Optical Absorption and Emission

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Outline

- Applications of solid-state optics: LED, etc.
- Mechanism for light emission and absorption.
- Theory.
- Recent developments in nanoscience:
  - Luminescence in solutions of CdSe nanocrystals.
  - Nanomotors based on azobenzene.

Why Study Optical Properties?

•One can test different theories for the interaction of light and matter and understand the physical phenomena involved.

•Knowing the physics behind emission/absorption of light, one can design new materials and devices.

Some Applications of Solid State Optics:

Solar cells

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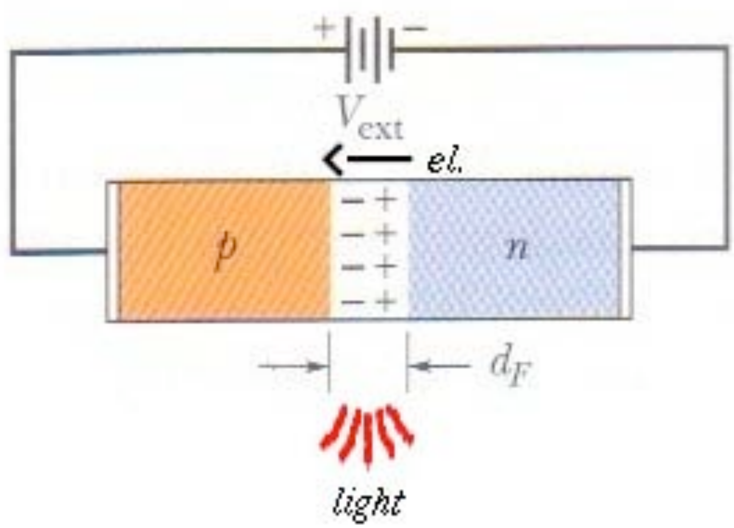
Lasers

LEDs

The Physics of a Laser-Emitting Diode (LED)



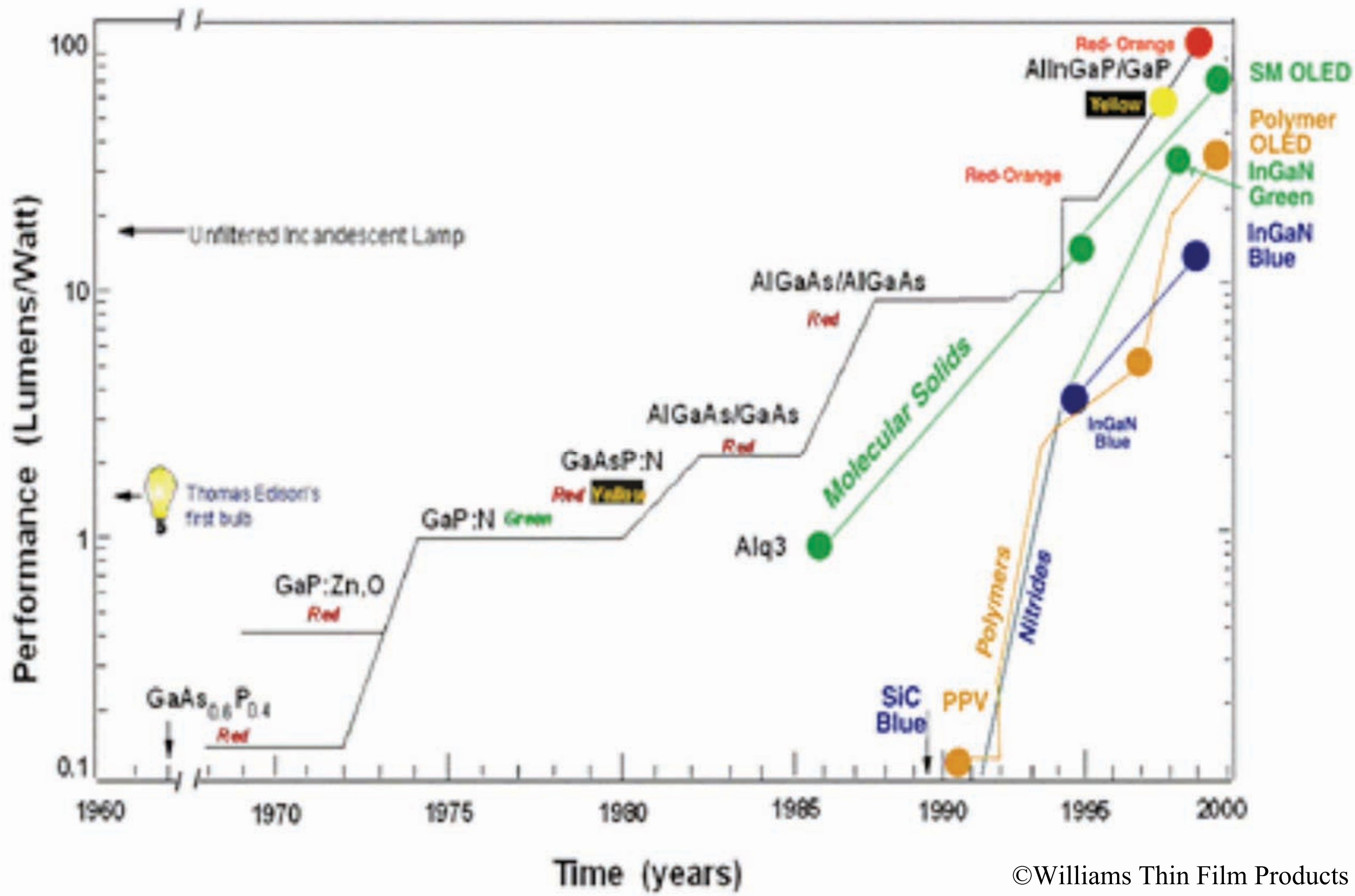
Cheap, low-power source of monochromatic light.

