Lattice Dynamics & Band Gaps: Exploring Material Properties Through Simulation

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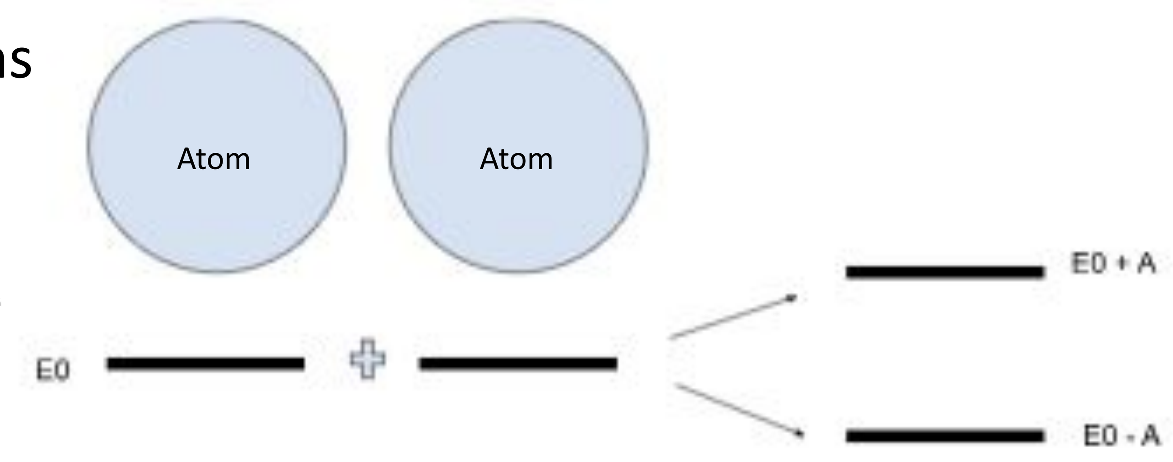
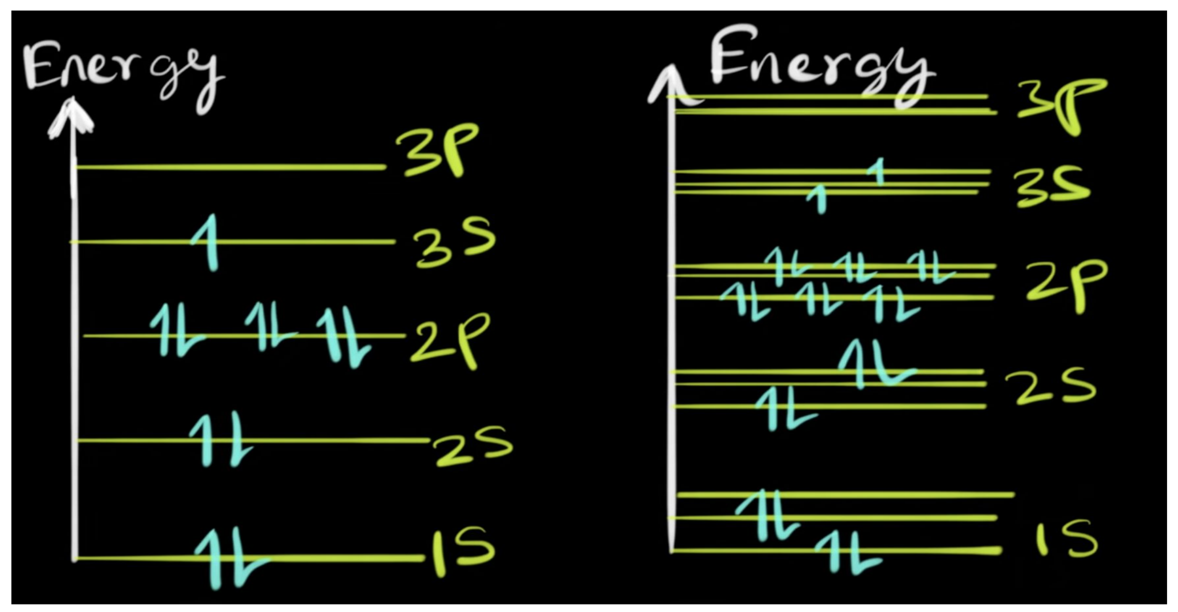
Band Formation:

Single atoms have discrete energy levels that electrons can occupy. When two atoms are bonded, individual energy levels in the atoms will interact and form two energy levels, one with higher energy and one with lower energy. This is caused by the interference of the wave functions of energy levels.





