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3.23 Electrical, Optical, and Magnetic Properties of Materials

Fall 2007

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3.23 Fall 2007 – Lecture 11

FERMI

Last time

1. Explicit solution of the Bloch equation, energy bands
2. Brillouin zone, Fermi surface
3. Energy of molecules and solids
4. Mean field approaches – Hartree and Hartree-Fock
5. Spin-statistics, Slater determinant, Pauli principle
6. Huckel approach (LCAO for aromatic compounds)

Study

- Chap. 5 Singleton
- Read Chap. 6 Singleton

Tight-binding (LCAO for solids)

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

Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

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

Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

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

$$\phi(\vec{r}) = \sum_{n} b_n \psi_n(\vec{r})$$

Some despicable algebraic workout

More workout

More

From *s* level to *s* bands

From *s* level to *s* bands

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

From *s* level to *s* bands

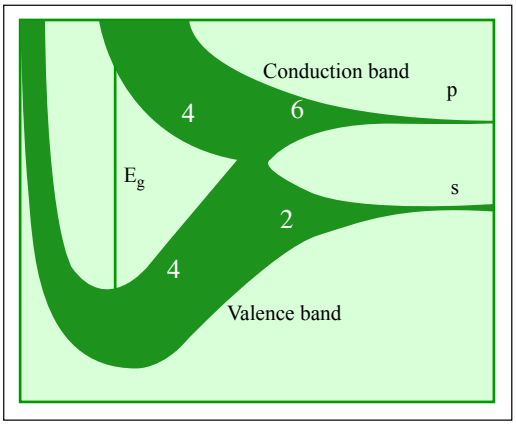
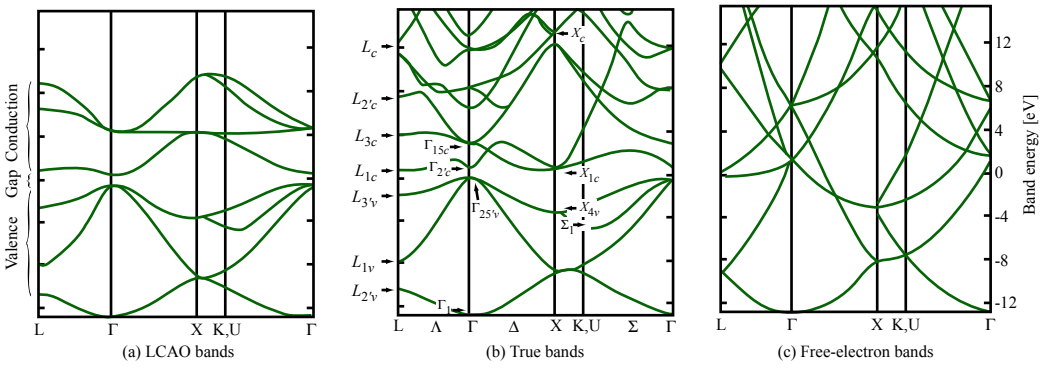


Figure by MIT OpenCourseWare.

Tight-binding vs. empirical psp

Image removed due to copyright restrictions. Please see: Fig. 2.24 in
Yu, Peter Y., and Manuel, Cardona. *Fundamentals of Semiconductors: Physics and Materials Properties*. New York, NY: Springer, 2001.

Tight-binding vs. empirical psp



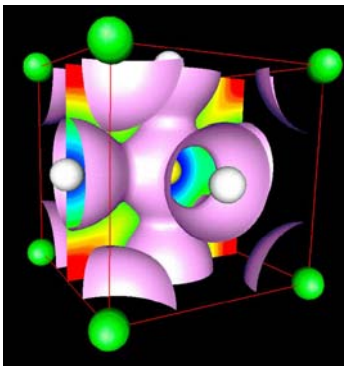
A comparison of the band structure of Ge as calculated by (a) the tight-binding, (b) the empirical pseudopotential, and (c) the nearly free electron methods.

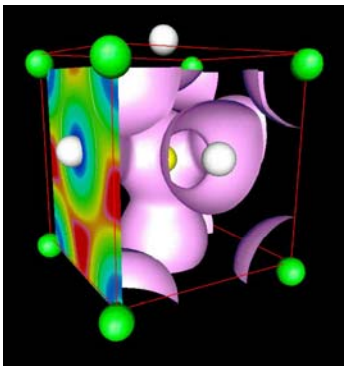
Figure by MIT OpenCourseWare.

Bands in Ge

Image removed due to copyright restrictions. Please see http://www.ioffe.ru/SVA/NSM/Semicond/Ge/Figs/221.gif

Ferroelectric perovskites





Ferroelectric perovskites

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King-Smith, R. D., and David Vanderbilt. "First-principles Investigation of Ferroelectricity in Perovskite Compounds." *Physical Review B* 49 (March 1994): 5828-5844.

Ferroelectric perovskites

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King-Smith, R. D., and David Vanderbilt. "First-principles Investigation of Ferroelectricity in Perovskite Compounds." *Physical Review B* 49 (March 1994): 5828-5844.