The first LED was a p-n junction made of doped GaAsP.

The semiconductor in the junction defines the color:
AlGaAs, **GaAsP**, **GaN**, **GaP**, **ZnSe**, etc.

AlGaAs LEDs also emit infrared light

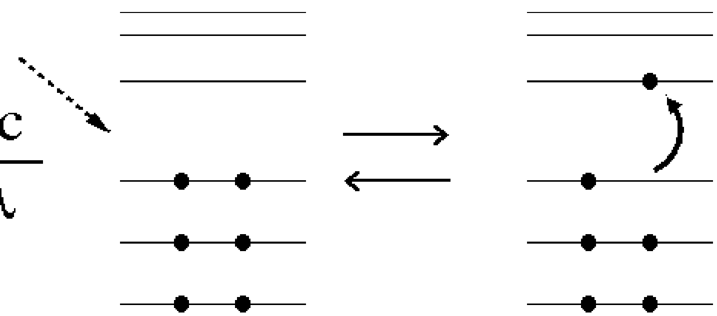
Evolution of LED Performance



How Do Materials Absorb and Emit Light?

Simple picture: Electrons gain energy from light and undergo a transition from an occupied orbital to an empty orbital.

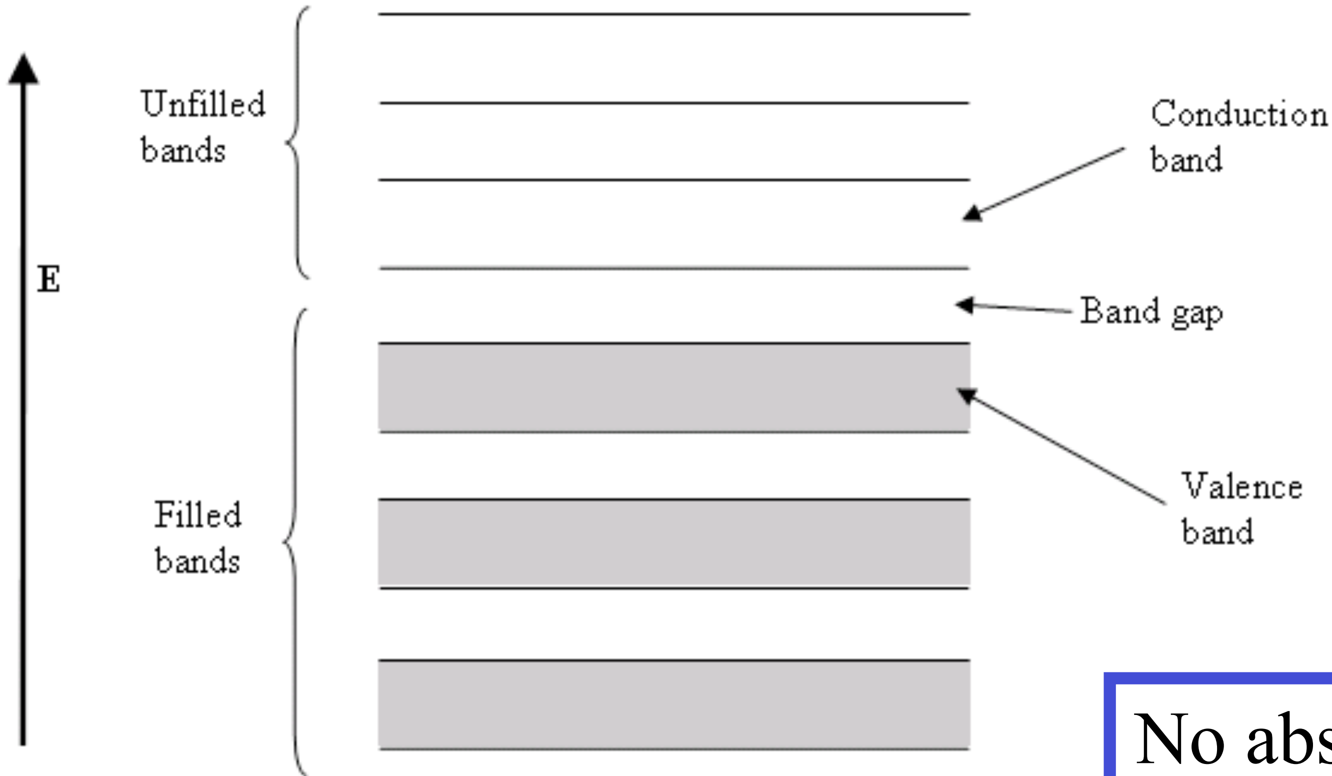
$$E = \frac{hc}{\lambda}$$



color	wavelength interval	energy interval
red	~ 625-740 nm	~ 1.7-2.0 eV
orange	~ 590-625 nm	~ 2.0-2.1 eV
yellow	~ 565-590 nm	~ 2.1-2.2 eV
green	~ 500-565 nm	~ 2.2-2.5 eV
cyan	~ 485-500 nm	~ 2.5-2.7 eV
blue	~ 440-485 nm	~ 2.7-2.8 eV
violet	~ 380-440 nm	~ 2.8-3.3 eV

No absorption with energy below the Gap!

In solids, orbitals split up in bands.



No absorption with energy below the Gap!