When more and more atoms combine to form a solid, their energy levels/orbitals get closer and closer together until they eventually become practically continuous. These continuous sections of energy levels are called bands and are separated by gaps. The size of these band gaps determine the structure and behavior of the material the atoms create.

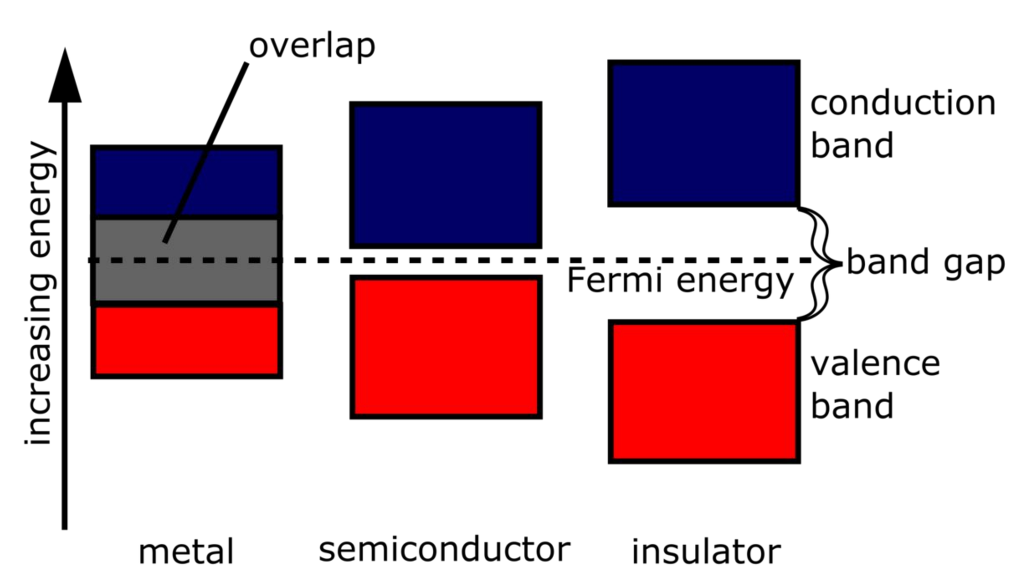
Band Gaps and Material Properties:

A key feature of band structures are band gaps, energies that electrons cannot occupy. The band below the gap is typically called the valence band while the band above is called the conduction band. The gap size determines the ease of electron flow with larger gaps requiring more energy to overcome.

Metals have partially filled bands so that electrons can easily be excited to higher energies. This lack of a band gap allows electrons to flow easily and create a highly conductive material.

Semiconductors have a fully filled valence band and a small band gap (<3 eV). A small, yet big enough gap allows for efficient switching between conductive and insulating behavior.

