

Modern Physics (Phys. IV): 2704

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

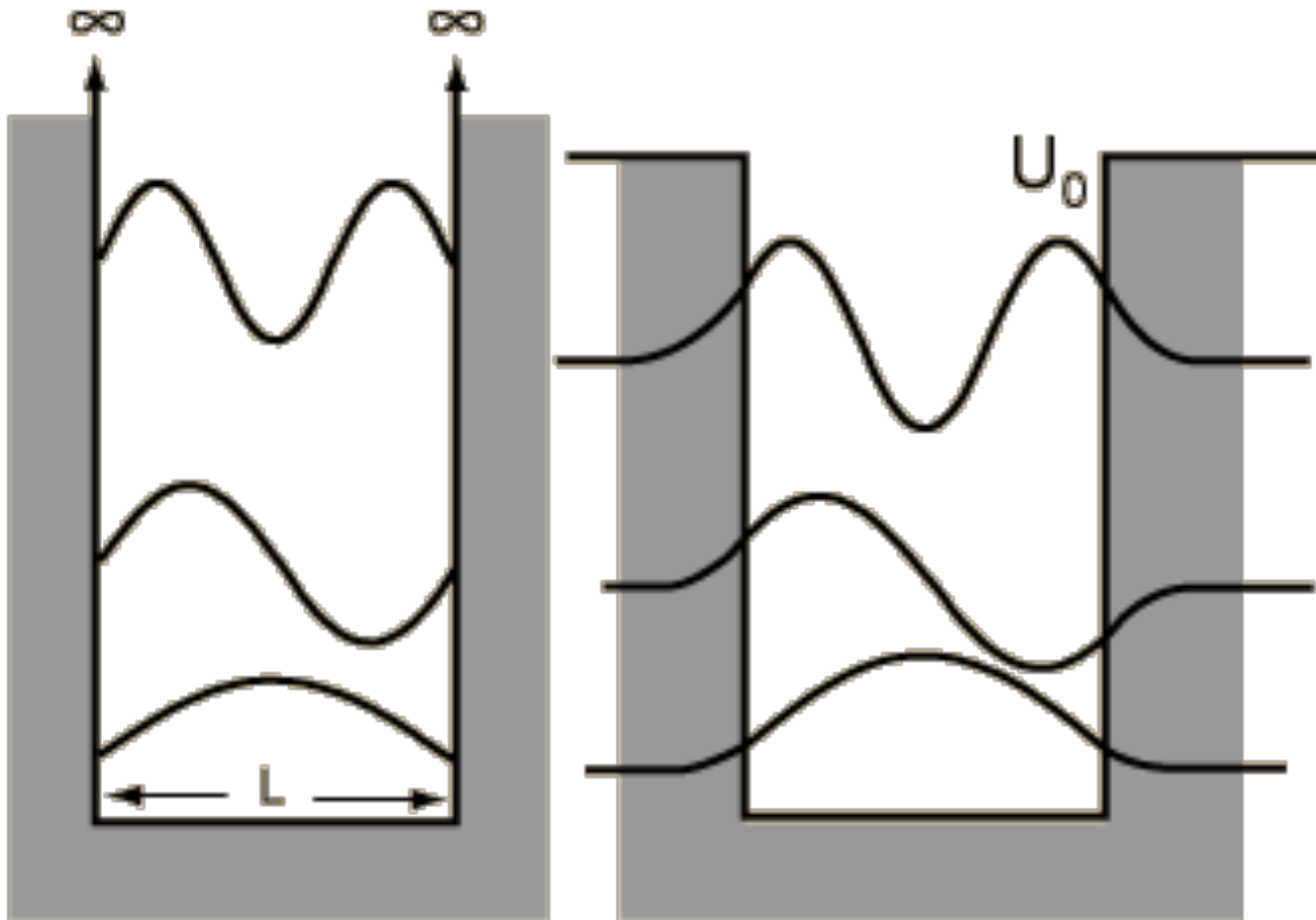
Sign of the Wave Function

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

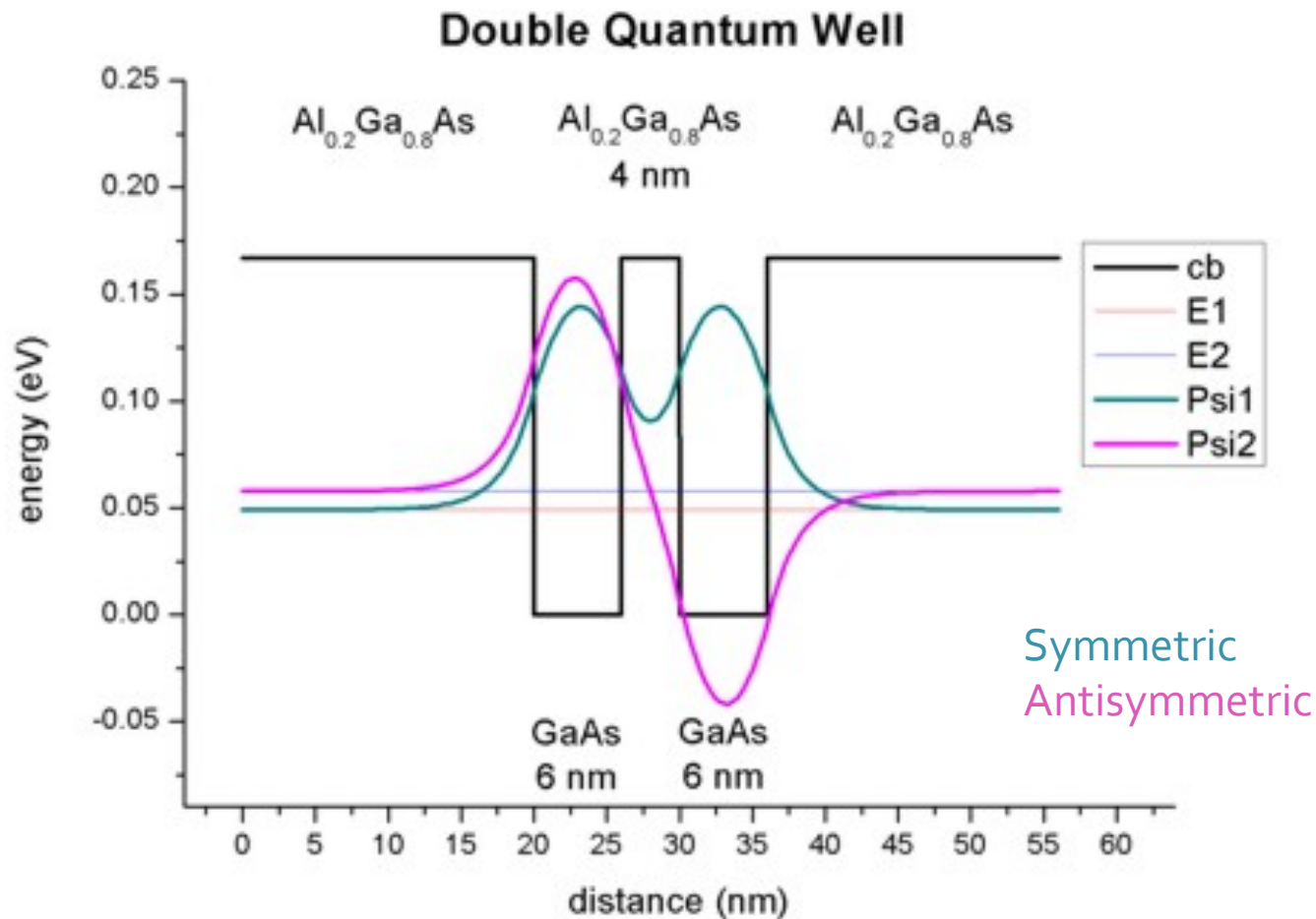
If the wave function Ψ solves this wave equation, so does $-\Psi$ (and there are no observable effects)

But, what about combinations of solutions...?

Single-Well Wave Functions



Double-Well Ground State Wave Functions



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?

