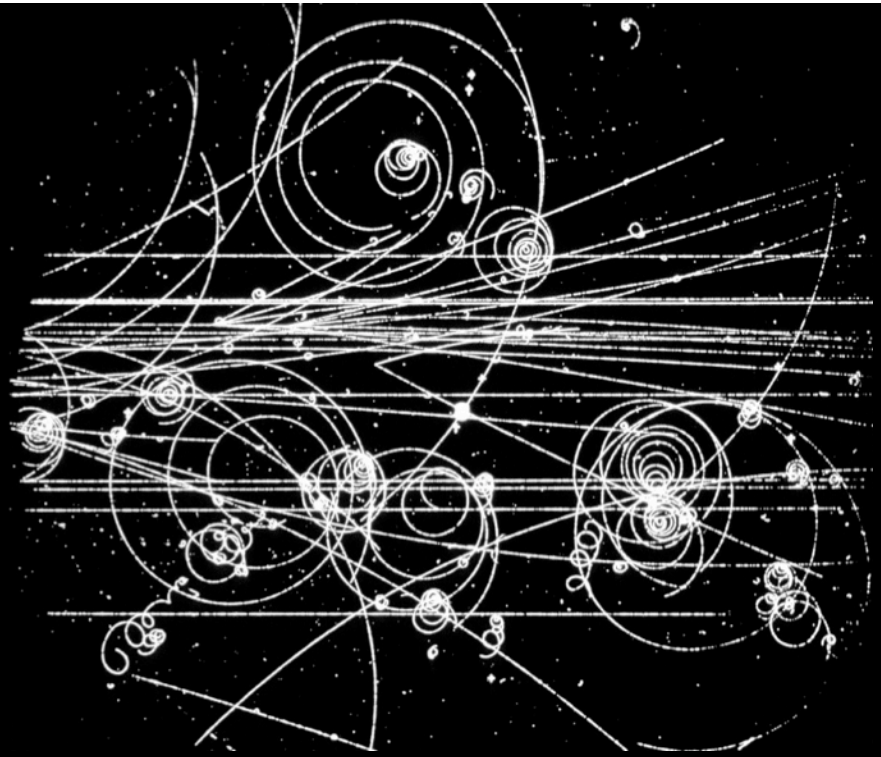
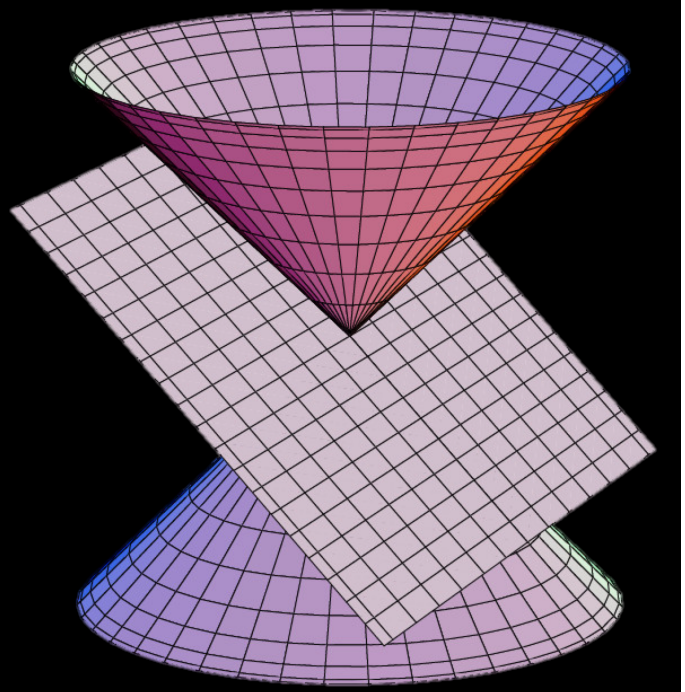




Modern Physics (Phys. IV): 2704

Professor Jasper Halekas
Van Allen 70
MWF 12:30-1:20 Lecture

Sign of the Wave Function

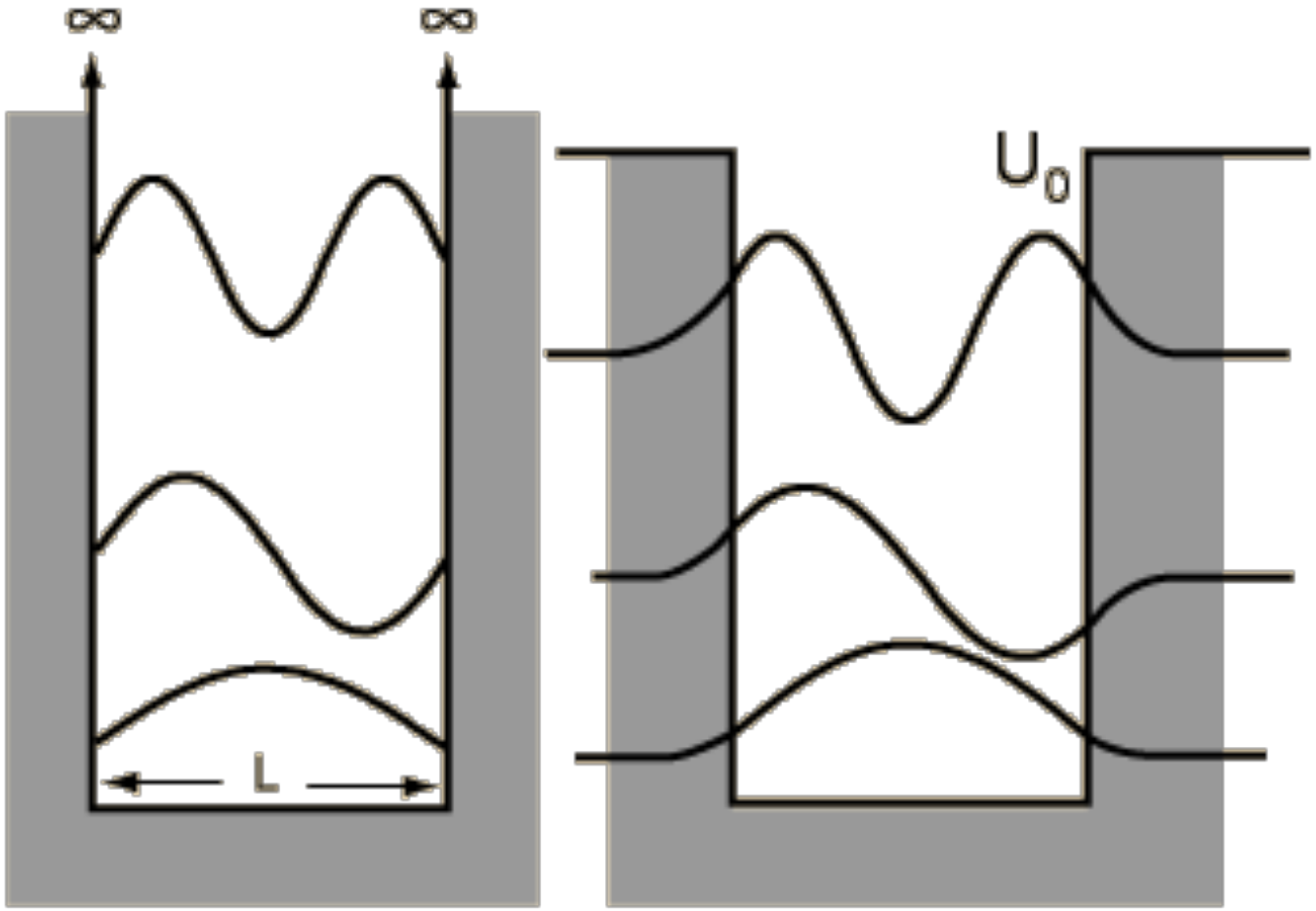
$$\frac{-\hbar^2}{2\mu}\frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{\sin\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]$$