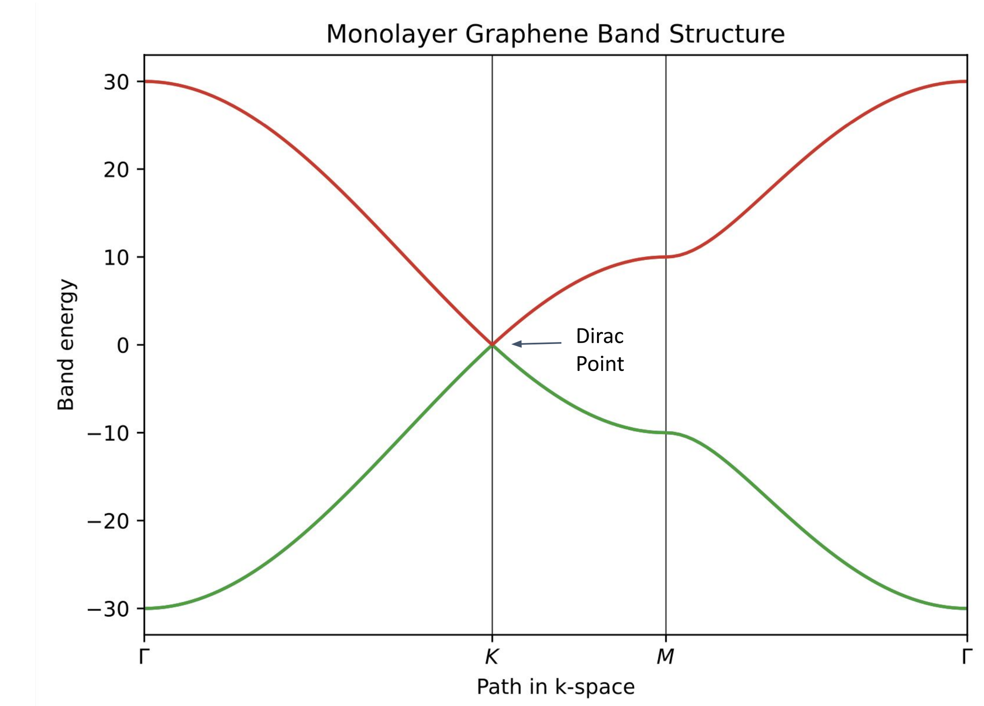
Insulators have a fully filled valence band and a large band gap (>3 eV). This large gap leads to increased difficulty in exciting electrons to the conduction band, leading to poor conductivity.



Real-World Applications:

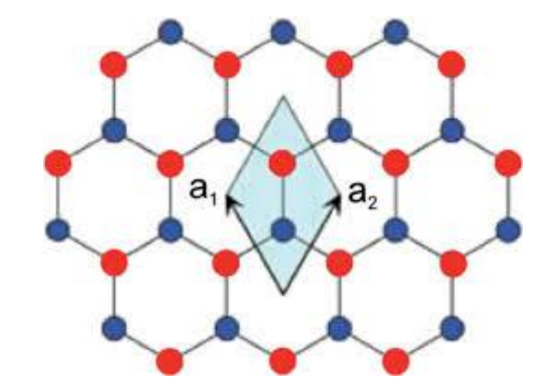
Band gap sizes are crucial for determining the material properties of substances. Devices such as LEDs use specific band gaps to emit different colored lights, with larger band gaps emitting shorter wavelengths compared to smaller band gaps. Transistors are made from semiconductors with relatively small band gaps so that currents are easily switched on and off.

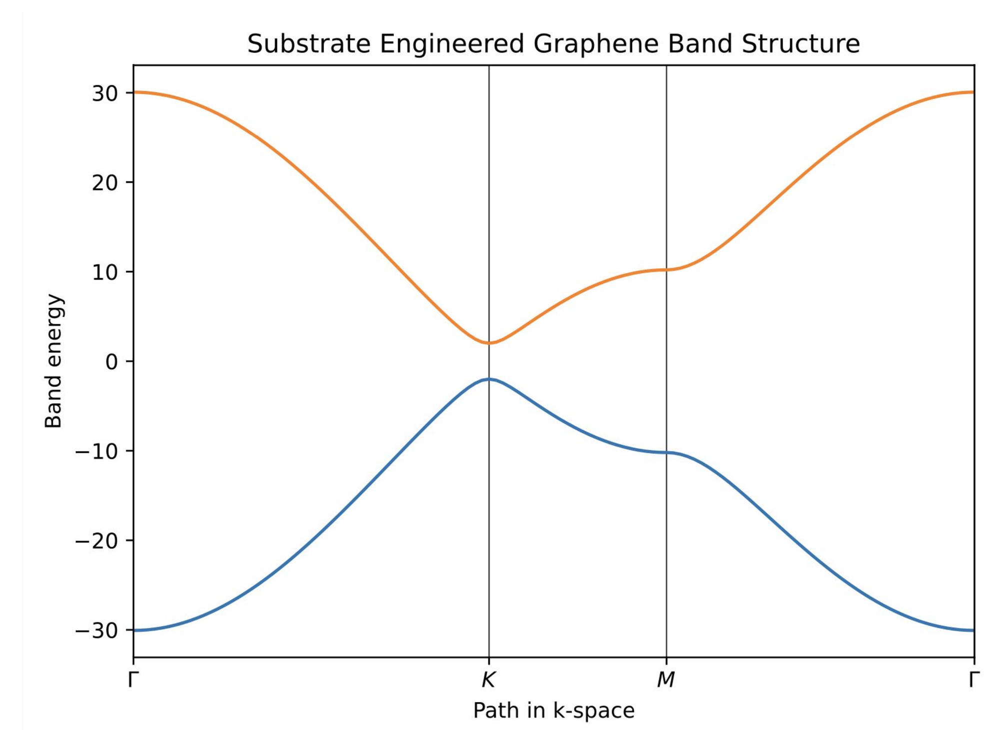
Visuals:



