Notes:

- **Exam next week!** Choices now are Weds (start early), Weds evening (start 6PM?) or maybe Friday afternoon. I will need to find a room, and I will email!

- Covers: Through ch. 10 (tight binding material, today). Format, open book (Ashcroft & Mermin) – you should have a paper copy!

Tight binding model

Reading: ch. 10

$$\psi_{\vec{k}}(r) = \frac{1}{\sqrt{N}} \sum_R \varphi_n(r-R) e^{i\vec{k}\cdot\vec{R}}$$

Bloch state with localized states as basis set

- LCAO ("Hückel") model; basis = atomic orbitals.
- More general tight binding: mutually orthogonal local orbitals; "Wannier functions" complete orthonormal set.
- May converge more quickly than plane waves for insulators & more localized systems.

$$H\psi_{\vec{k}}(r) \approx \frac{E_n}{\sqrt{N}} \sum_R \varphi_n(r-R) e^{i\vec{k}\cdot\vec{R}}$$

1st order: E_n energy of isolated state

$$\varepsilon_{\vec{k}} = \left\langle \psi_{\vec{k}} \middle| H \middle| \psi_{\vec{k}} \right\rangle \qquad \varepsilon_{\vec{k}} = E_n + \frac{1}{N} \sum_R \sum_i \left\{ \left\langle \varphi(r-R) \middle| H \middle| \varphi(r-R_i) \right\rangle + c.c. \right\} e^{i\vec{k}\cdot(\vec{R}-\vec{R}_i)}$$

$$\Rightarrow \quad \varepsilon_{\vec{k}} = E_n - \gamma \sum_i e^{i\vec{k}\cdot(\delta\vec{R}_i)}$$

Assume only nearest neighbor matrix elements, all equal to $-\gamma$

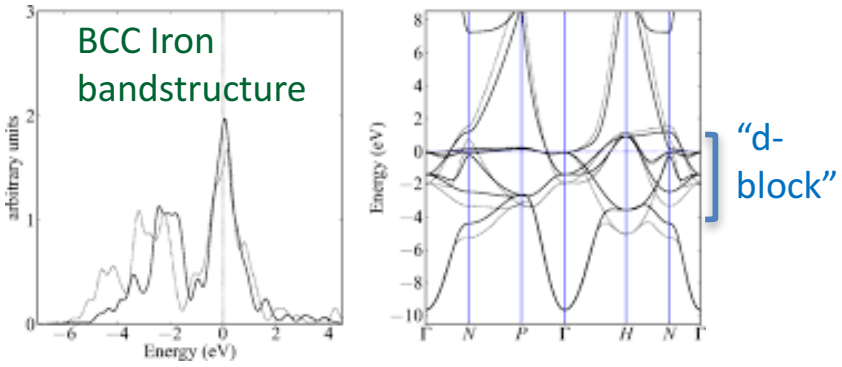
$$E_n - 2\gamma\cos(ka)$$

simple 1D case

Tight-Binding method:

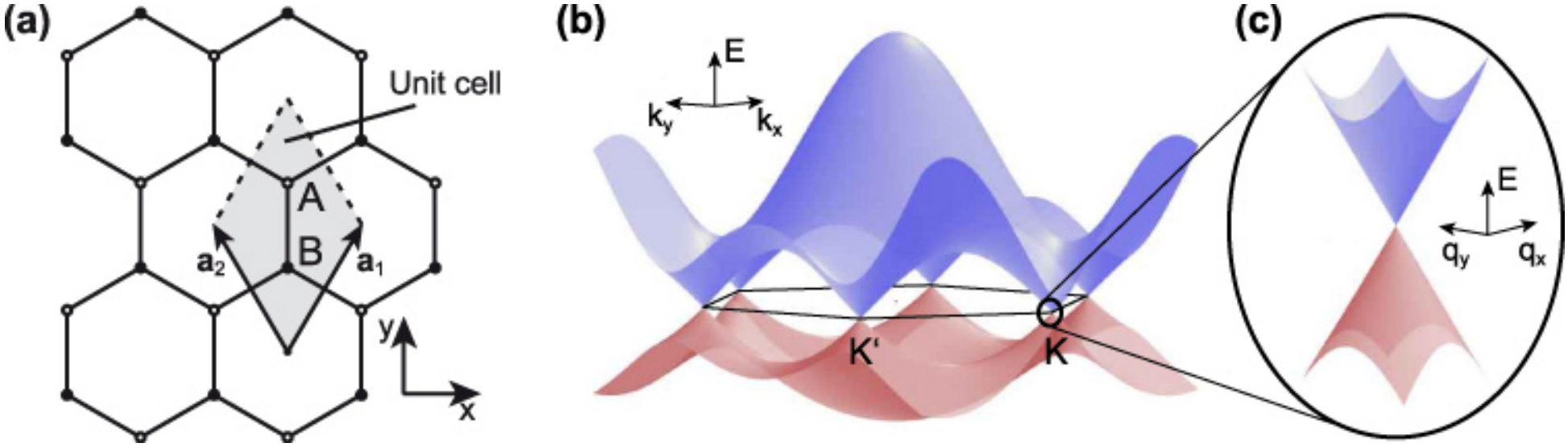
- Particularly useful for:
  - Naturally small-radius states (*d-electrons, core states* …)

Borghi, et al., Phys Rev B 2014

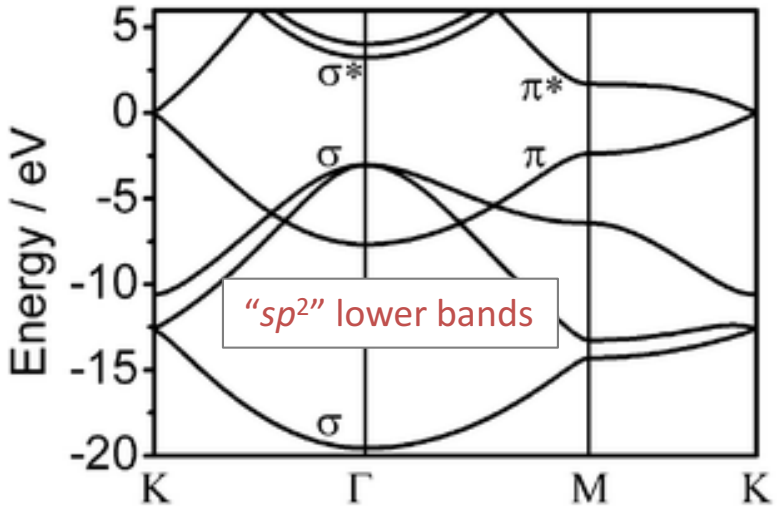


  - Fast calculations ("Empirical Tight-binding"; energy parameters fitted to sets of experimental results)—e.g. large nanostructures, or part of Molecular Dynamics (MD) code.

Graphene -- & see handout



Guttinger et al. Rep. Prog. Phys. 2012



Li et al. PhysChemChemPhys 2012

Semimetal with zero effective mass

$$m^* = \hbar^2 \left(\partial^2 \varepsilon / \partial k^2 \right)^{-1}$$

will see later in course

- "Dirac electrons and holes"
- Contact points: zero gap, required by symmetry!
- Very large mobility $\mu = \frac{e\tau}{m}$

See e.g. Das Sarma et al., Reviews of Modern Physics 83, 407-470 (2011); Schwierz, Nature Nanotechnology 5, 487-496 (2010).