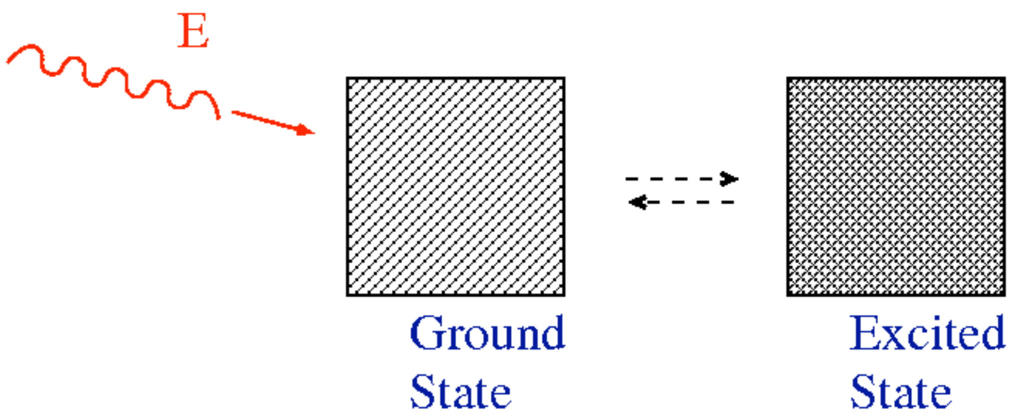
But not all materials have an energy gap...

Metals have no gap.
They absorb light at all frequencies. Opaque.

Insulators have gap:

- water, gap = 6.7 eV
- glass, gap > 5 eV (colored glass is obtained by mixing metals and other impurities).

Failure of the simple picture: It does not include interactions among electrons.



Direct approach: solve the Schrödinger equation

$$H\Psi = i(\partial/\partial t)\,\Psi$$

Are there simpler methods?

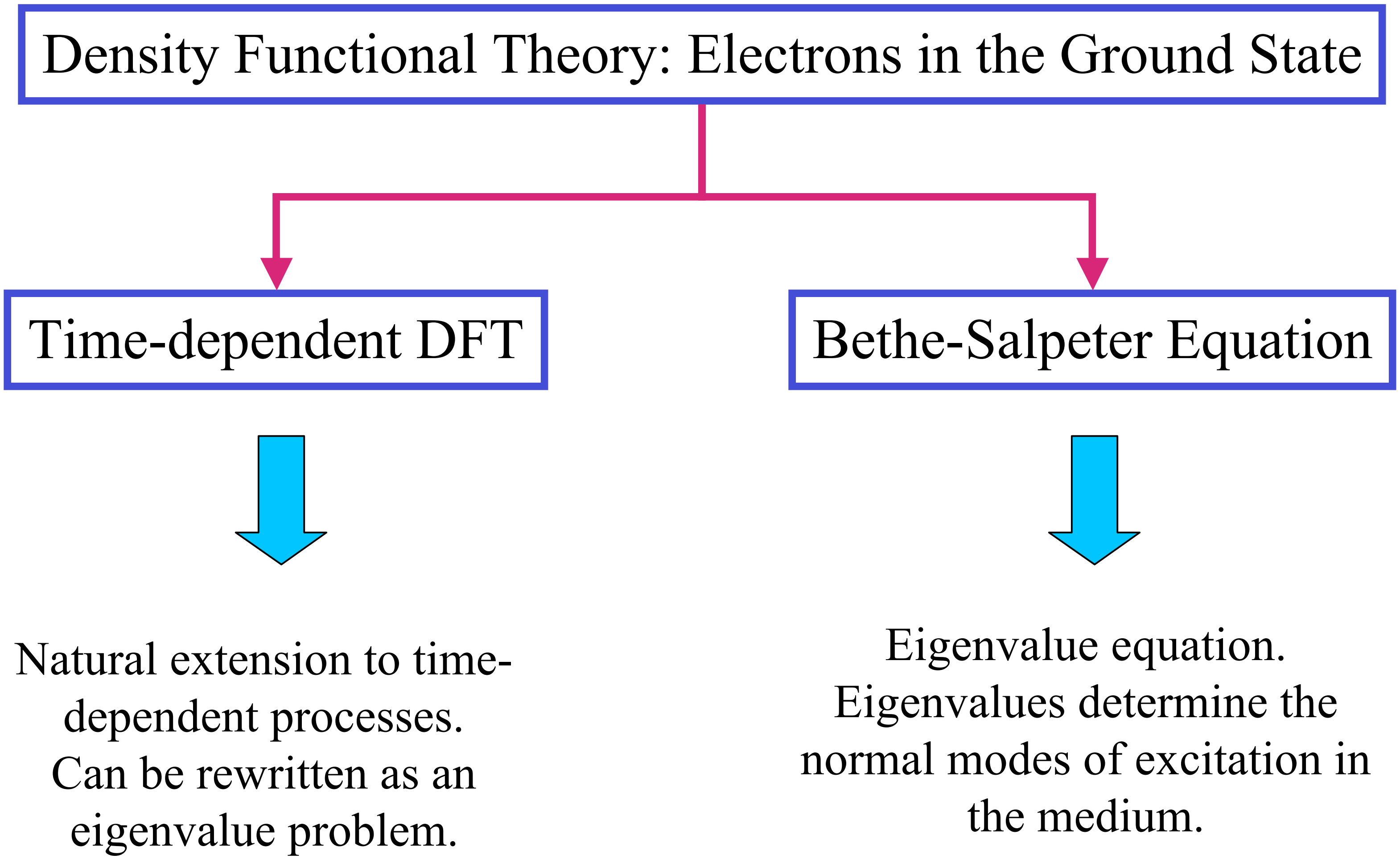
First-principles Calculations

Optical absorption can be predicted very accurately from numerical simulations with no input information except for the chemical composition of the material.

