

MSE 423 Fall 2025 – Week 12

Semi-conductors



MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2025)

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

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Tight-binding (LCAO for solids)

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

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Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

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

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Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

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

$$\phi(\vec{r}) = \sum_n b_n \varphi_n(\vec{r})$$

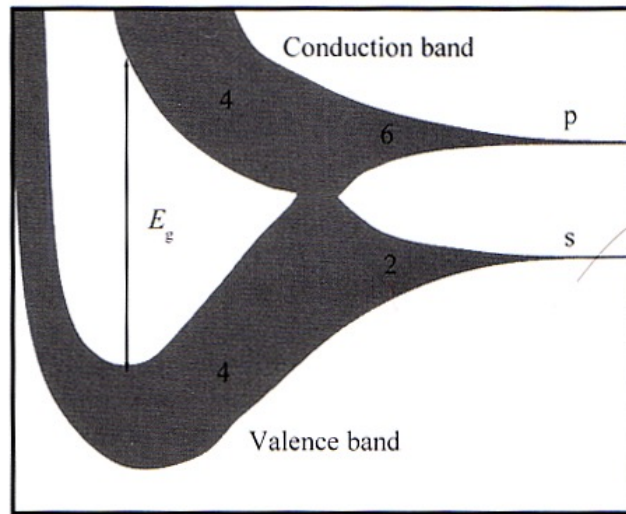
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From levels to bands

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

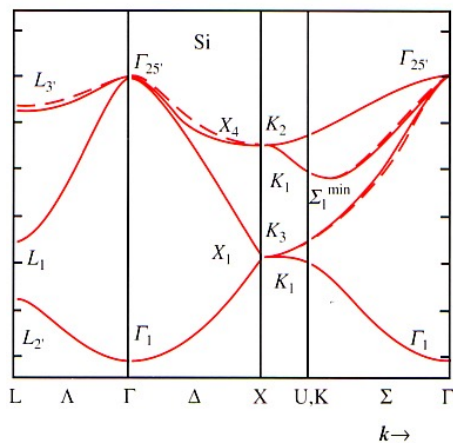
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From levels to bands



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How many bands in silicon ?



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Tight-binding vs. empirical psp

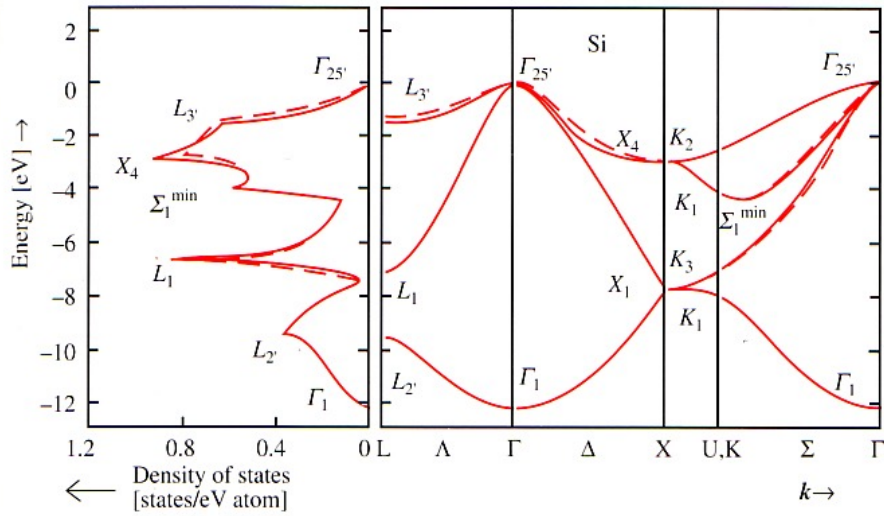


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

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Tight-binding vs. empirical psp

