

Bandstructure Calculation: General Considerations

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Electrons and Phonons

- Total Hamiltonian of the System -

$$H = \underbrace{\sum_j \frac{p_j^2}{2m_j} + \frac{1}{2} \sum_{j,j'} \frac{e^2}{|\bar{r}_j - \bar{r}_{j'}|}}_{\text{Over all e's}} + \underbrace{\sum_i \frac{P_i^2}{2M_i} + \frac{1}{2} \sum_{i,i'} \frac{e^2 Z_i Z_{i'}}{|\bar{R}_i - \bar{R}_{i'}|}}_{\text{Over all nuclei}} - \underbrace{\sum_{i,j} \frac{e^2 Z_i}{|\bar{r}_j - \bar{R}_i|}}_{\text{e-nuclei}}$$

➤ **1st Approximation:** core vs. valence e's

Still Eq. Above Applies with:
 Core e's + nucleus → ion core
 e's → valence e's

IV Semiconductor

C $1s^2 2s^2 2p^2$

Si $1s^2 2s^2 2p^6 3s^2 3p^2$

Ge $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$

semicore

III-V Semiconductor

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$

As $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$

Electrons and Phonons

- Adiabatic Approximation -

➤ **2nd Approximation: Born-Oppenheimer or adiabatic approximation**

✓ **Ions are much heavier (> 1000 times) than e's**

So,

for e's: ions are essentially stationary (at eql. Lattice sites $\{R_{j0}\}$)

for ions: only a time-averaged adiabatic electronic potential is seen

In other words,

using the adiabatic approximation, we separate the (in principle non-separable) perfect crystal Hamiltonian

Electrons and Phonons

- Application of the Adiabatic Approximation -

Under adiabatic approximation...

$$H = H_{ion}(\bar{R}_i) + H_e(\bar{r}_j, \bar{R}_{i0}) + H_{e-ion}(\bar{r}_j, \delta\bar{R}_i)$$

phonon spectrum

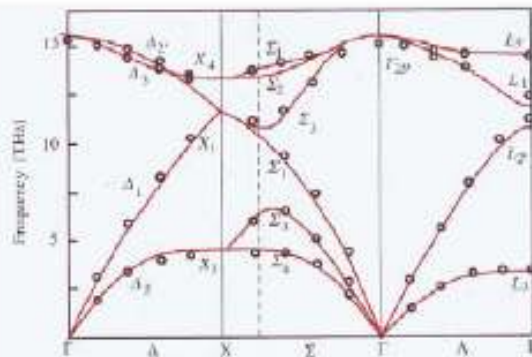
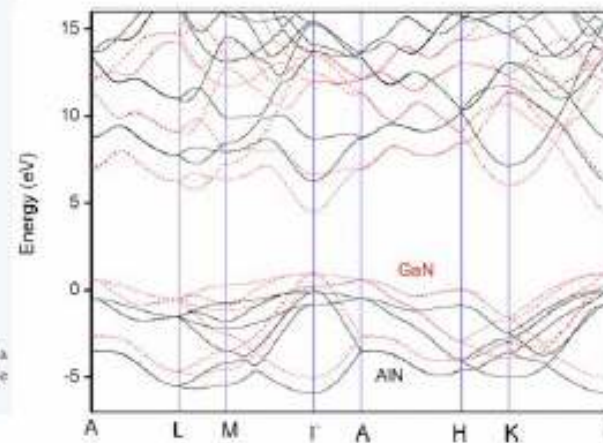


Fig. 3.1. Phonon dispersion curves in Si along high-symmetry axes. The circles are data points from [3.3]. The continuous curves are calculated with the adiabatic bond charge model of Weber [3.4].

Ref: Yu-Cardona

electronic band structure



e-phonon interaction
(resistance, superconductivity...)