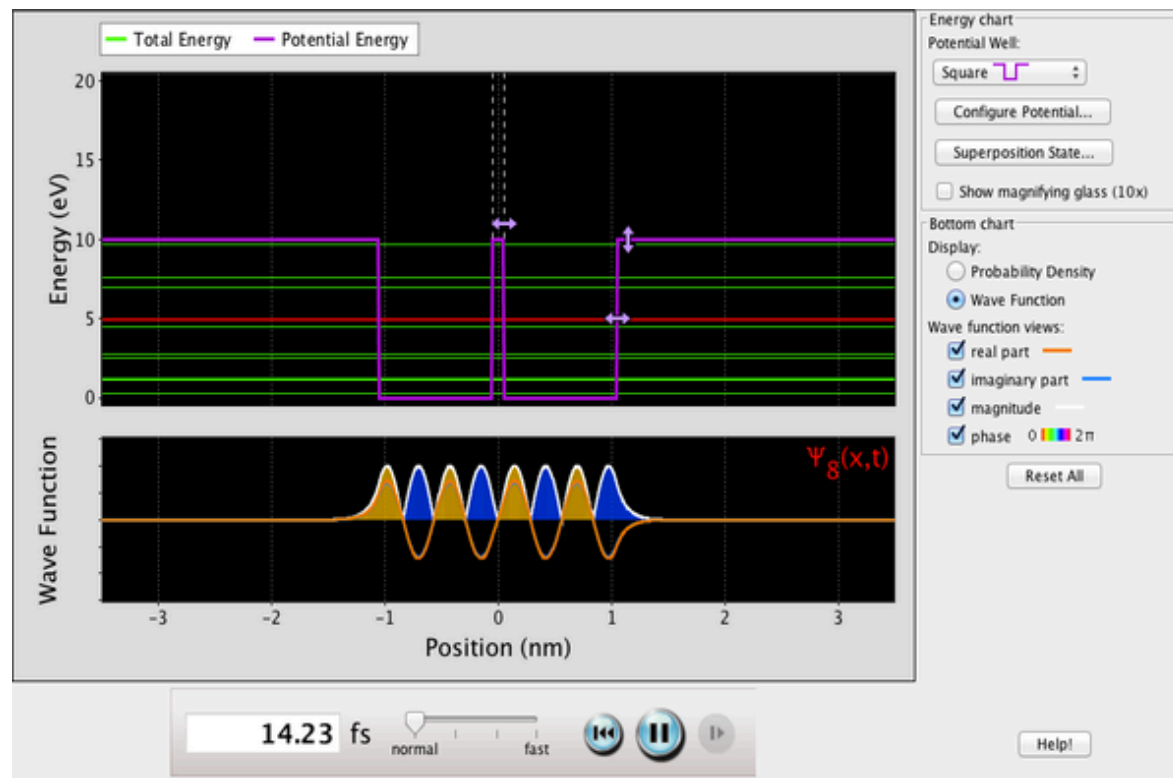
A. Symmetric

B. Antisymmetric

C. No difference

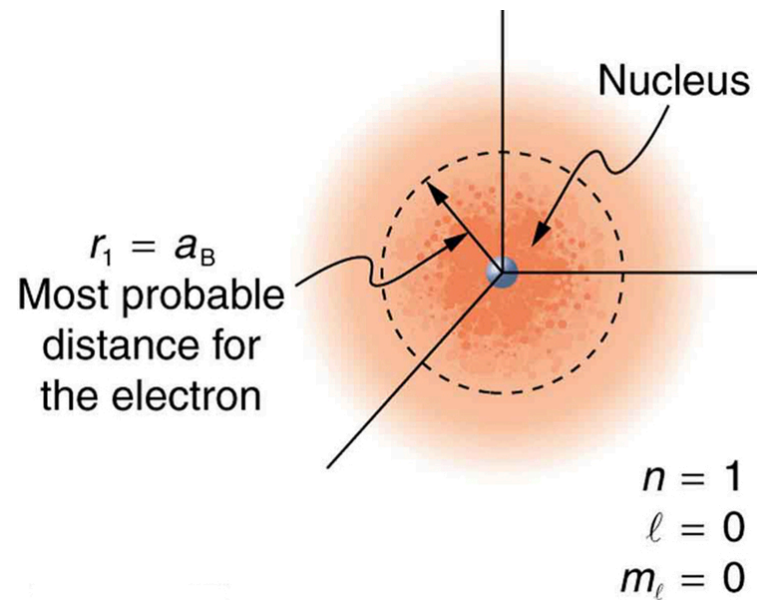
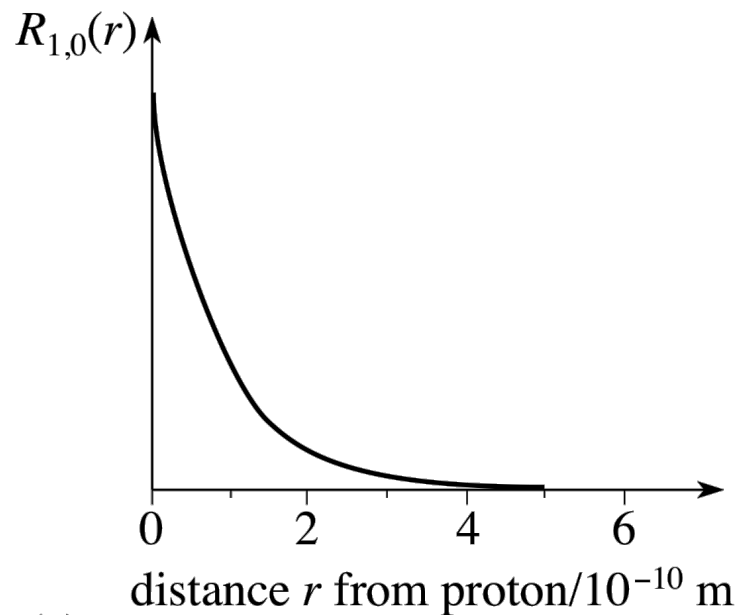
Double Well Potential

