

Band Theory

Extensions (Optional)

■ We need to know the periodic $V(\vec{r})$ to do band structure calculations. How do we know $V(\vec{r})$?

- This is a difficult question.
- Same question is valid for atomic problems (except hydrogen)
- Many ways have been developed to handle $V(\vec{r})$, especially the part of $V(\vec{r})$ reflecting the effects of the other electrons when we reduce the solid (atomic) problem to a single-electron Schrödinger problem.

These approaches include:

- Hartree and Hartree-Fock approximations
- Self-consistent Hartree-Fock approximation

- Density Functional Theory

- Kohn won the Chemistry Nobel Prize for establishing this theory

Reference: For students who want to become a band theorist, the book to read is:

Richard M. Martin, "Electronic Structure: Basic Theory and Practical Methods"

- Special Band Structure of Graphene