From Atoms to Materials: Predictive Theory and Simulations

Week 2: Electronic Structure and Bonding of Molecules and Crystals
Lecture 2.4: Electronic Structure of Crystals

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Wave functions of crystals

- Let’s consider a 1D chain of atoms
- Combination of atomic orbitals to make the wavefunction of the crystal
Molecules vs. solids

Energy

$E_0$

Inverse separation between atoms

Anti-bonding

Bonding

$\sim 10^8$ states
Remember: bring 2 Si together

Adapted from: W. Harrison, “Electronic structure and the properties of solids”
Images from Wikipedia
Making a crystal: lots of Si atoms together

The s and p states overlap

- C: 5.5 eV
- Si: 1.2 eV
- Ge: 0.6 eV
- Sn: 0.0 eV
  - Low T: a-Sn (diamond)
  - High T: b-Sn (tetragonal)
- Pb: fcc metal

Column IV band gaps
Making a crystal: lots of Si atoms together

- Bonding/anti-bonding splitting larger than s-p splitting:
  - Covalent bonding dominates, insulators and semiconductors
  - s-p splitting larger than bonding anti-bonding splitting
    - Metallic bonding, closed packed structures

### Column IV band gaps
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