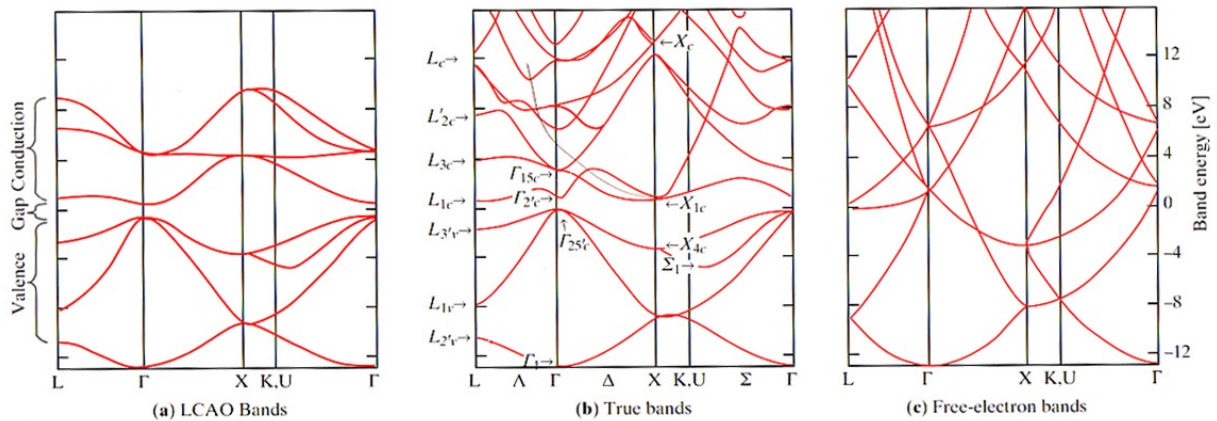
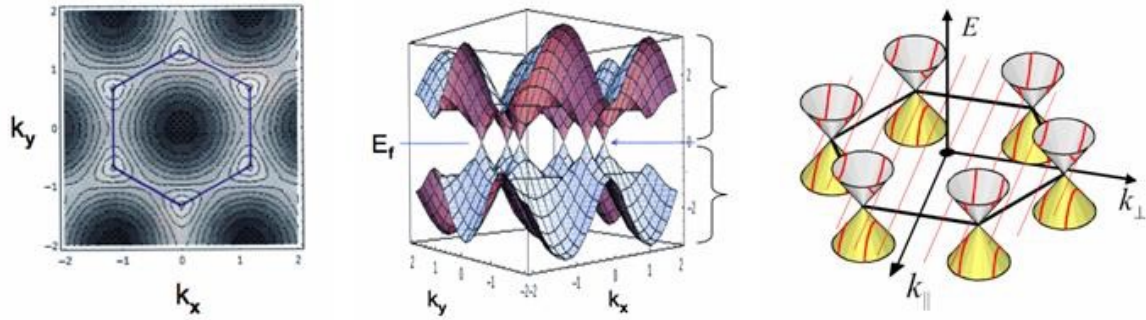


Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.18, p. 79]