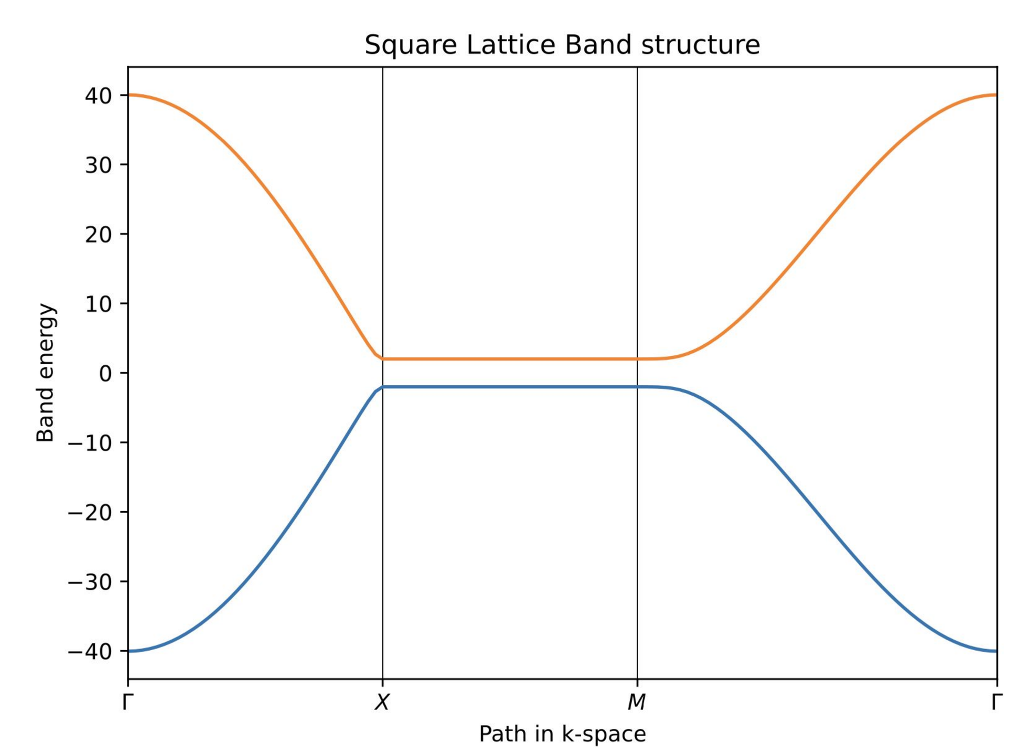
Using Python to execute a tight-binding model, the band structure of three lattices were explored.

Materials:
Monolayer graphene, made up of carbon atoms arranged in a hexagonal lattice, is a highly conductive semimetal with no band gap.





By making the energies of the two atoms in the graphene unit cell different (red and blue atoms in rhombus above), a gap in the band structure can be created, generating a fully filled valence band and empty conduction band. One way to achieve this is by placing graphene on a lattice-matched substrate where the red and blue carbon atoms lie on top of different types of atoms.



Lattice Structures:
The lattice structure of a material affects how the orbitals (wavefunctions) interfere, determining the shape of energy bands. These differences in band shapes can be seen between the square lattice structure and the hexagonal graphene structures.

Acknowledgements:

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