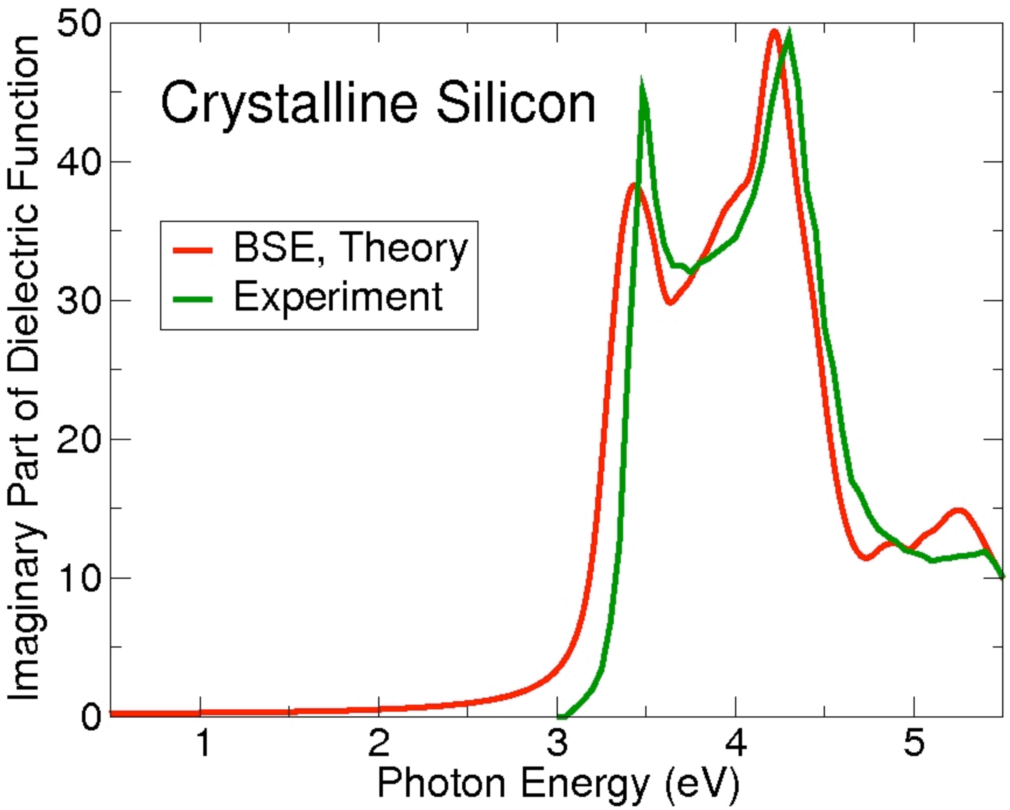
Various theories for electron-electron interactions in the excited state:

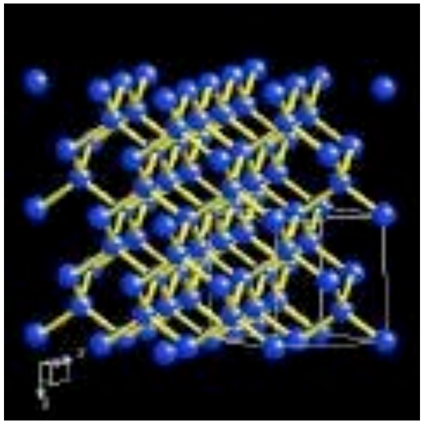
- semi-empirical models;
- Time-dependent density-functional theory (TDDFT);
- Bethe-Salpeter equation (BSE);
- Multiconfiguration methods.

Overview of the Theory:



