.4×10^{16}
25	1.2×10^{17}
26	1.3×10^{17}
27	2.7×10^{17}
29	9.5×10^{17}

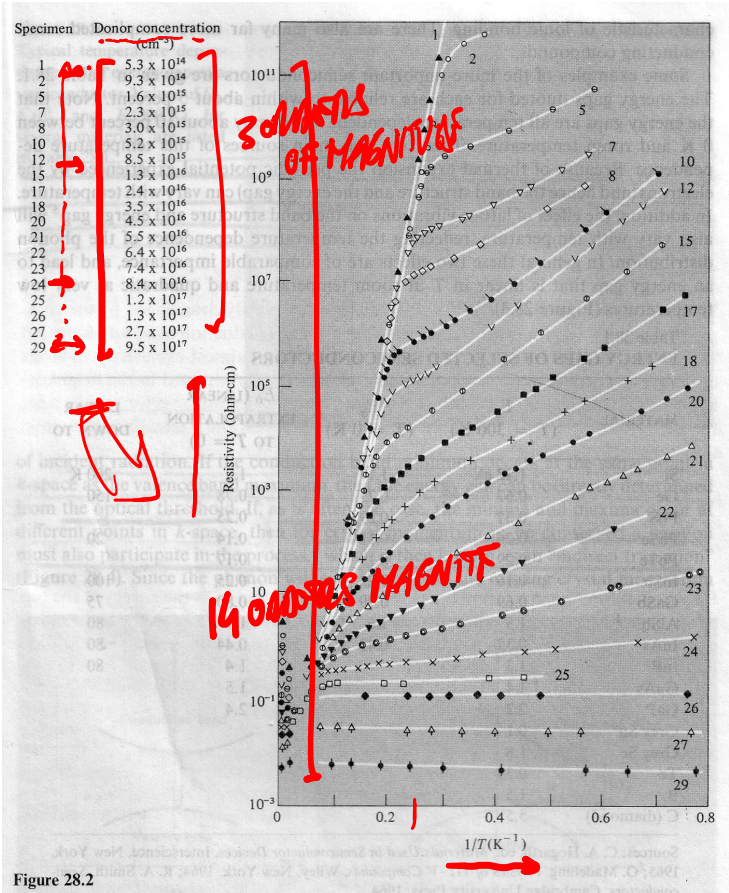


Figure 28.2
The resistivity of antimony-doped germanium as a function of $1/T$ for several impurity concentrations. (From H. J. Fritzsche, *J. Phys. Chem. Solids* **6**, 69 (1958).)