$$+U(r)\Psi(r,\theta,\phi)=E\,\Psi(r,\theta,\phi)$$

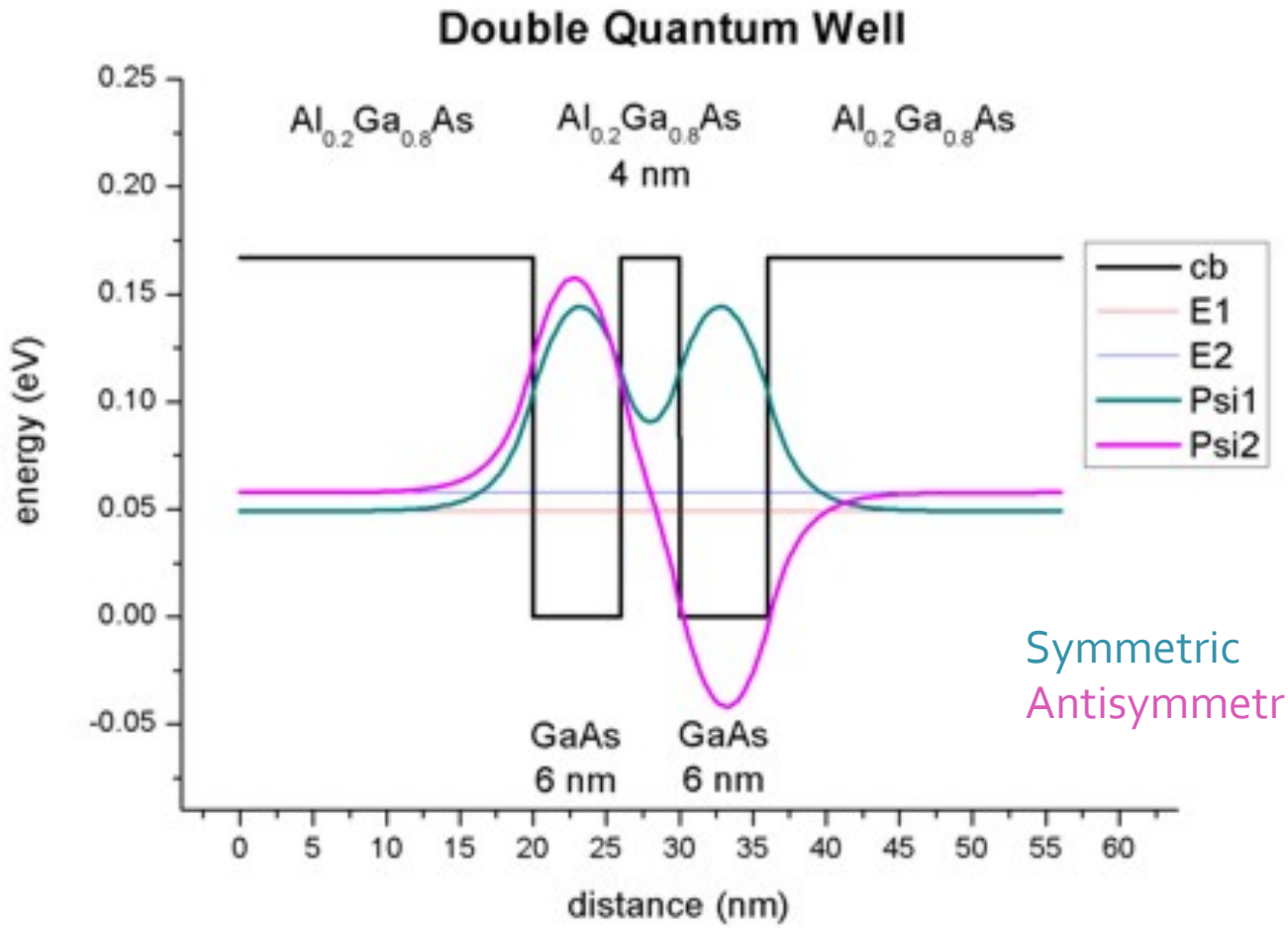
If the wave function Ψ solves this wave equation, so does -Ψ (and there are no observable effects)

But, what about combinations of solutions…?

Single-Well Wave Functions



Double-Well Ground State Wave Functions



Symmetric
Antisymmetric

Concept Check

- For which wave function does the electron have a higher probability of being in the space between the two wells?

A. Symmetric
B. Antisymmetric
C. No difference

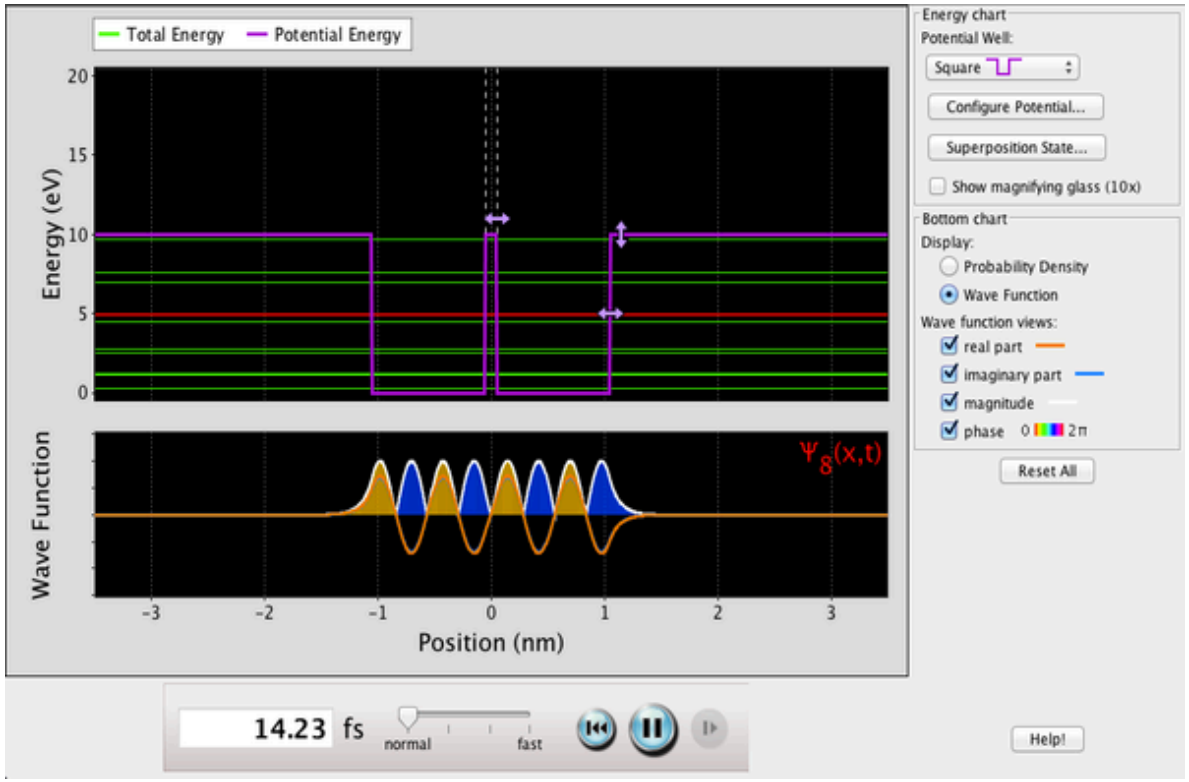
Concept Check

- For which wave function does the electron have a higher probability of being in the space between the two wells?