Mean Field Approximation

Electronic Hamiltonian

$$H_e = \underbrace{\sum_j \frac{p_j^2}{2m_j} + \frac{1}{2} \sum_{j,j'} \frac{e^2}{|\vec{r}_j - \vec{r}_{j'}|}}_{\text{over all valence e's } > 10^{23} \text{ cm}^{-3}} - \sum_{i,j} \frac{e^2 Z_i}{|\vec{r}_j - \vec{R}_{i0}|}$$

over all valence e's $> 10^{23} \text{ cm}^{-3}$

- 3rd Approximation: **Mean-field Approximation**

$$H_{1e} = \frac{p^2}{2m} + V(\vec{r}); \quad V(\vec{r} + \vec{R}) = V(\vec{r})$$

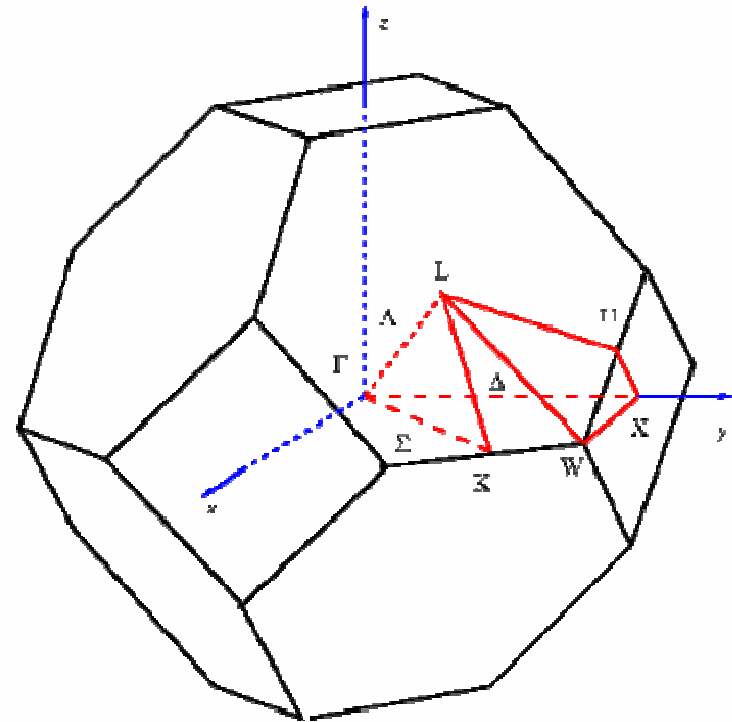
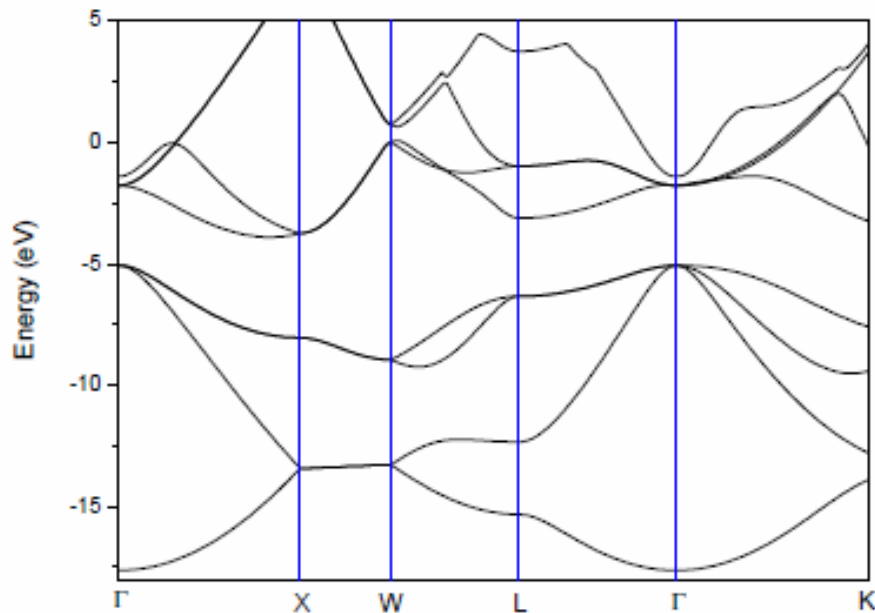
Density Functional
Theory