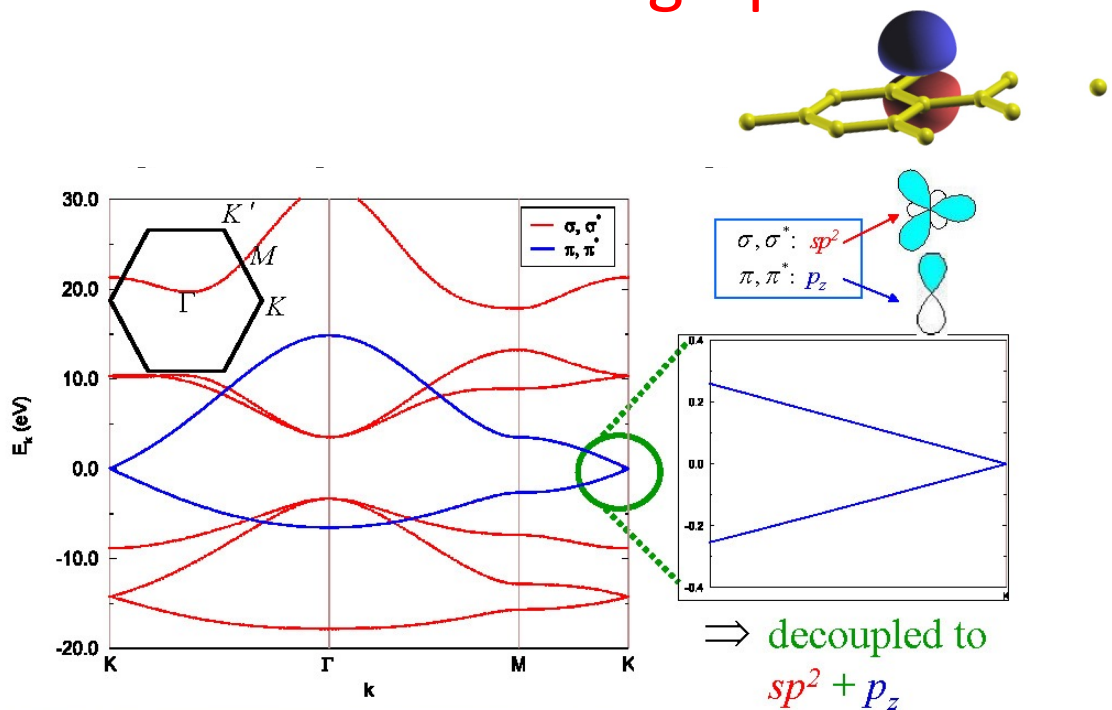
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Band structure of graphene



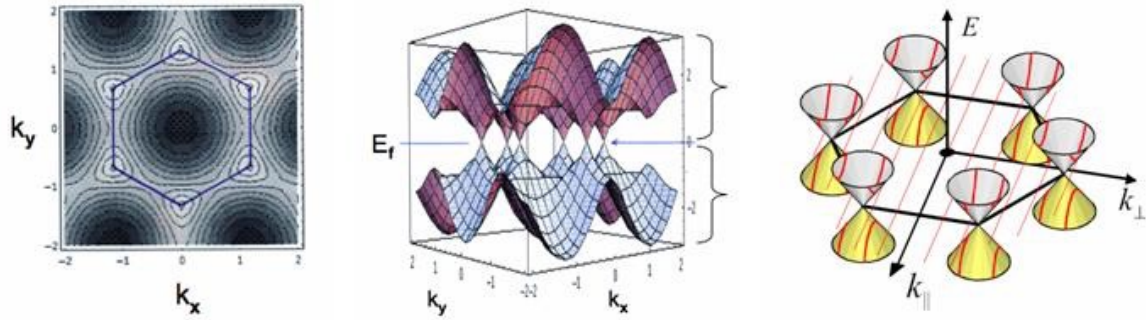
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Band structure of graphene



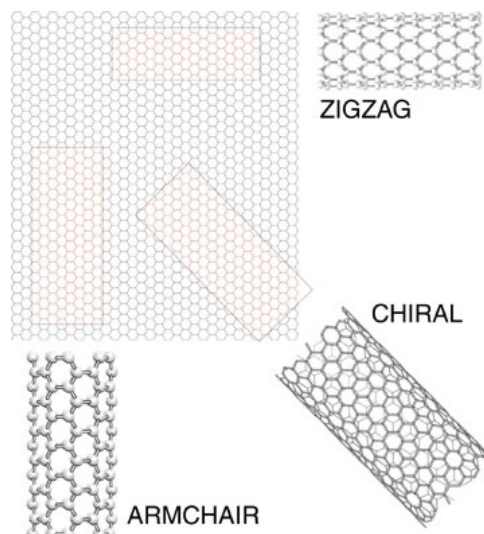
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Band structure of graphene