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

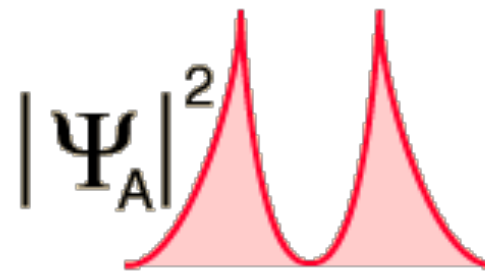
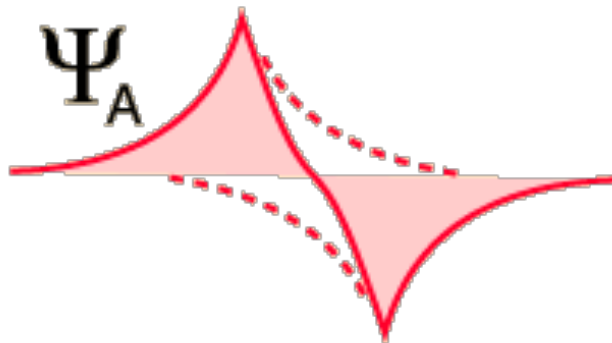
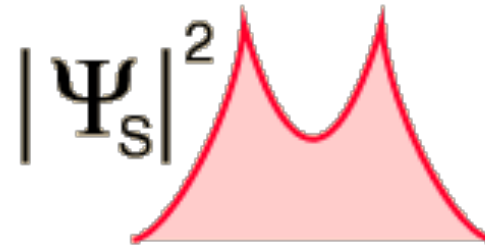
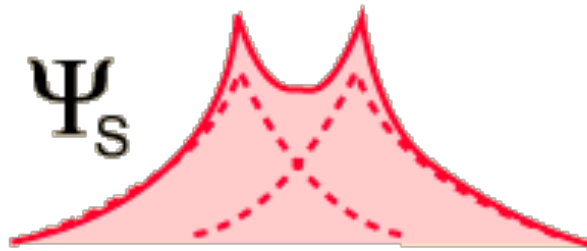


Ground State of Electron in H Atom

$$\Psi_{1,0,0} = \Psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$$



Symmetric and Antisymmetric Electron Wave Functions in H₂



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

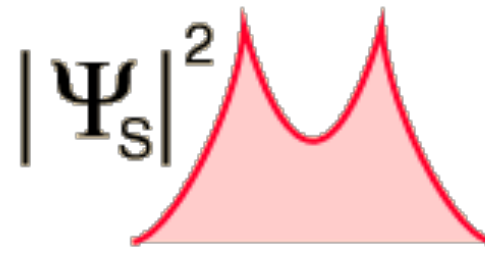
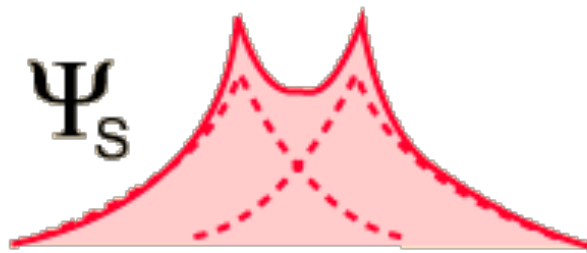
- Imagine that we have a system of two protons and one electron. For which electron wave function will the system be more likely to be stable?