A. Symmetric
B. Antisymmetric
C. No difference

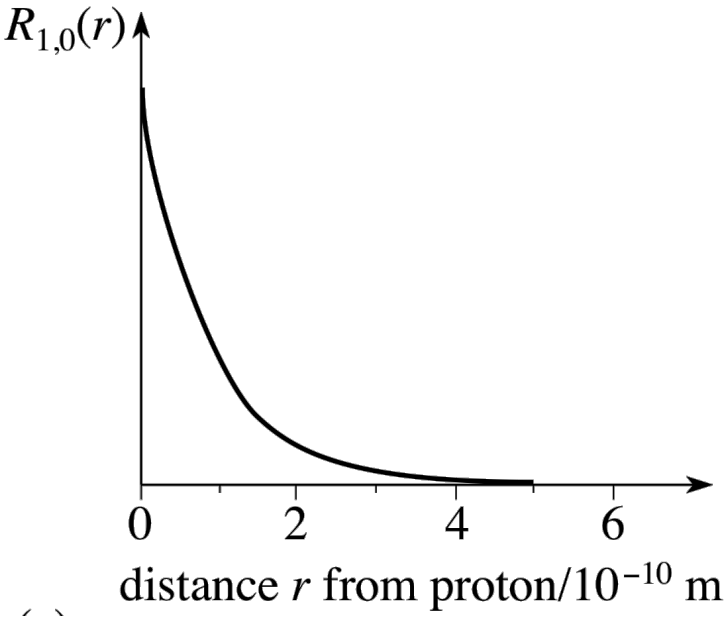
Double Well Potential

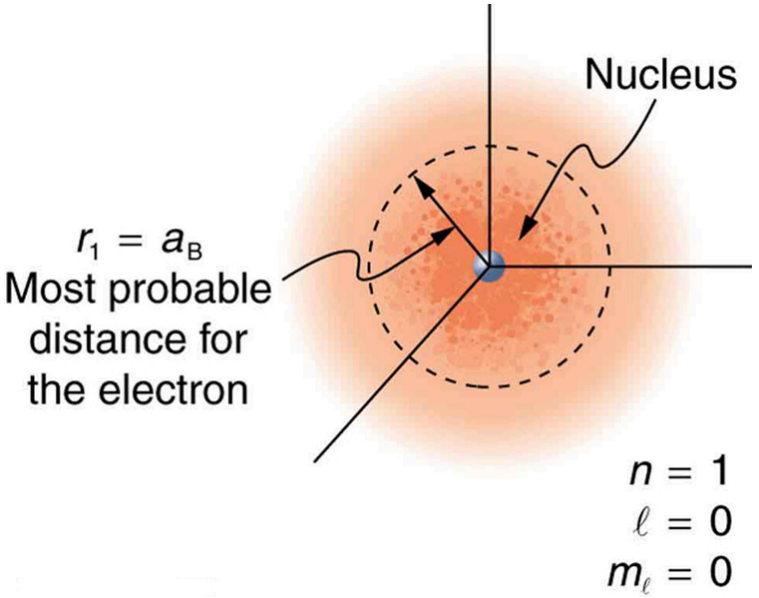
- https://phet.colorado.edu/en/simulation/legacy/covalent-bonds



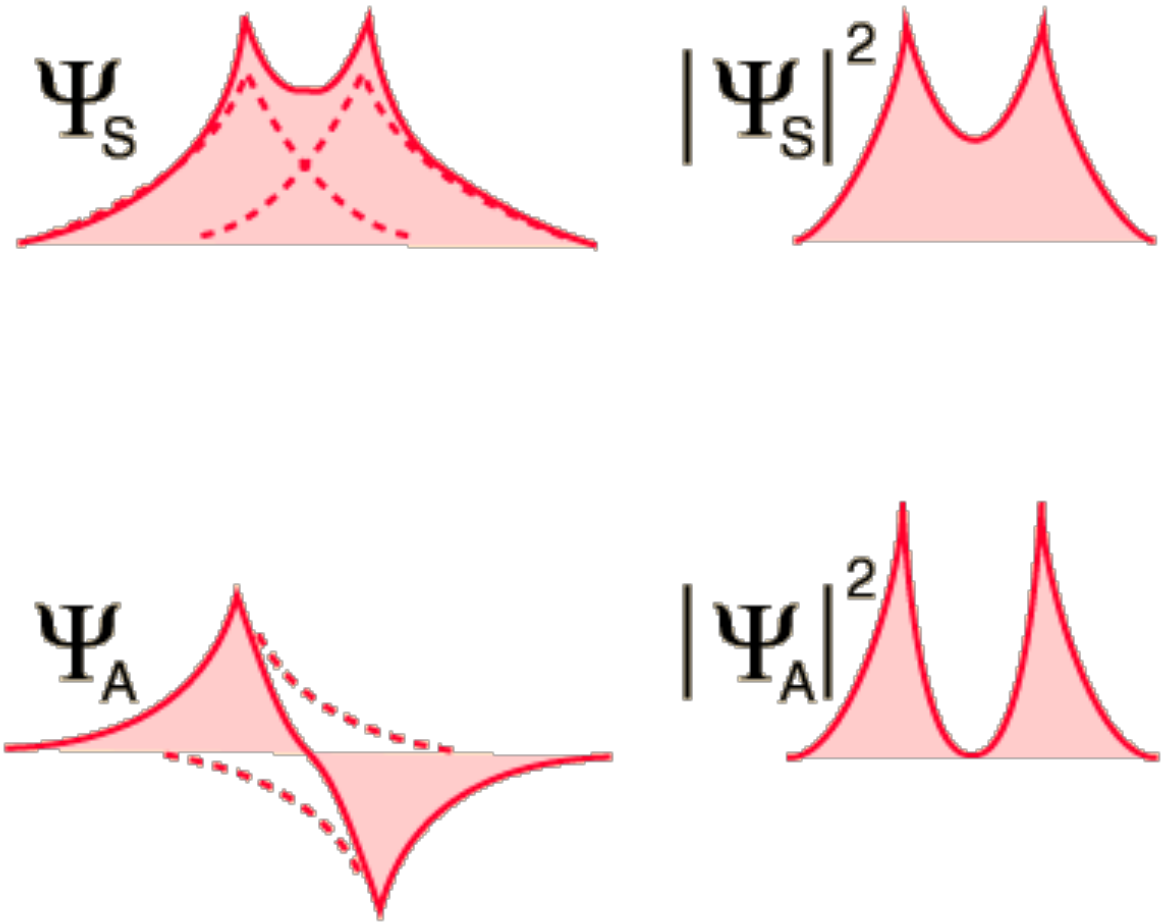
Ground State of Electron in H Atom

$$\Psi_{1,0,0} = \Psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o}\right)^{3/2} e^{-r/a_o}$$





Symmetric and Antisymmetric Electron Wave Functions in H_2



Concept Check

- Imagine that we have a system of two protons and one electron. For which electron wave function will the system be more likely to be stable?

A. Symmetric
B. Antisymmetric
C. No Difference

Concept Check

- Imagine that we have a system of two protons and one electron. For which electron wave function will the system be more likely to be stable?