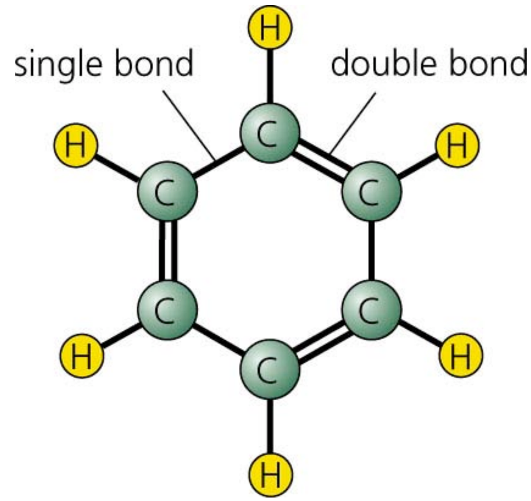
Accurate description of solid materials

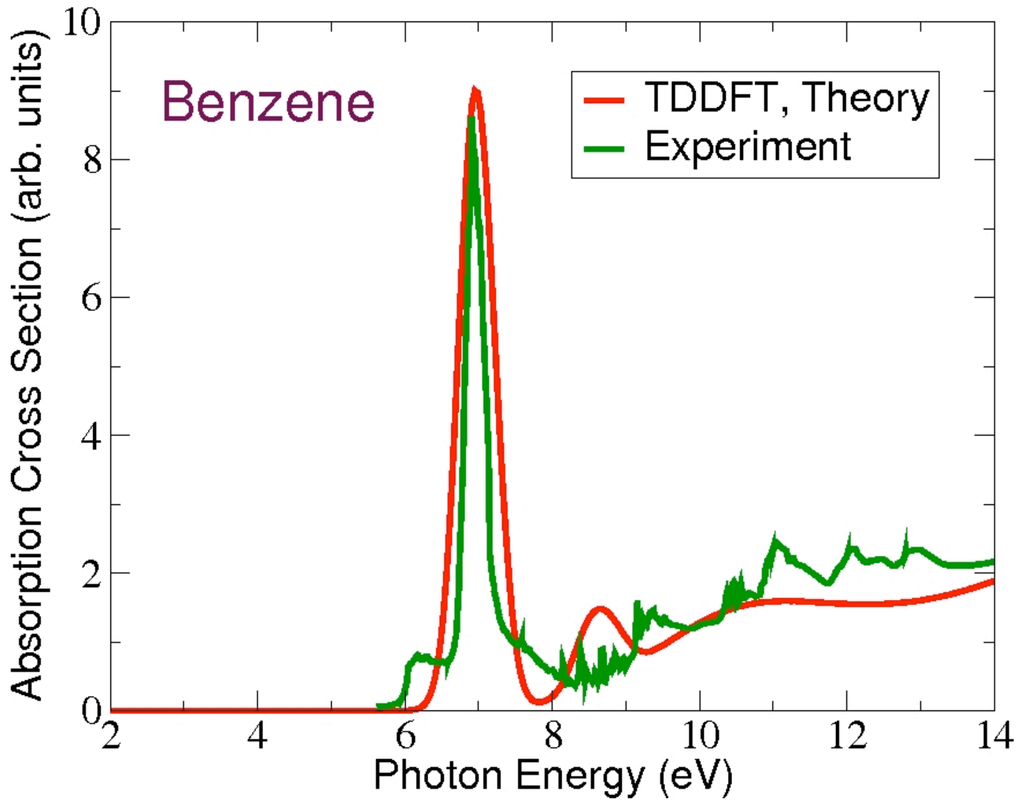




Single Crystal Silicon Ingot

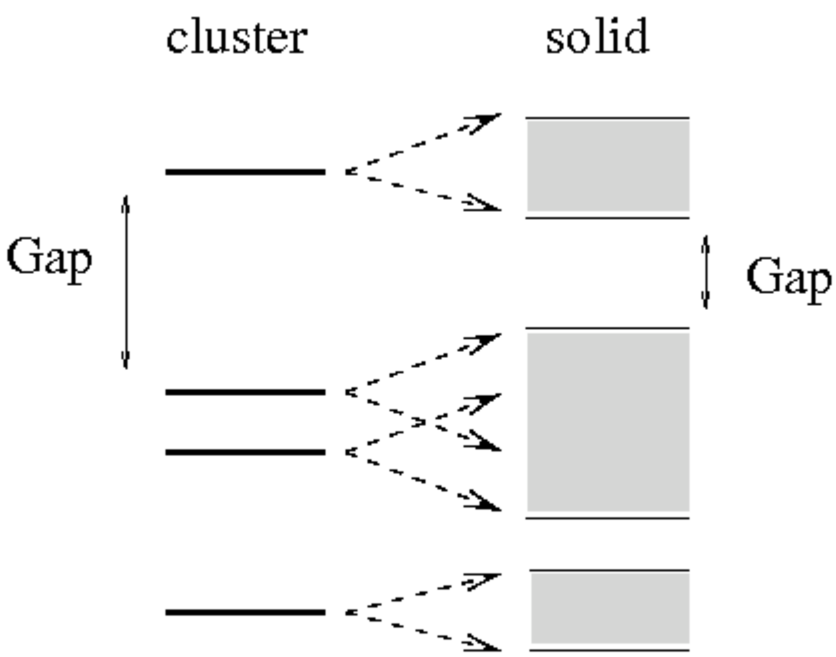
Accurate description of molecules





Quantum confinement in nanosystems

Electrons confined to a nanocluster behave differently from free electrons in a solid.



- Gap widening
- Surface effects
- Reduced screening

CdSe nanocrystals

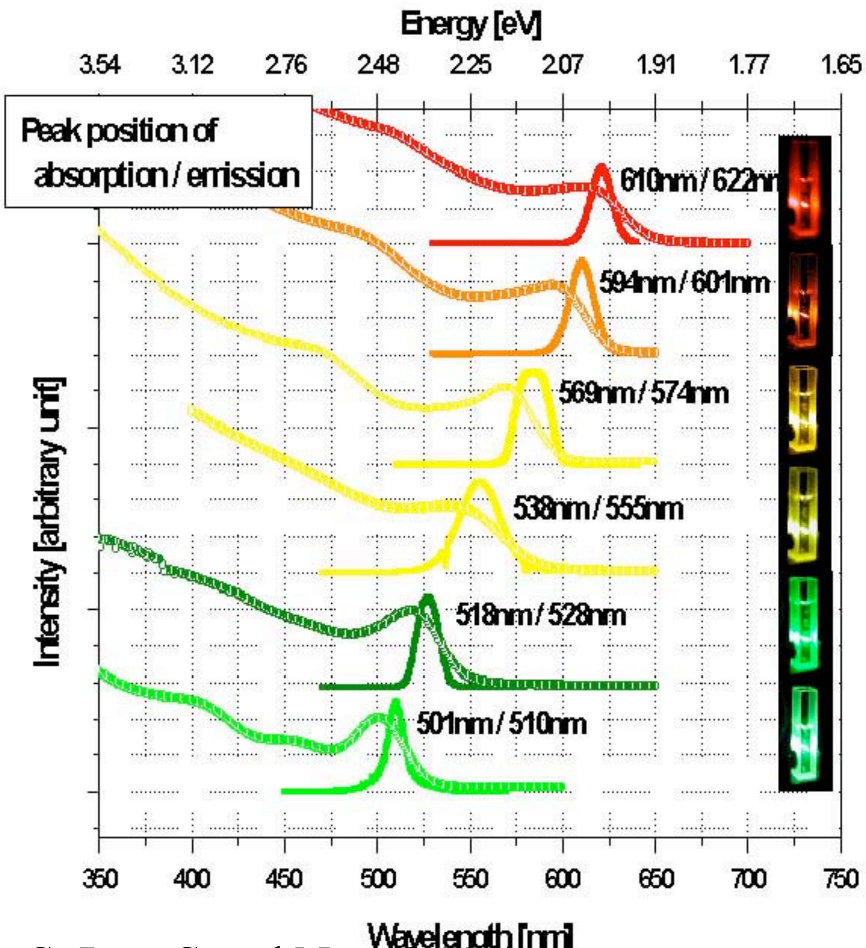
Cd_nSe_m , n+m = 10^3 to 10^4 atoms

Cluster Size →

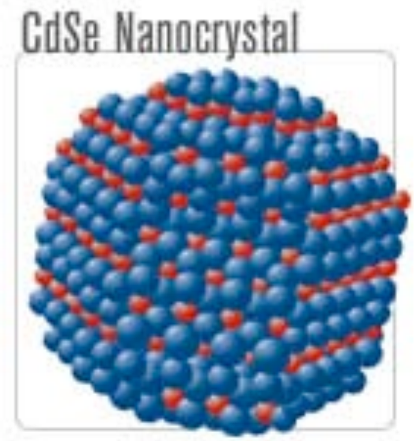
Optical activity is highly sensitive to the size of the dot.