A. Symmetric

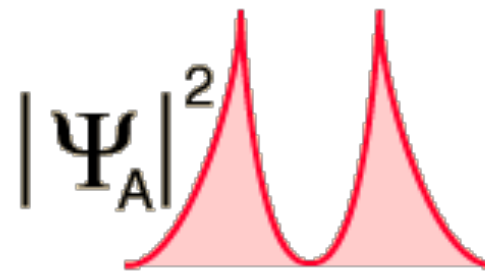
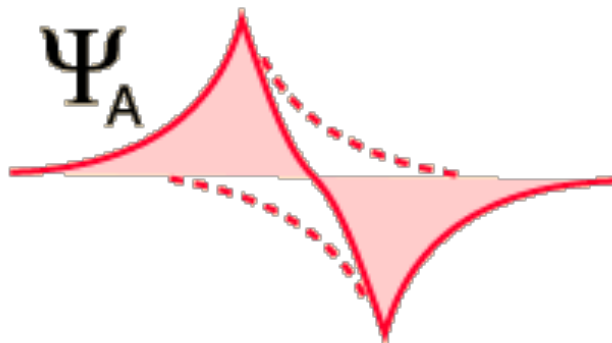
B. Antisymmetric

C. No Difference

Bonding and Antibonding Wave Functions

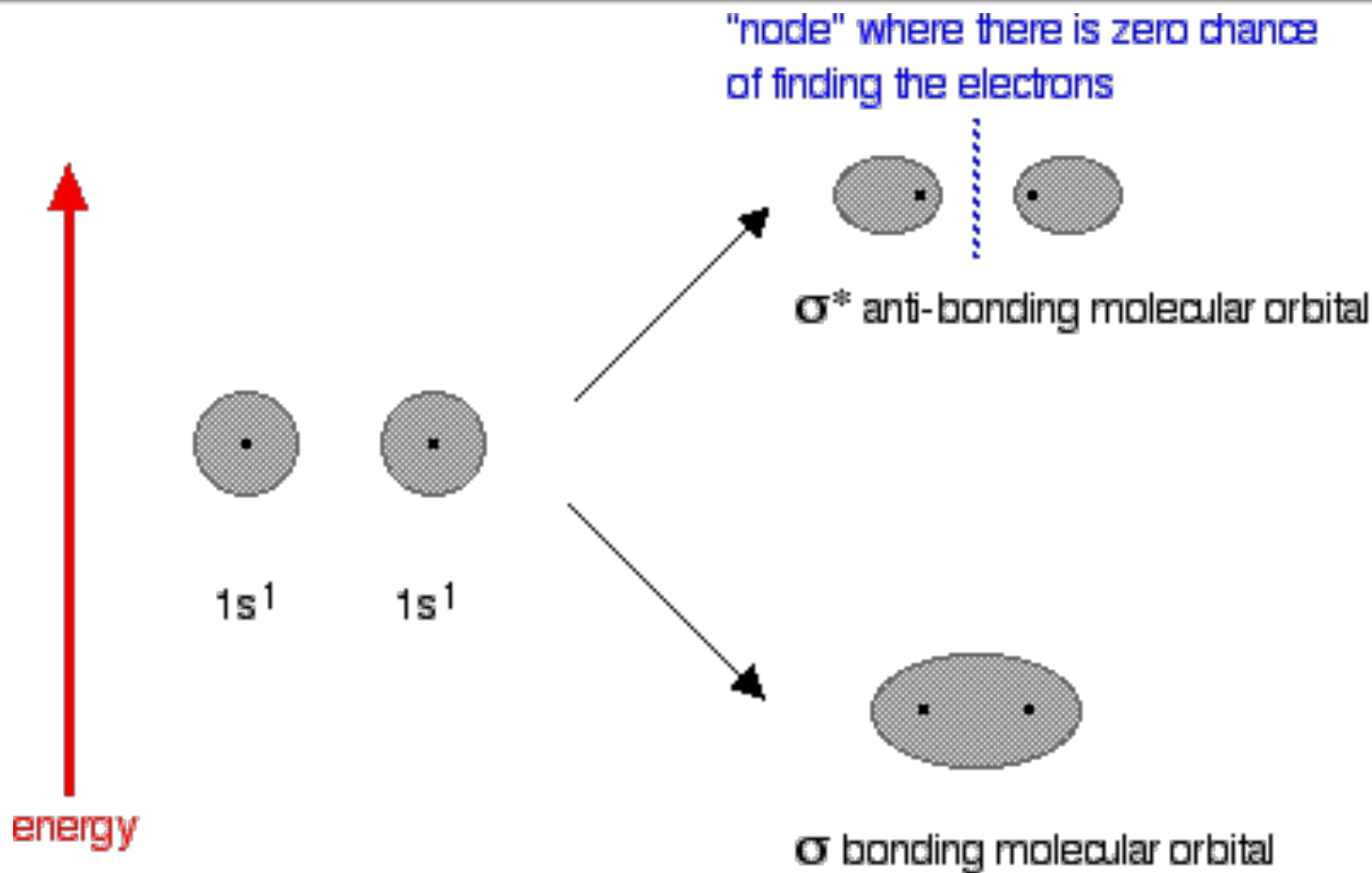


Bonding