A. Symmetric
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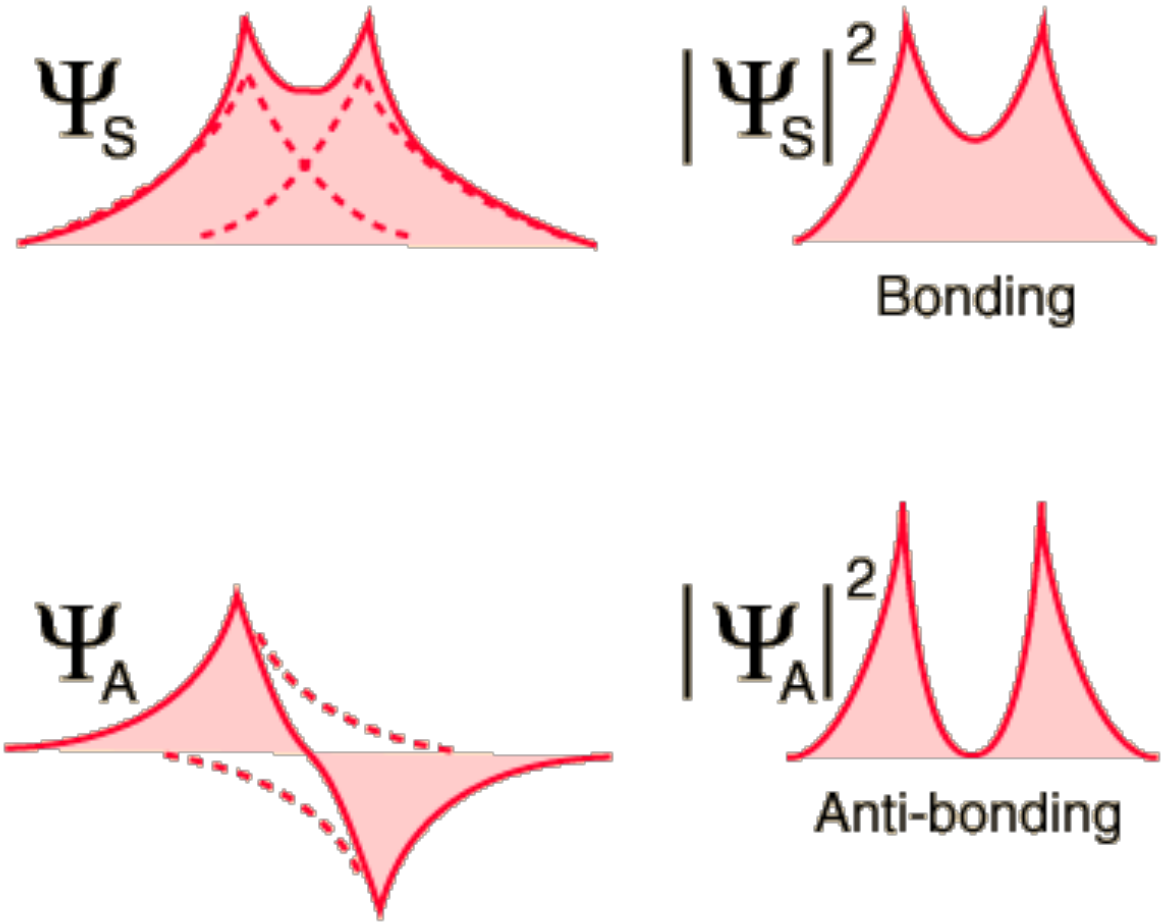
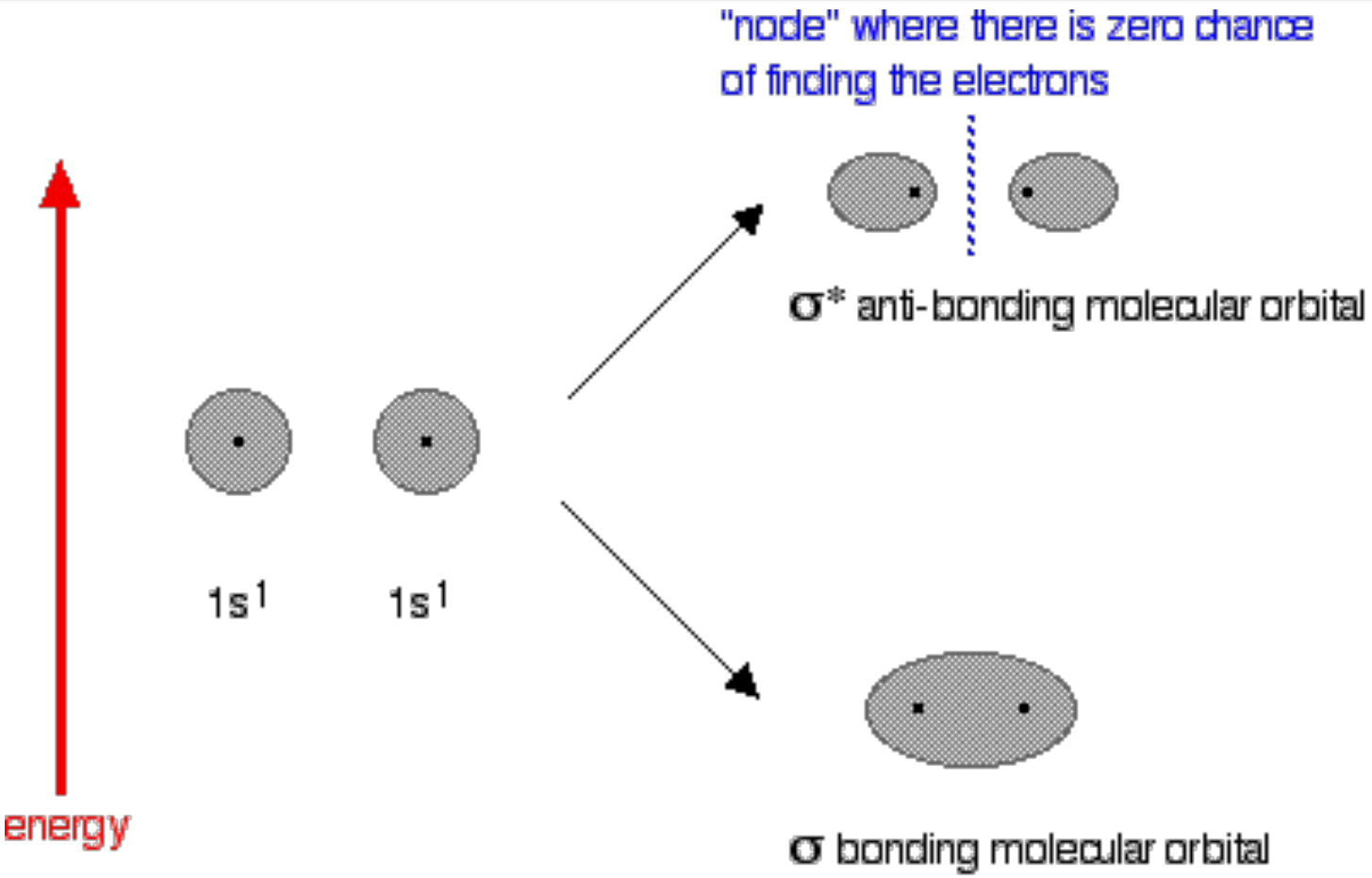
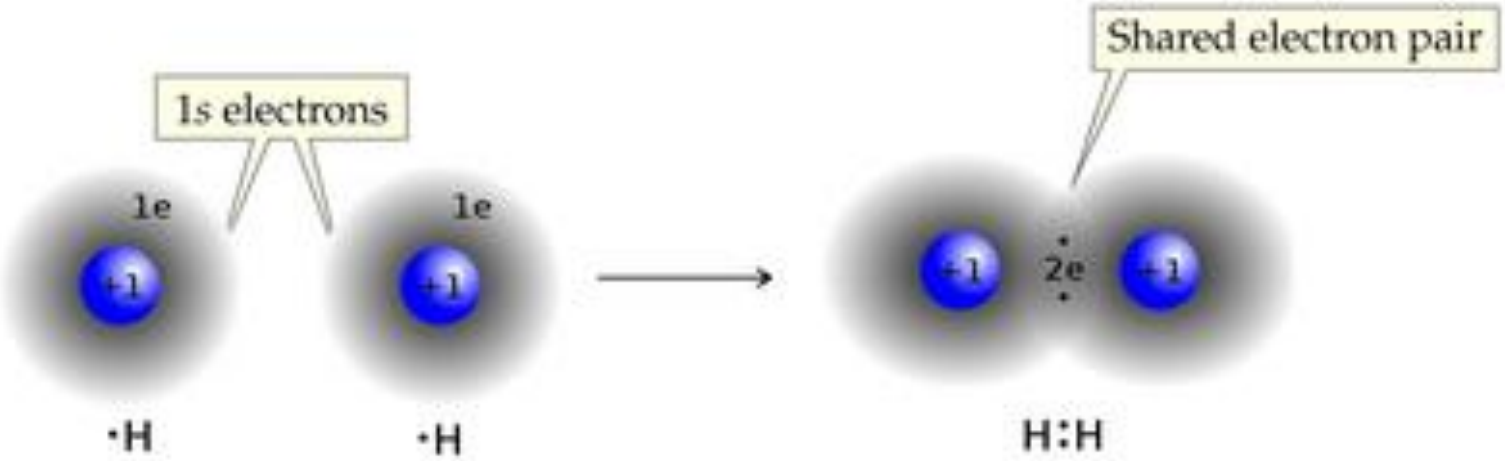
Bonding and Antibonding Wave Functions



