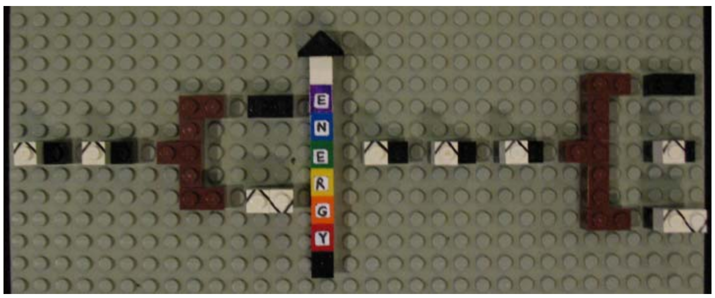
Band Theory Illustrated with LEGO® Bricks

Dean J. Campbell & Stephen J. Bannon, Bradley University

From atomic orbitals to bands

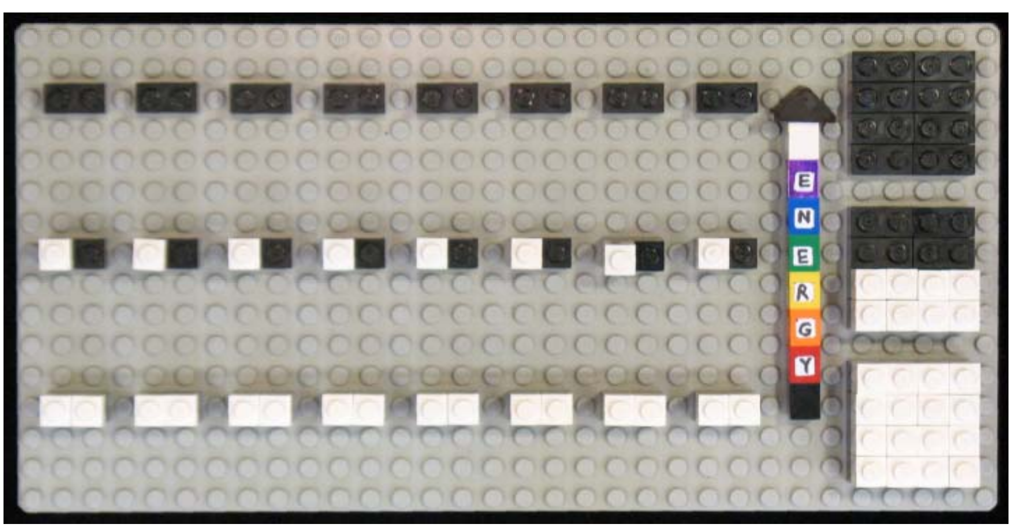
- When atoms bond together, the atomic orbitals involved in bonding combine to produce molecular orbitals.
- Both atomic and molecular orbitals can hold up to two electrons.
  - Orbital energy levels are represented by black 1x2 bricks.
  - Electrons are represented by white 1x1 bricks, arrows on the bricks represent electron spins.
- Electrons will tend to occupy the lowest energy orbitals first.
  - Lower energy is represented as lower positions on the energy diagram.
- The number of atomic orbitals combined equals the number of molecular orbitals produced.

Two atomic orbitals combine to produce two molecular orbitals.



Three atomic orbitals combine to produce three molecular orbitals.

- The combination of many atomic orbitals in a solid produces a nearly continuous distribution of many molecular orbitals known as a band.
- In order for materials to be electrically conductive, electrons must be able to move in the band.
  - The combination of empty orbitals produces an empty band.
  - Completely empty bands have no electrons to move.
  - The combination of half-filled orbitals produces a half-filled band.
  - Half filled bands have electrons that can move and materials containing these bands can conduct electricity.
  - The combination of full orbitals produces a full band.
  - Completely full bands are too crowded with electrons to allow electrons to move.