Blue CdS/ZnS nanocrystal lasers, Bawendi *et al.* (2005)

✓Absorption & Emission Spectra of CdSe Quantum Dot



S. Lee, Seoul Natn'l. Univ.



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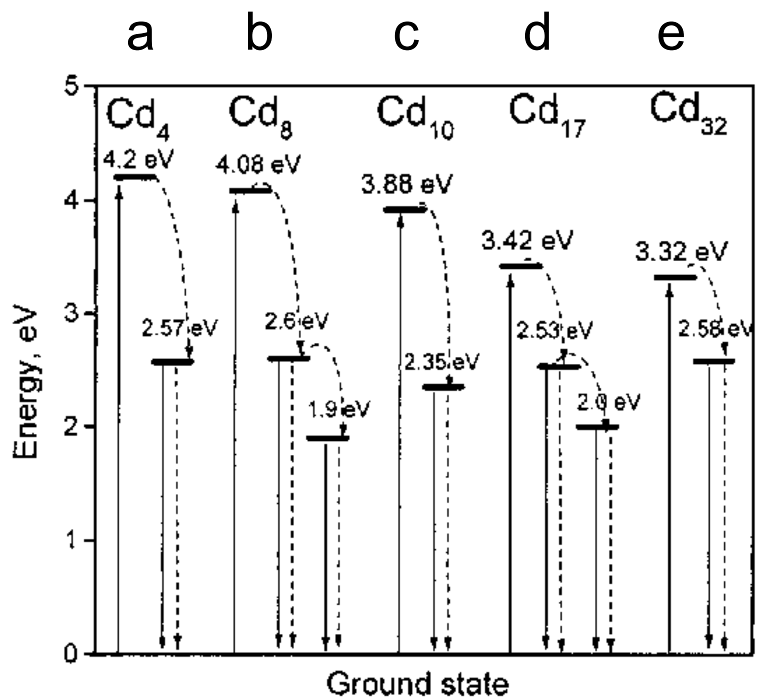
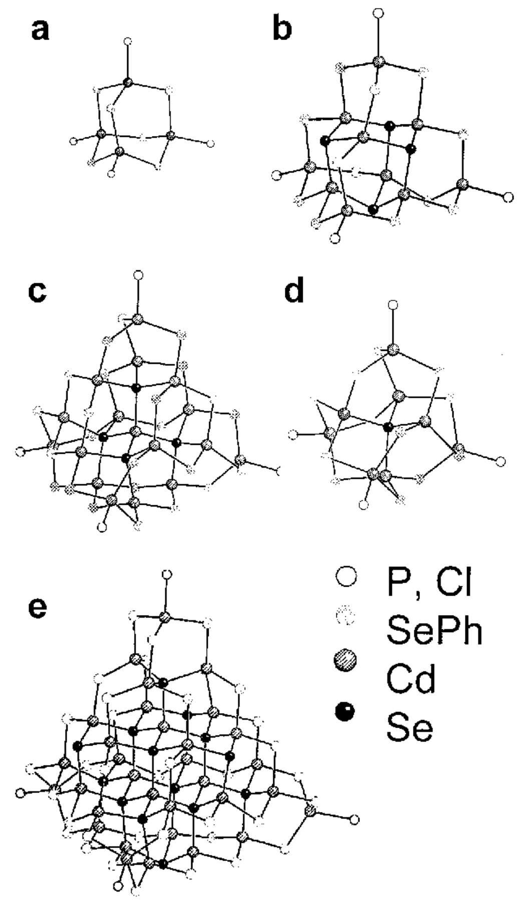
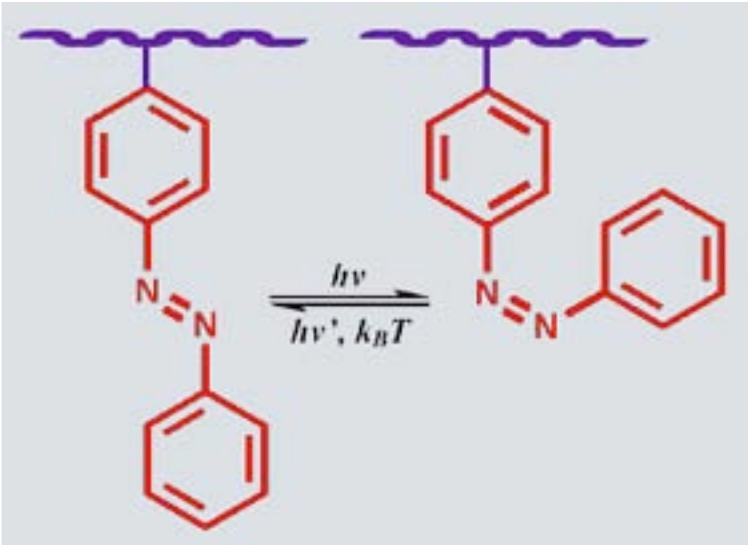
Small nanoclusters do not necessary have spherical shape





Banin *et al.* (2001)

Azobenzene ($C_{12}H_{10}N_2$)