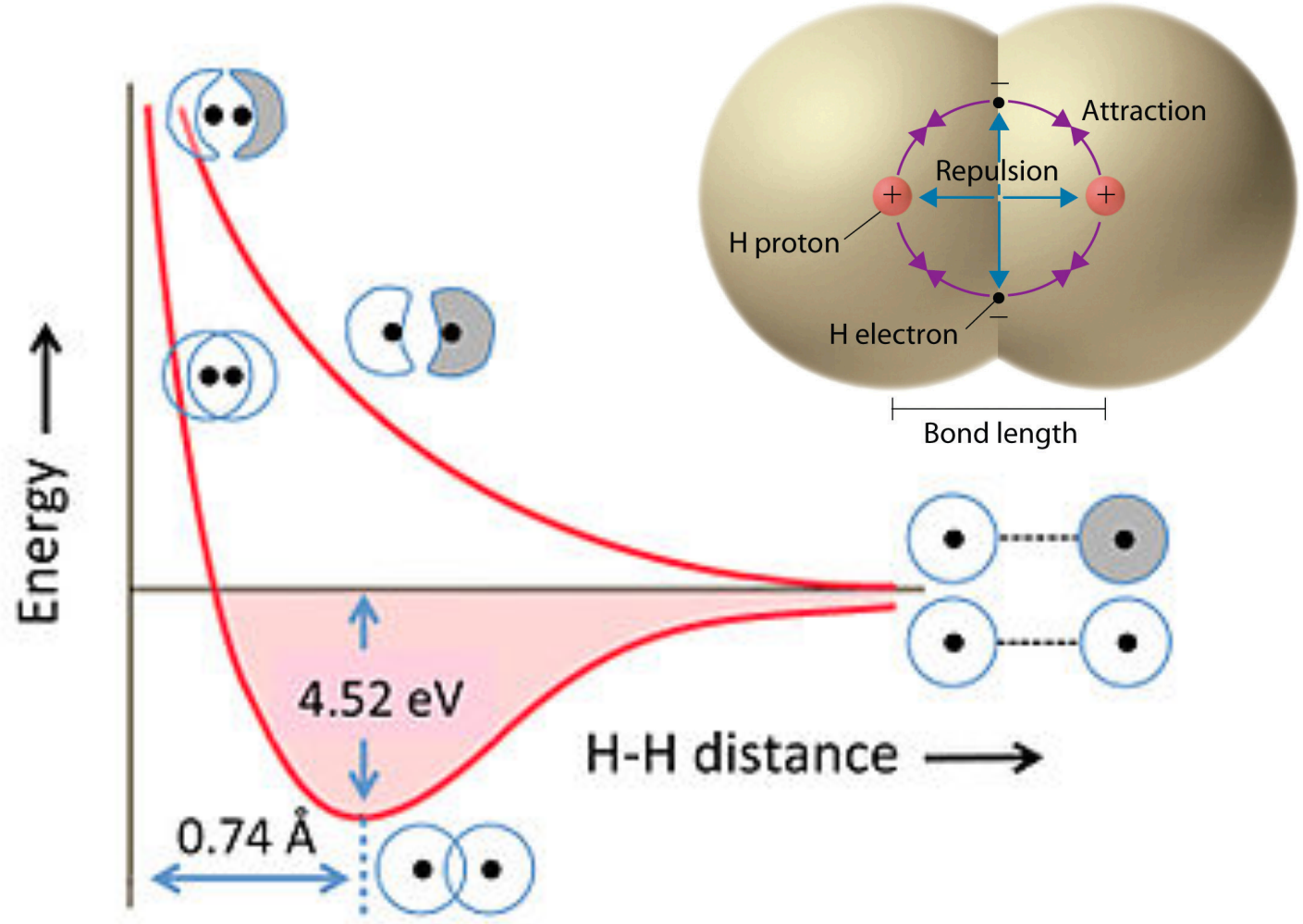
Bonding and Antibonding Orbitals



Covalent Bonding



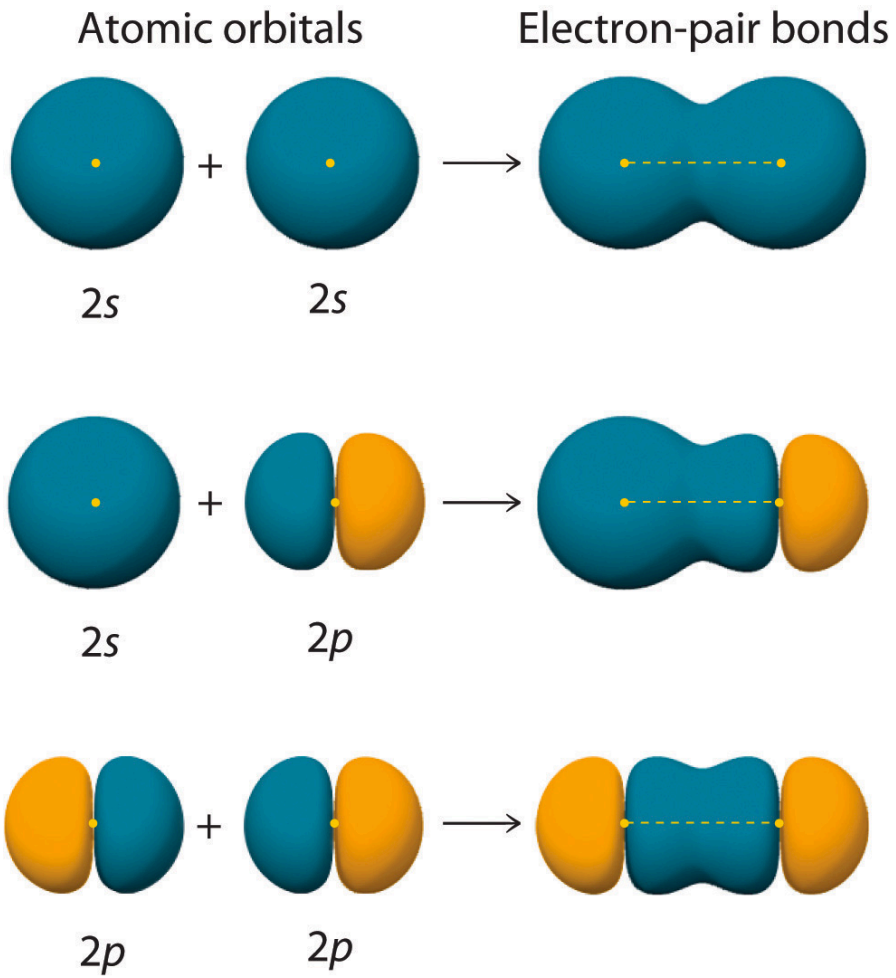
Hydrogen Molecule Covalent Bond Energy



Covalent Bonding

I. Wave function of electrons near two nuclei are (approximately) a combination of the individual wave functions
II. Symmetric combinations (bonding states) are energetically favorable
III. Antisymmetric combinations (antibonding states) do not lead to stable molecules
IV. Each molecular state has a maximum occupancy of two electrons (spin up and spin down)