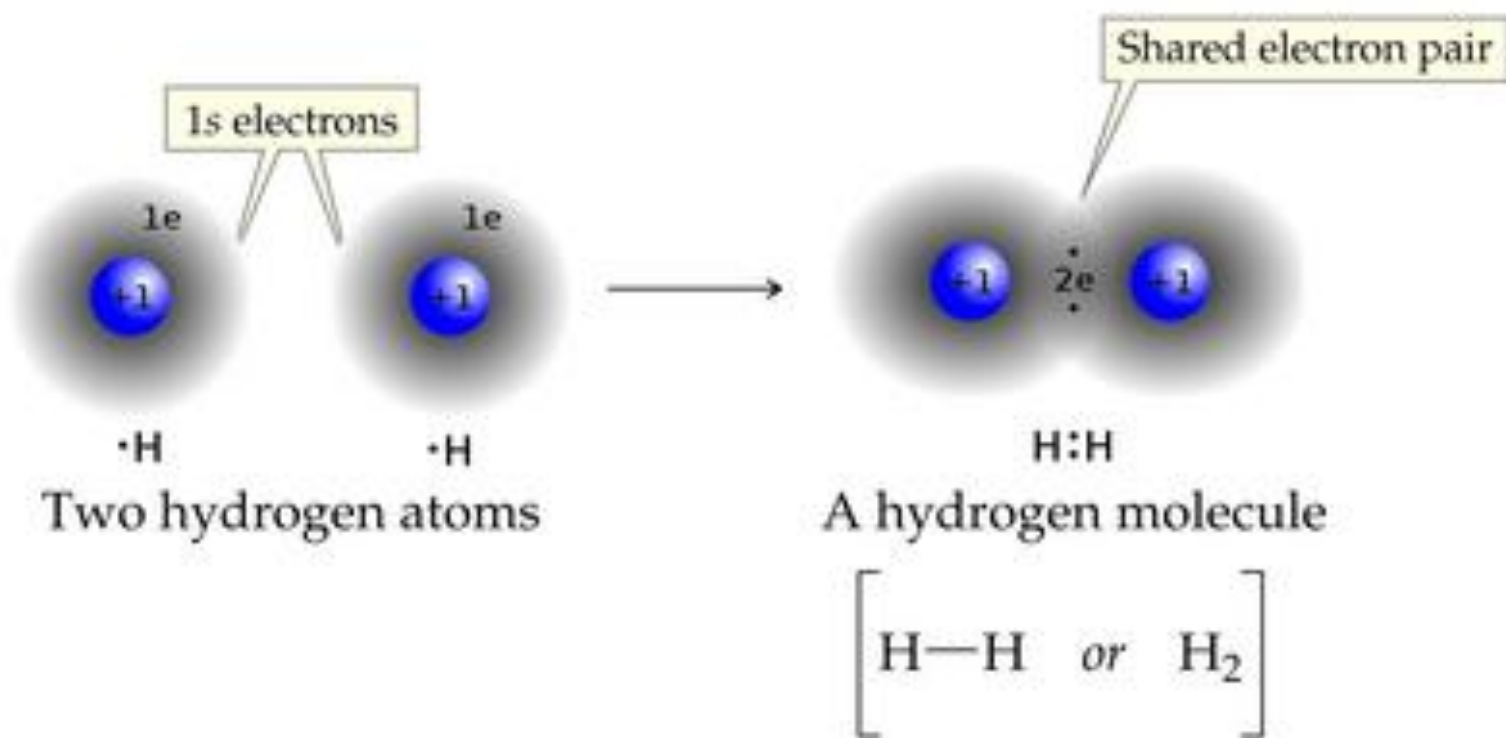


Anti-bonding

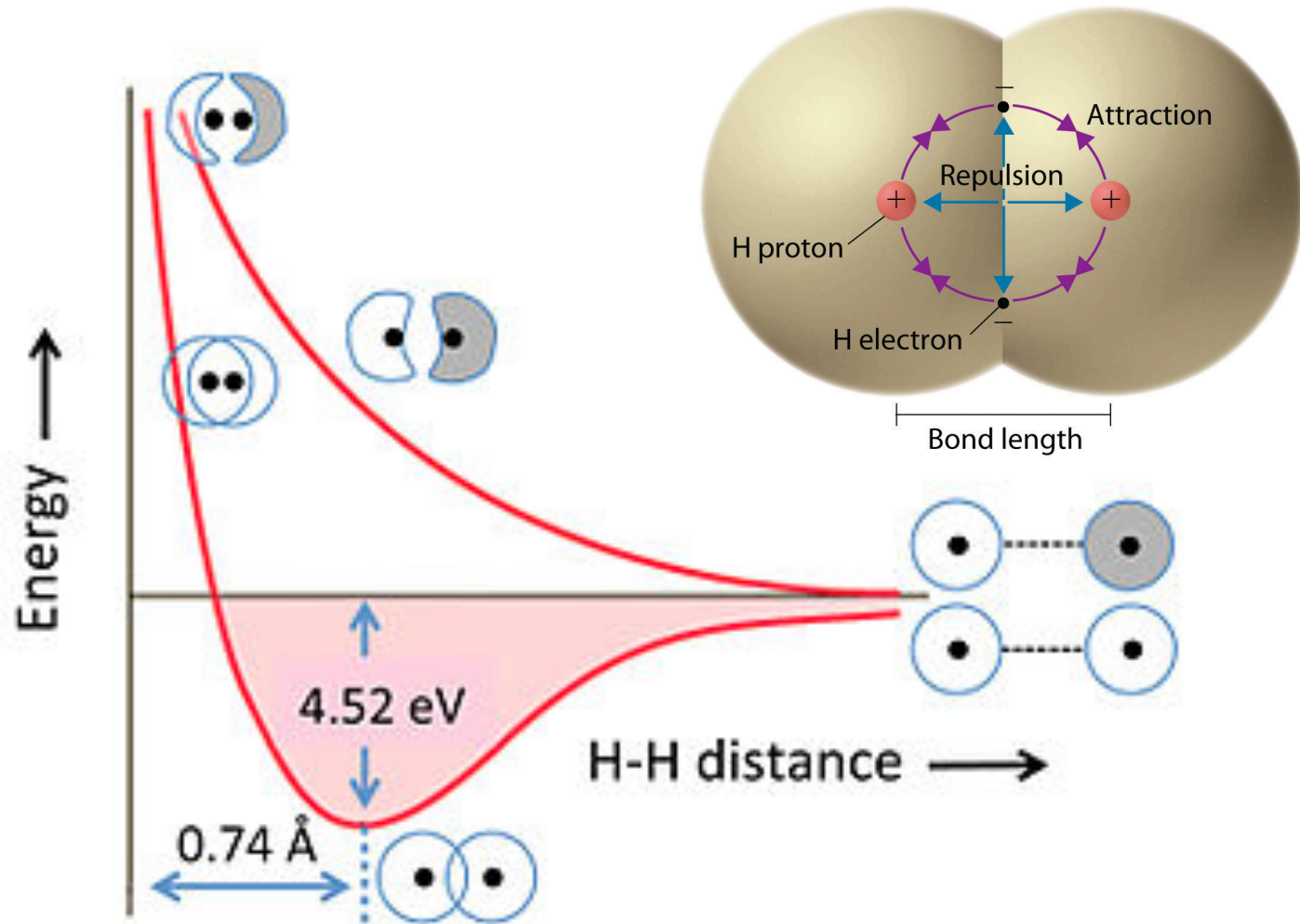
Bonding and Antibonding Orbitals



Covalent Bonding



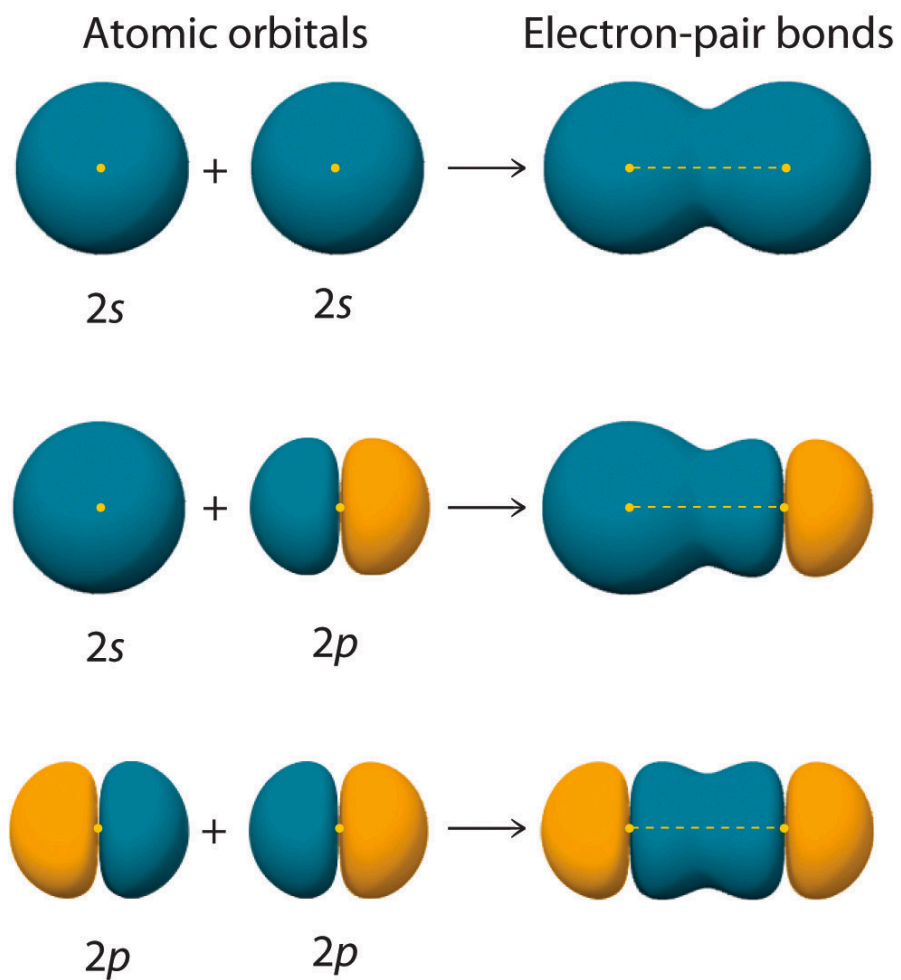
Hydrogen Molecule Covalent Bond Energy