$$V_H + V_x + V_c$$

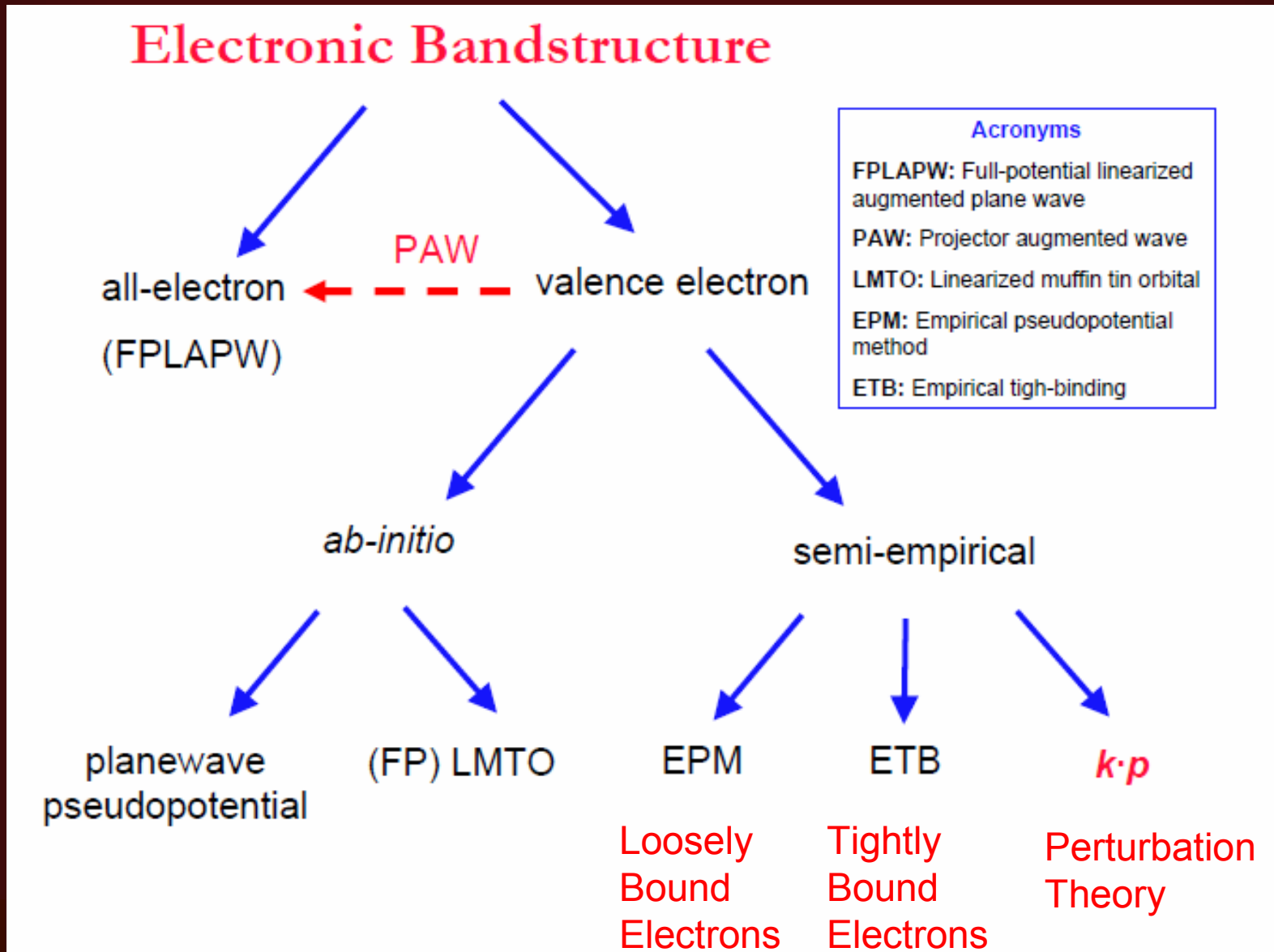
A direct lattice
vector

Symmetry Points and Plotting the Bandstructure

EPM Bandstructure of Si



Bandstructure Calculation Methods



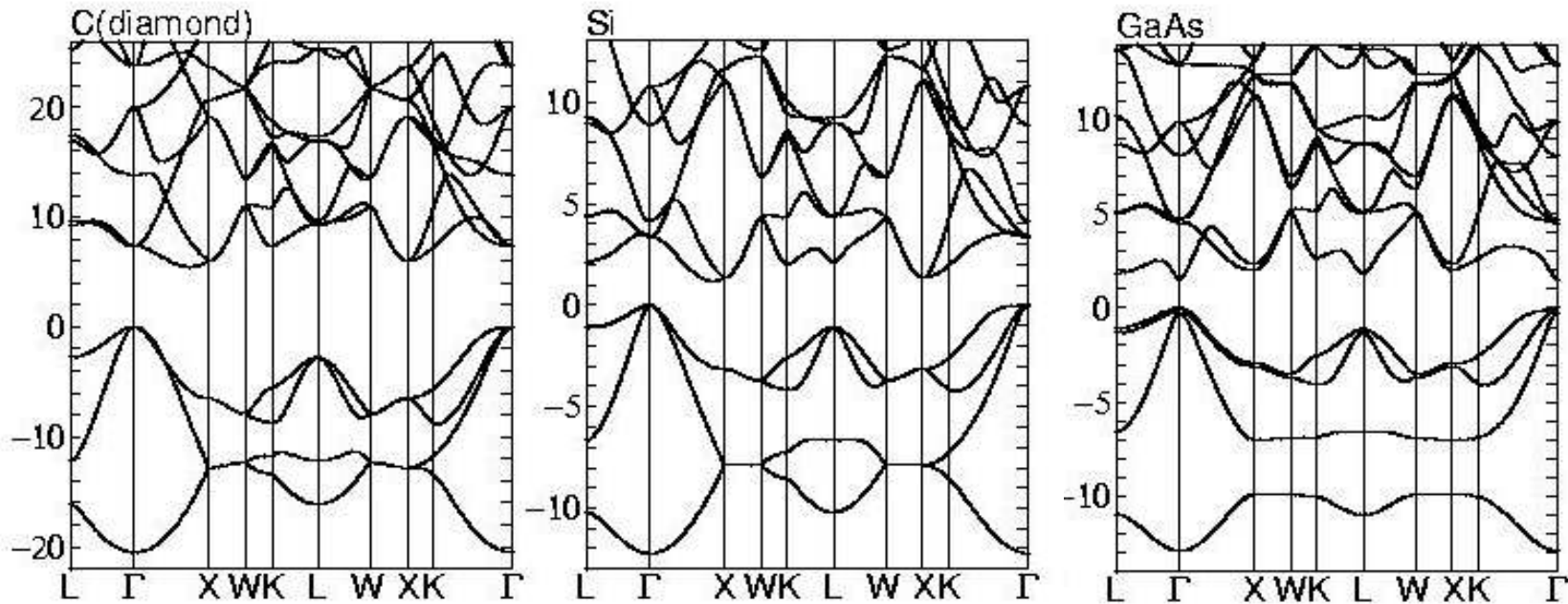
Advantages of Particular Methods

- **Semi-Empirical Methods**
 - Empirical Pseudopotential Method
 - Predicts optical gaps
 - **k.p Method**
 - Predicts effective masses
 - **Tight-Binding Method**
 - Can include strain and disorder, can simulate finite structures (not just bulk or infinite 2D or 1D)
- ***Ab Initio* Methods**
 - **GW Method**
 - Predicts Energy gaps of Materials correctly

The $sp^3d^5s^*$ Tight-Binding Hamiltonian

- [Jancu et al. PRB 57 (1998)] -

Many parameters, but works quite well !



QPscGW *Ab Initio* Results

- Mark van Schilfgaarde -