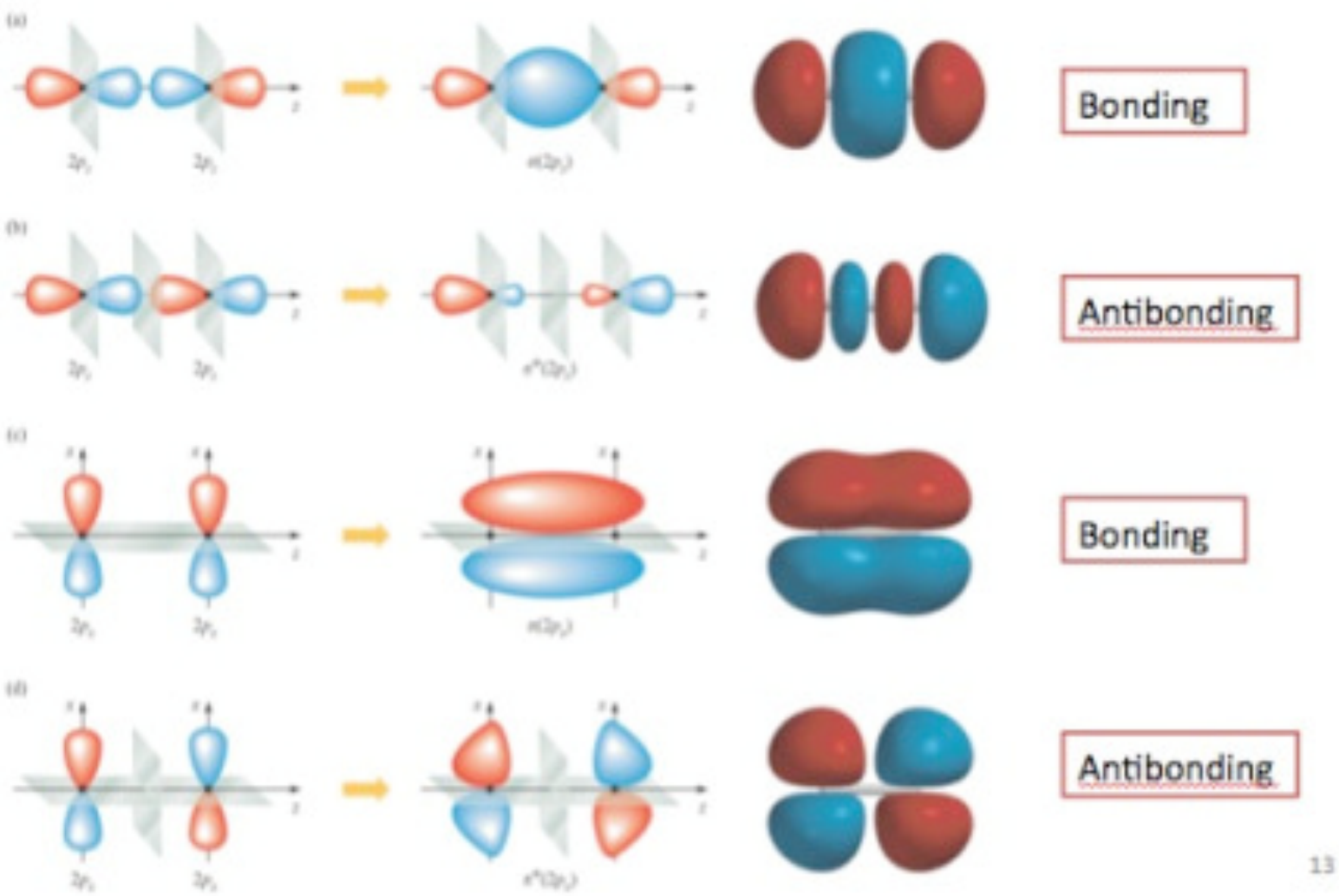
ss, sp and pp covalent bonds



pp covalent bonding

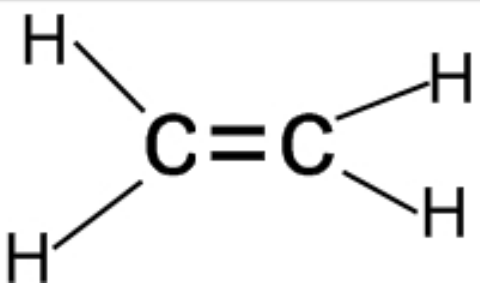
σ

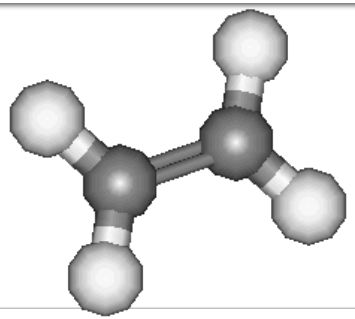
π

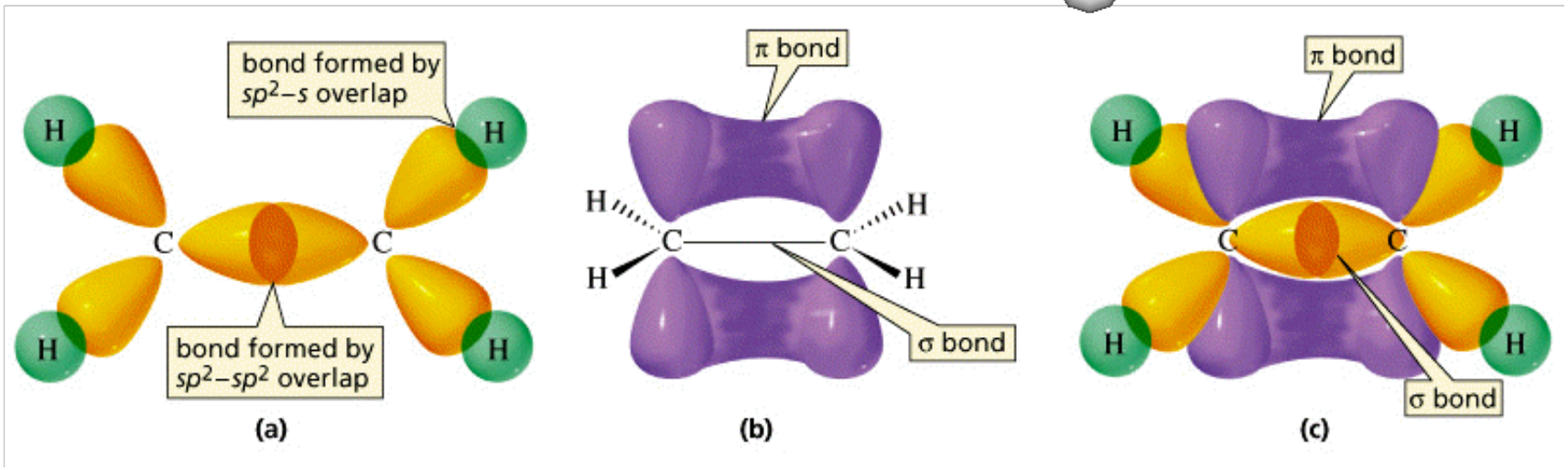


Multiple Bonds

Ethene

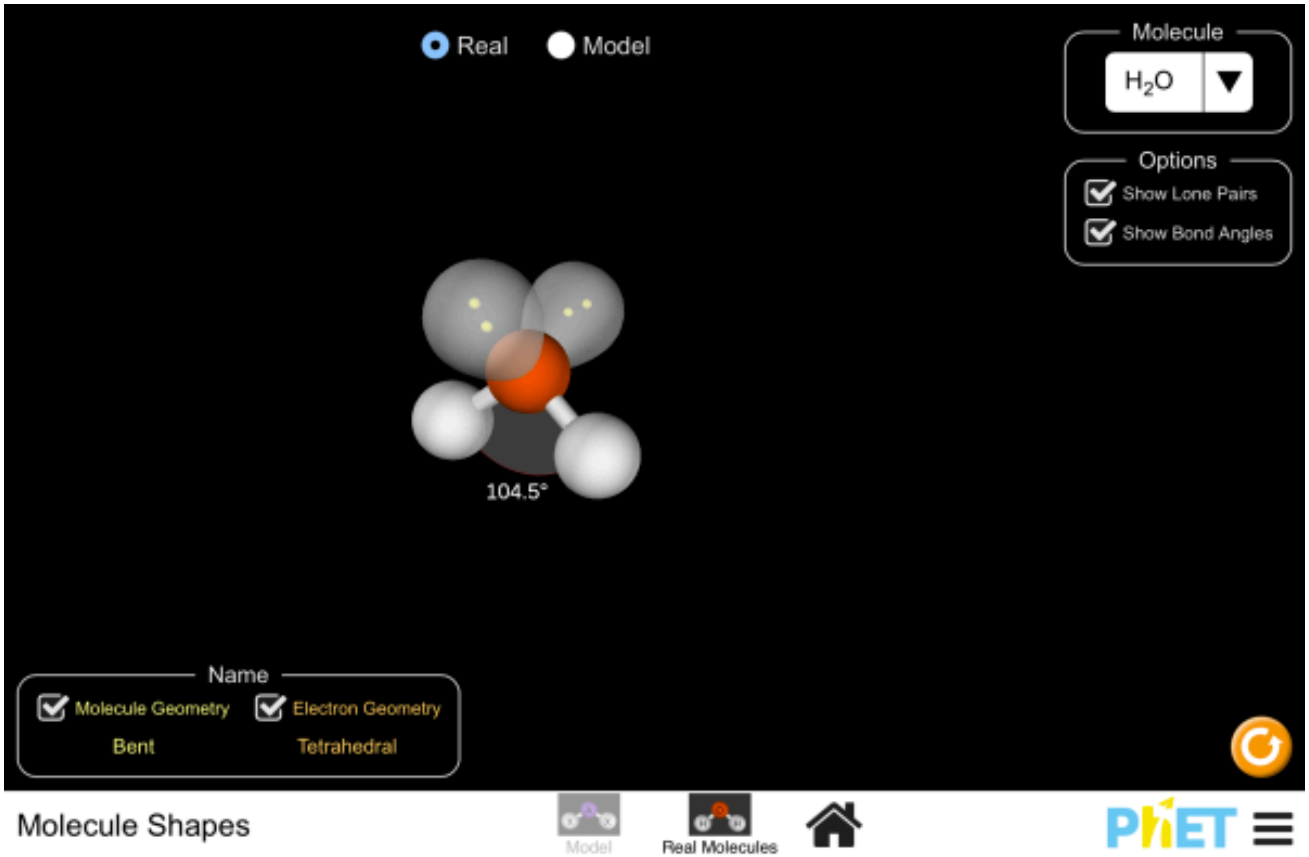




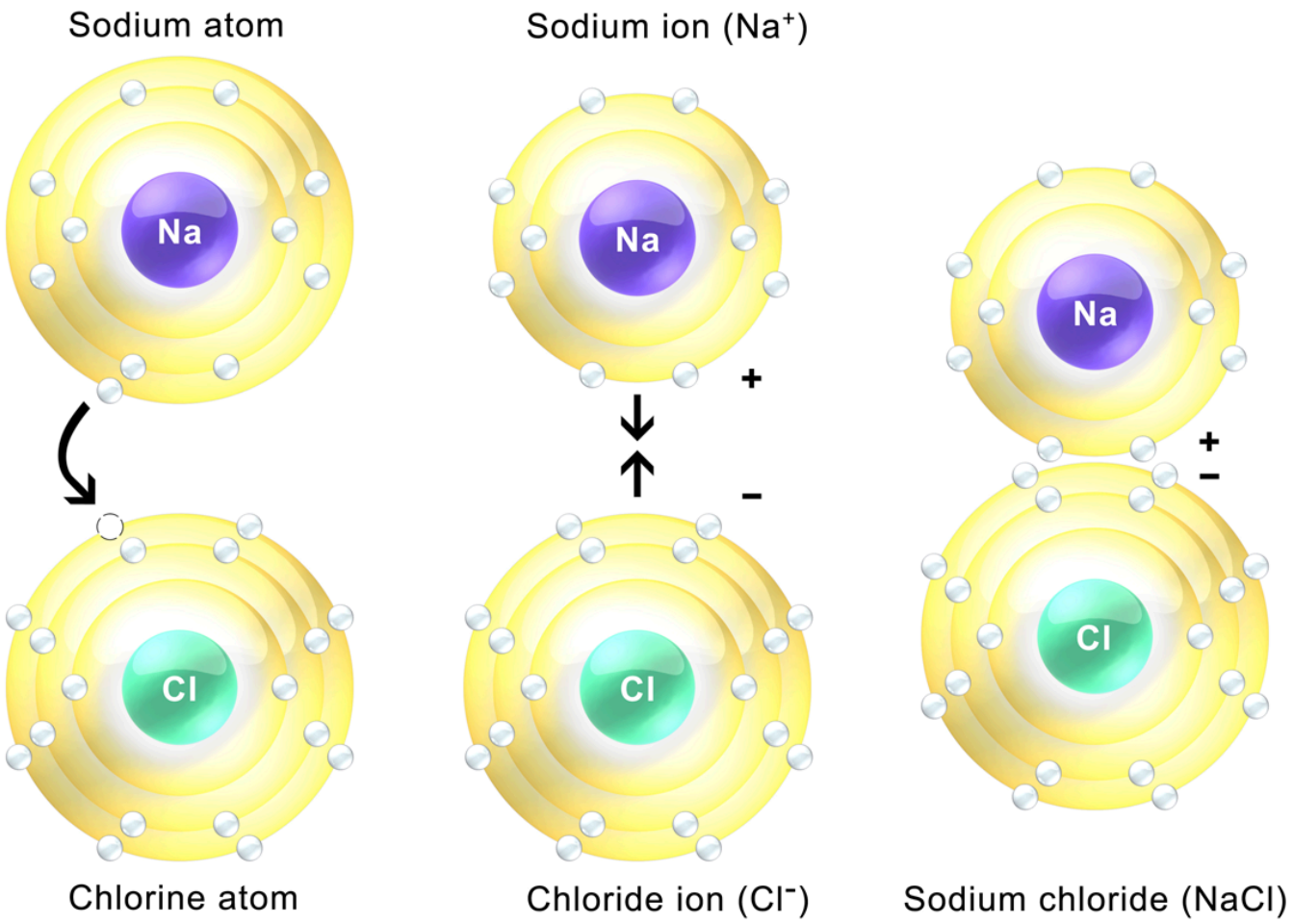