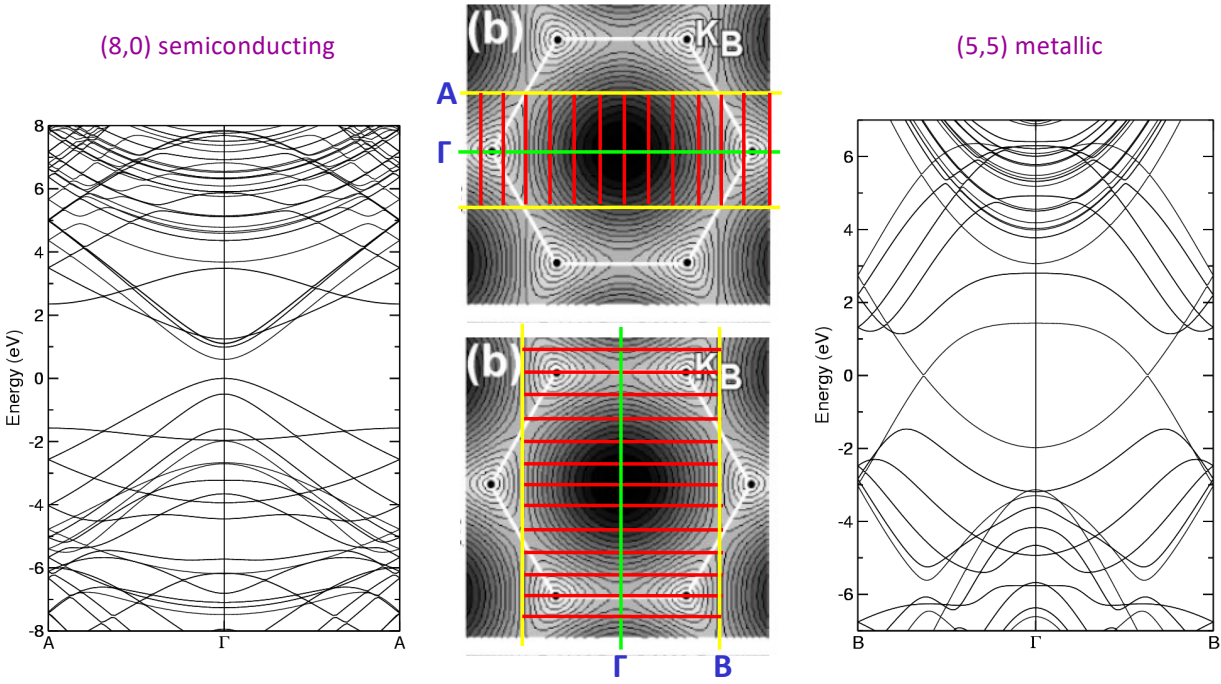
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Carbon nanotubes



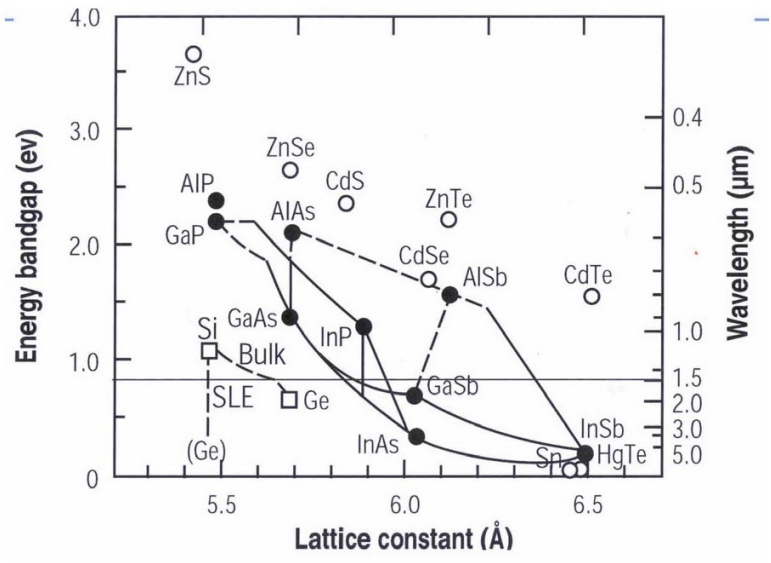
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Zone folding: Band structure of nanotubes



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