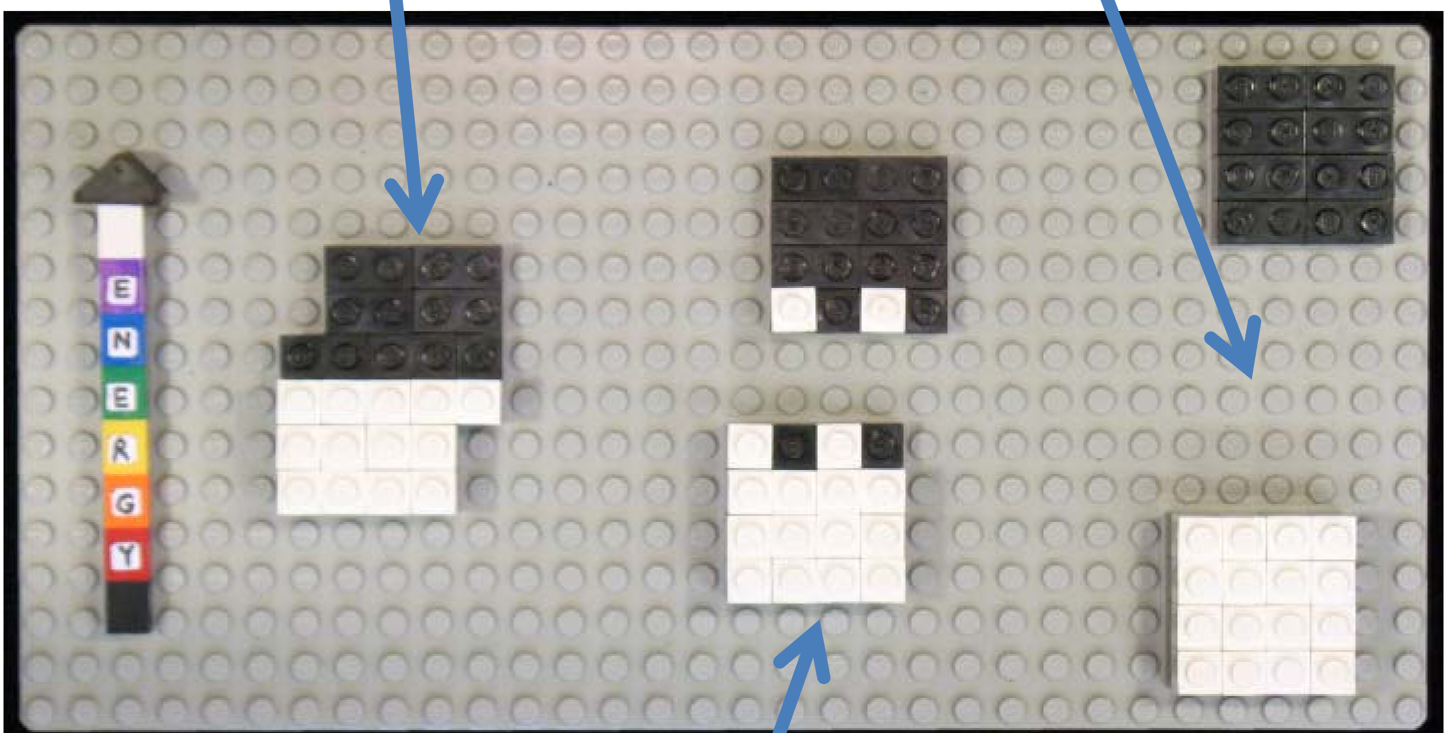


Bands can interact to affect electrical conductivity

•When an empty band overlaps in energy with a full band, the two bands behave effectively as one half-filled band, electrons are able to move, and the material is an electrical conductor.

•When there is a large energy separation between the top edge of the full band (called the valence band) and the bottom edge of the empty band (called the conduction band), electrons stay crowded into the full band, and the material is an electrical insulator.

- •The energy separation is referred to as a band gap, E_g.



•When there is only a small energy separation between the top edge of the full valence band and the bottom edge of the empty conduction band (small E_g), a few electrons can migrate from the full band into the empty band and are able to move, and the material is a semiconductor.