Molecule Shapes

- https://phet.colorado.edu/en/simulation/molecule-shapes

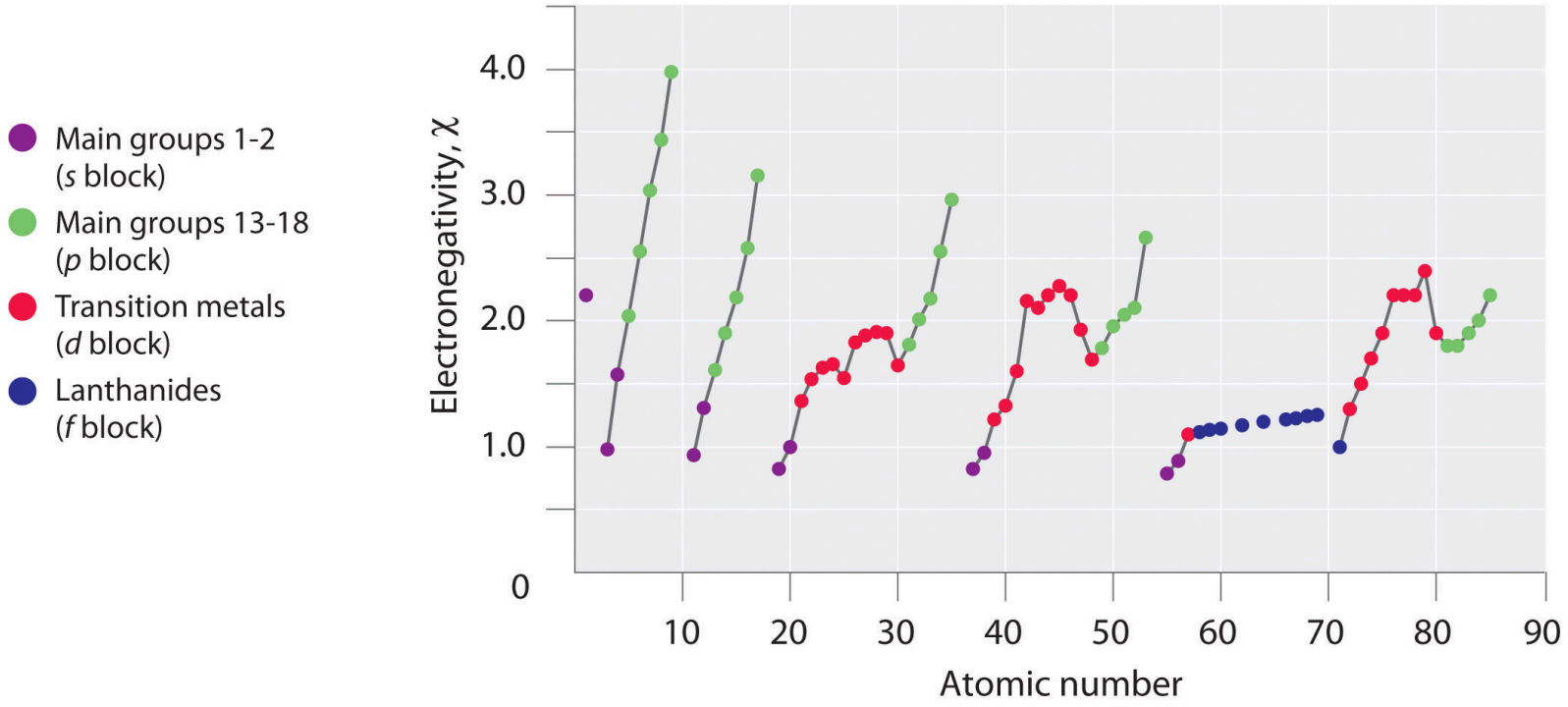


Ionic Bonds

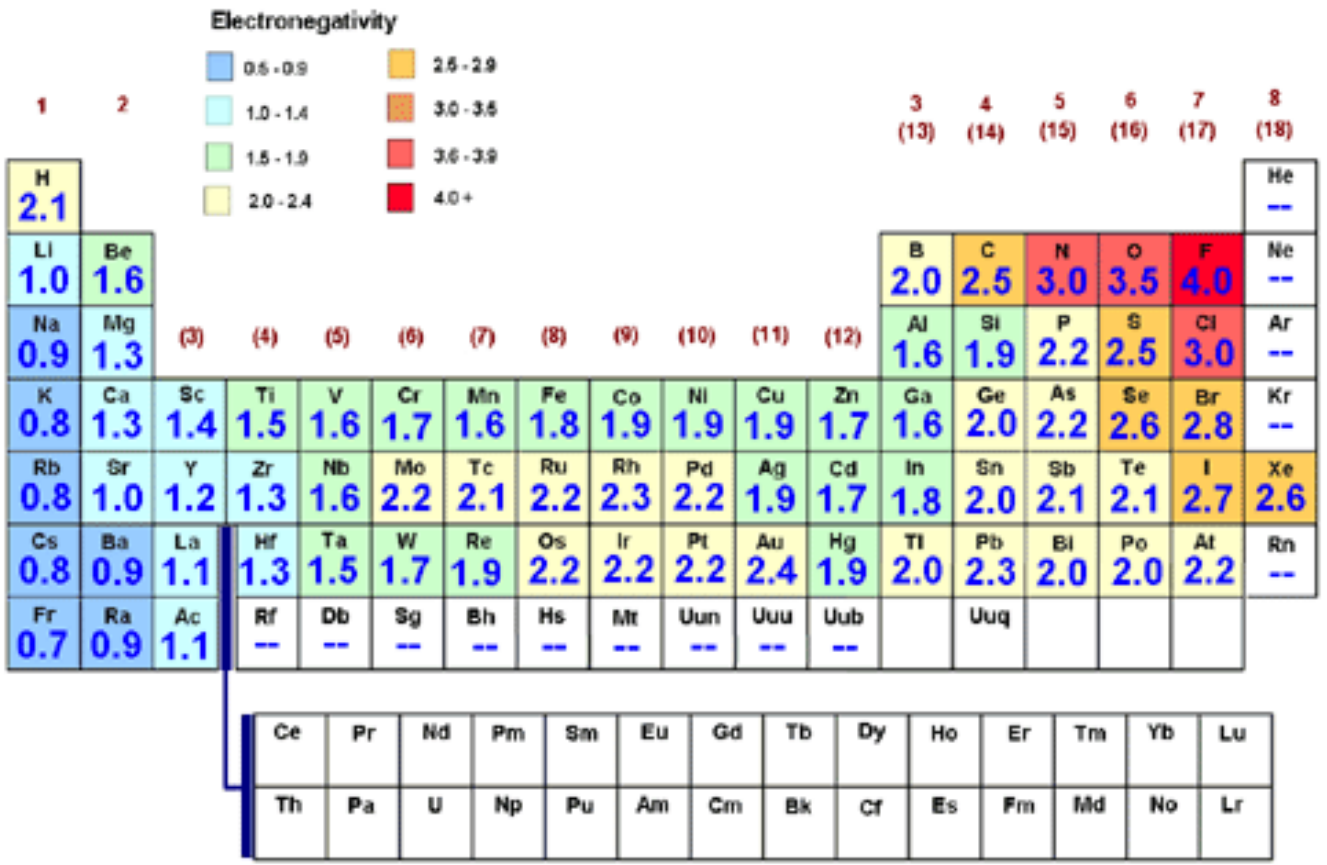

Sodium atom
Sodium ion (Na^+)
Na
Na
Na
+
−
+
−
Cl
Cl
Cl
Chlorine atom
Chloride ion (Cl^-)
Sodium chloride (NaCl)

Electronegativity