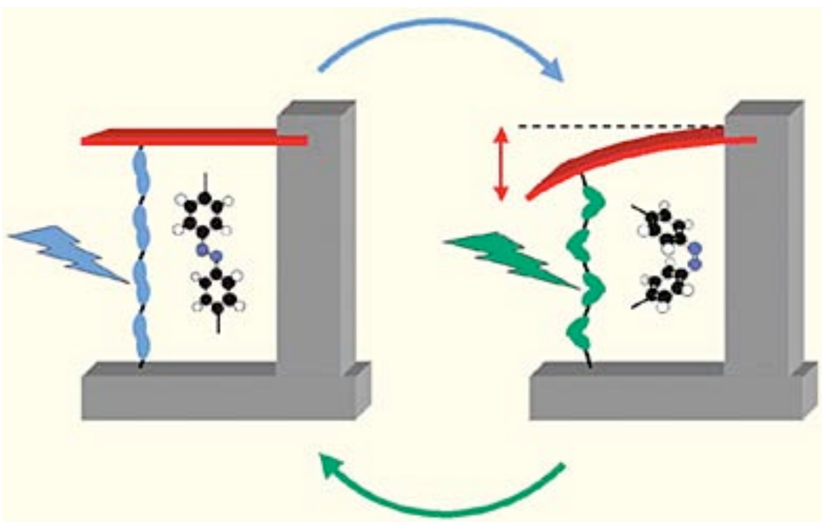


Shows photo- or thermo-induced isomerization.

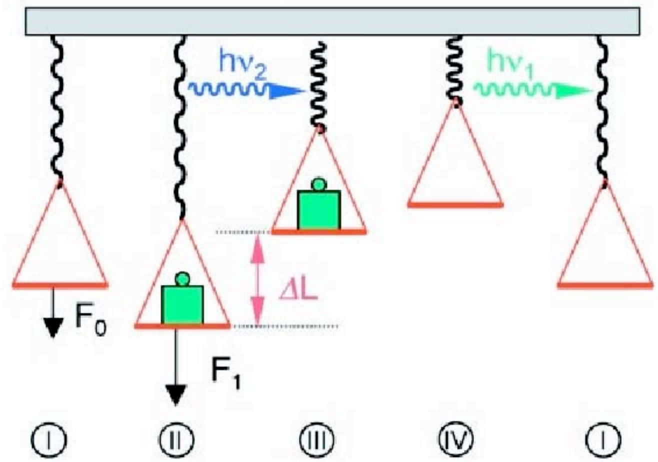
Length changes by 30% during isomerization.

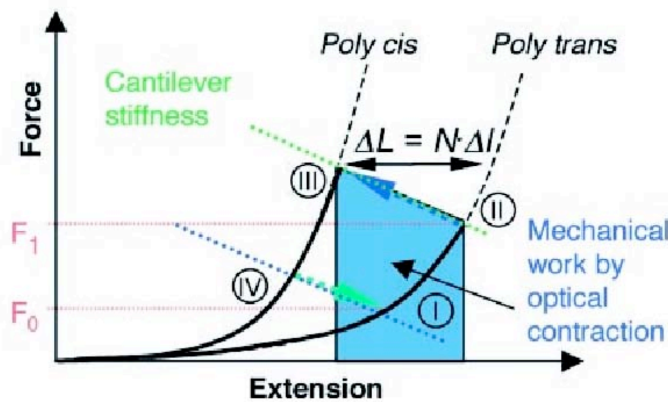
"engine" in a nanomotor.