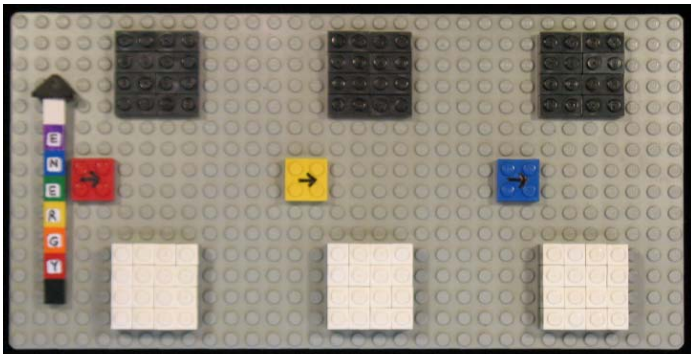
- •The gaps left by the electrons lost from the full band are called “holes”. These holes allow electrons to move in the full band.

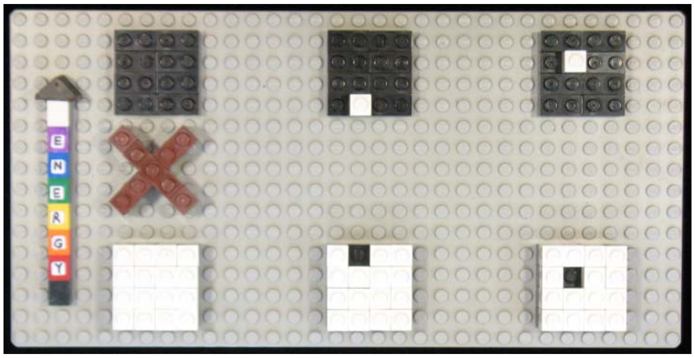
Semiconductor band interactions with light

•Recall that the colors of light arranged in increasing energy are: red, orange, yellow, green, blue, and violet.

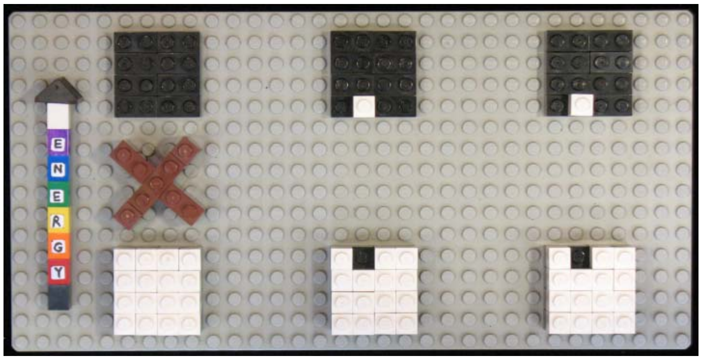
•Low energy photons of light (represented by a red brick) do not have sufficient energy to promote electrons from the valence band to the conduction band.

•Photons of light of light with higher energies (represented by yellow and blue bricks) have sufficient energy to promote electrons from the valence band to the conduction band.

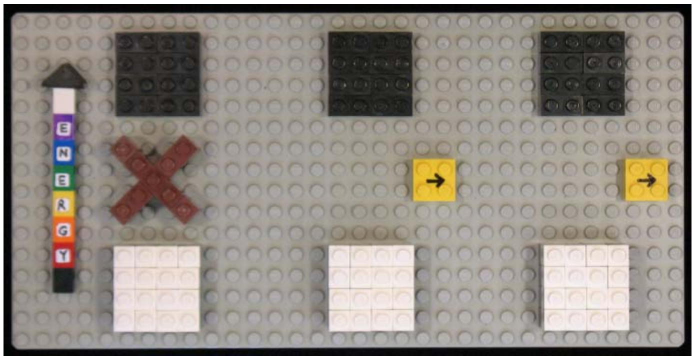




•Electrons that have promoted into the conduction band eventually relax to the bottom edge of the conduction band. Holes that have been created in the valence band eventually rise to the top edge of the valence band.



•Electrons that move back from the conduction band to re-fill the holes in the valence band tend to emit a fairly narrow range of wavelengths (represented by the yellow bricks), corresponding to the size of the band gap.



Doping semiconductors

•n-type semiconductors contain elements which have discrete energy levels within the bandgap of the semiconductor near the conduction band. These energy levels donate electrons to conduction band, which increases the conductivity of that band.

•p-type semiconductors contain elements which have discrete energy levels within the bandgap of the semiconductor located near the valence band. These energy levels accept electrons from the valence band, and the resulting holes produced increases the conductivity of that band.