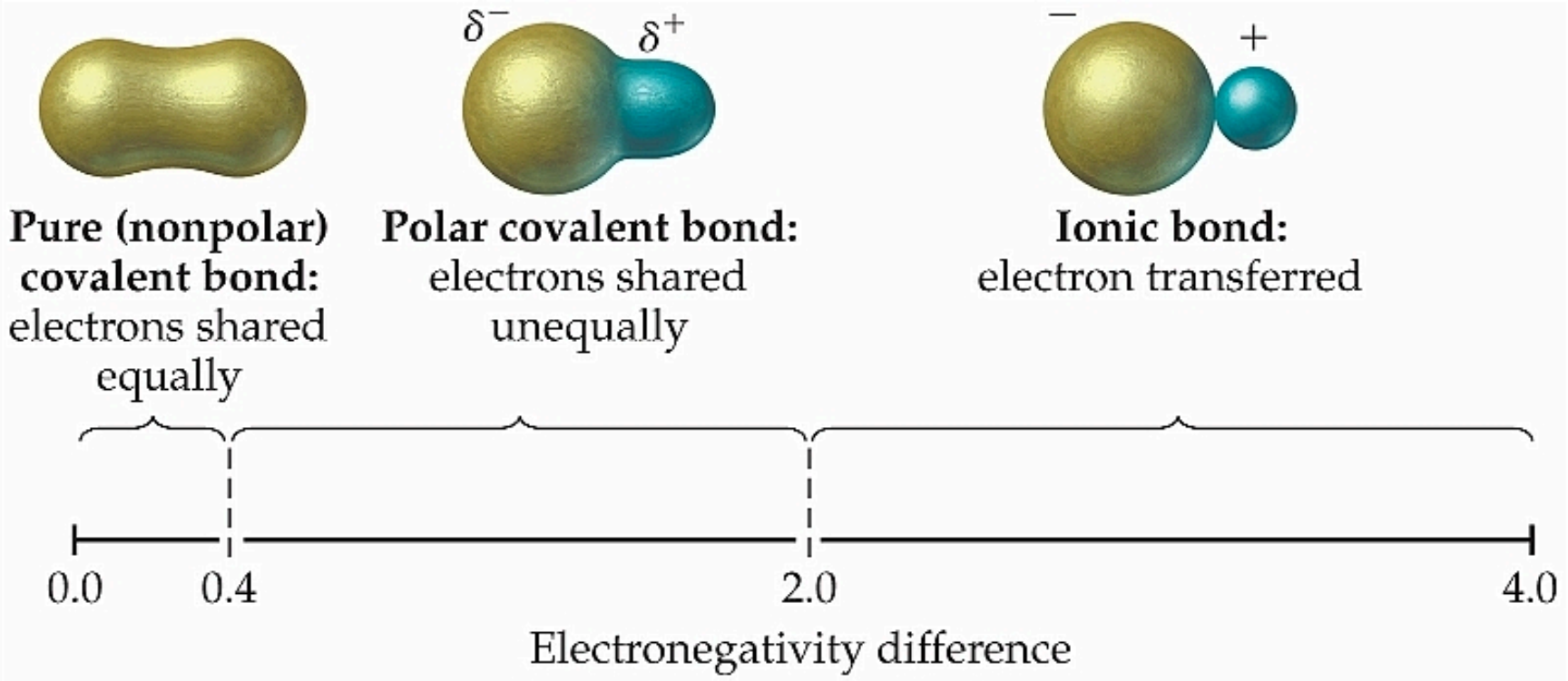
- Defined as: the tendency to attract electrons
  - Increases as you fill each shell since nuclear attraction increases faster than electron screening with a shell



Electronegativity



Covalent Vs Ionic Bonding



Covalent Vs. Ionic Bonds

- https://phet.colorado.edu/en/simulation/molecule-polarity