Nanocantilever from polymerized azobenzene

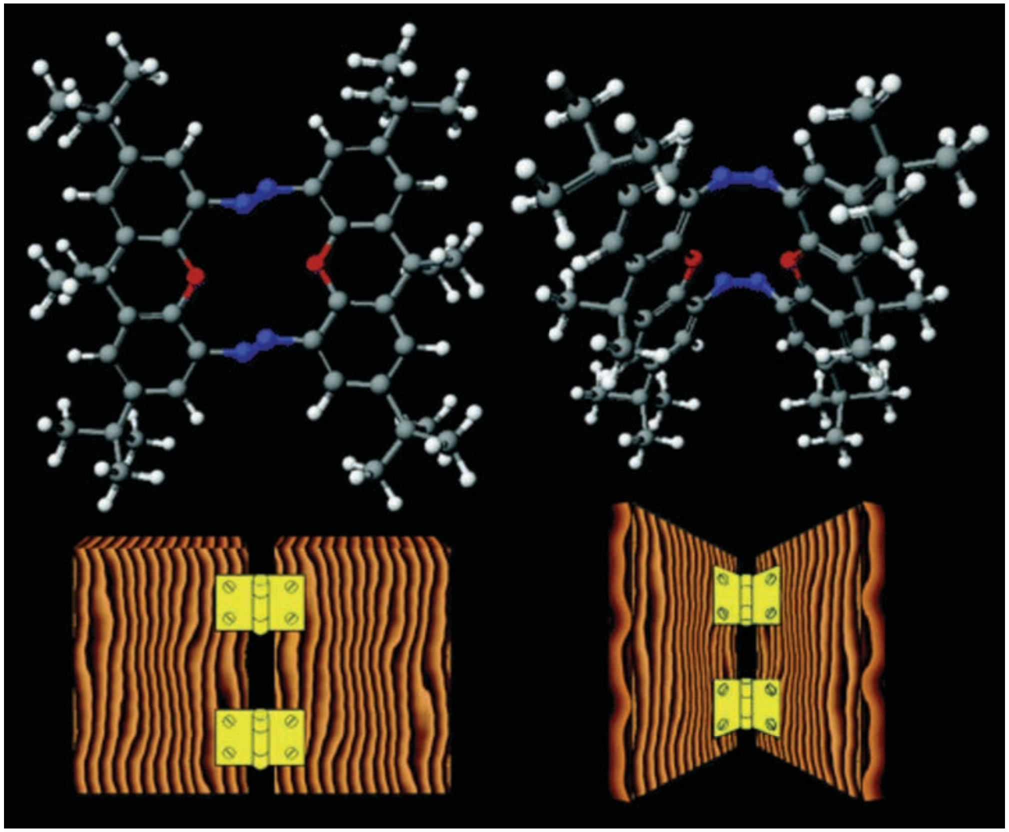


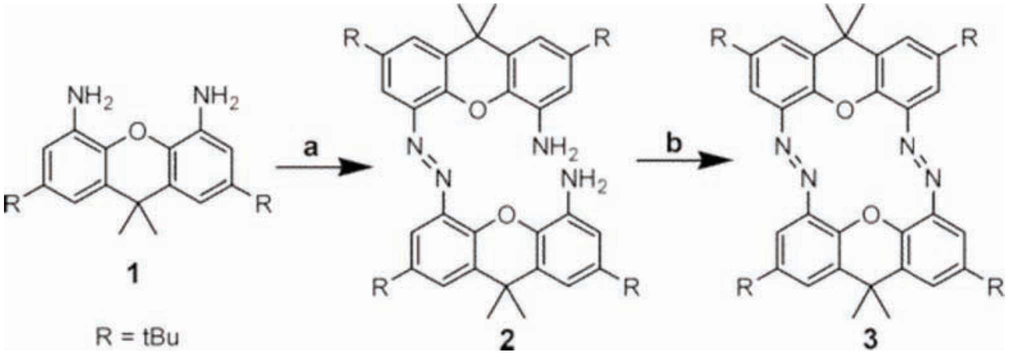
Gaub *et al.* (2002).





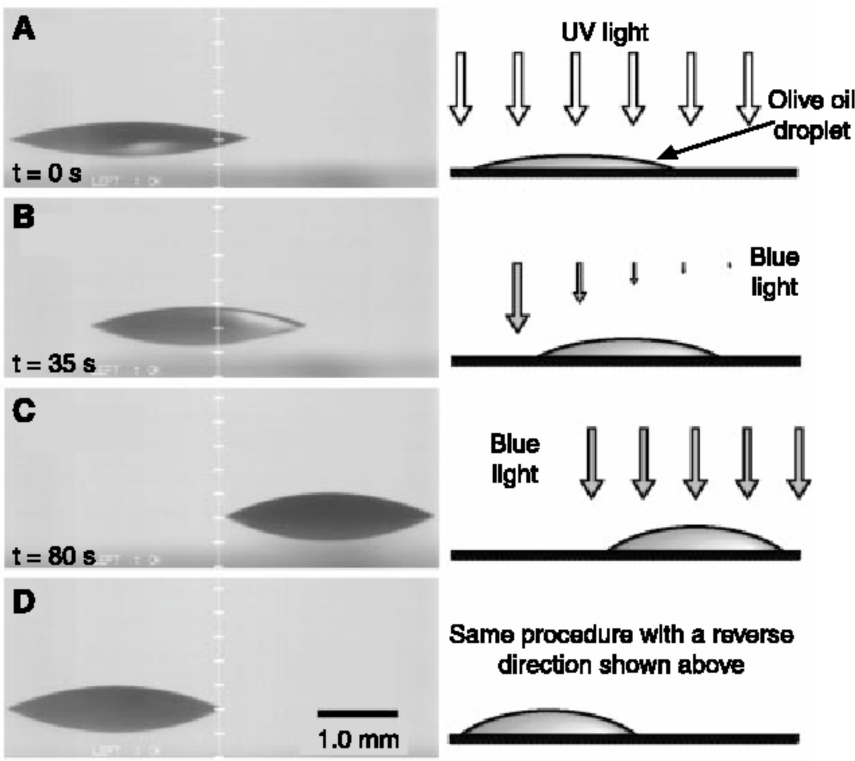
Light-driven molecular hinge.

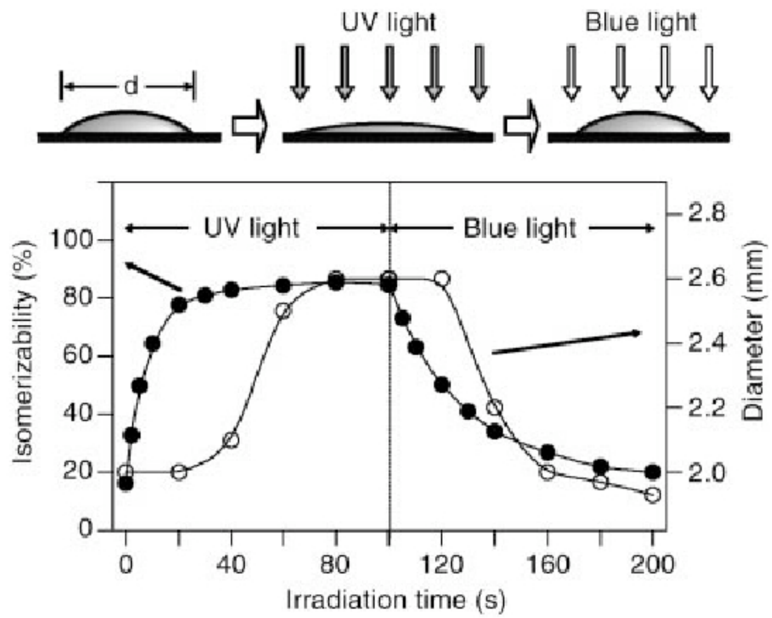




Norikane and Tamaoki (2004)

Light-driven motion of liquids on a photoresponsive surface





Ichimura *et al.* (2000)