Covalent Bonding

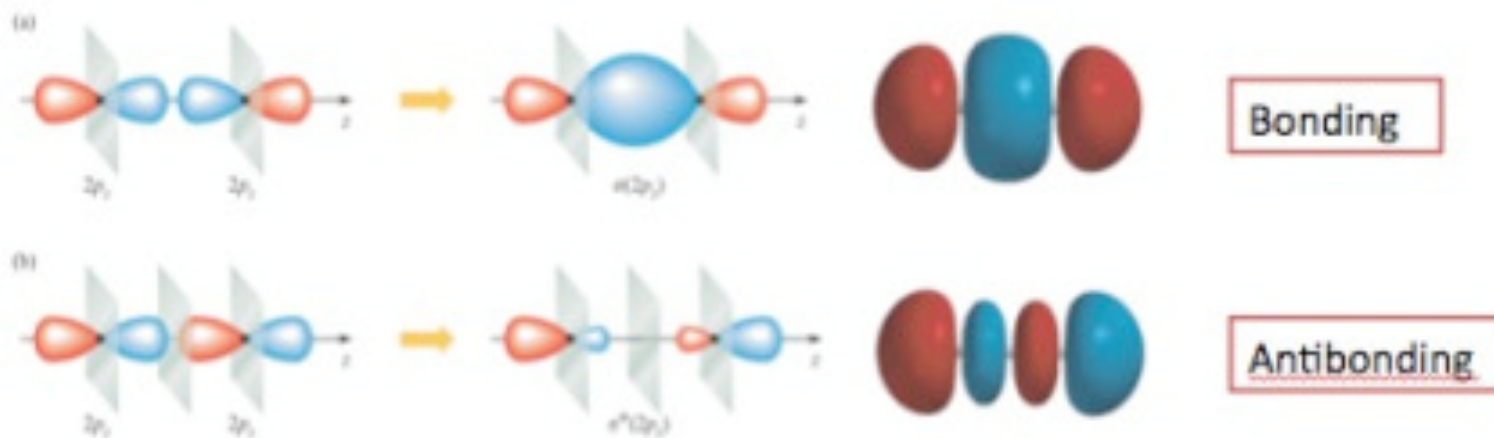
- I. Wave function of electrons near two nuclei are (approximately) a combination of the individual wave functions
- II. Symmetric combinations (bonding states) are energetically favorable
- III. Antisymmetric combinations (antibonding states) do not lead to stable molecules
- IV. Each molecular state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

ss, sp and pp covalent bonds

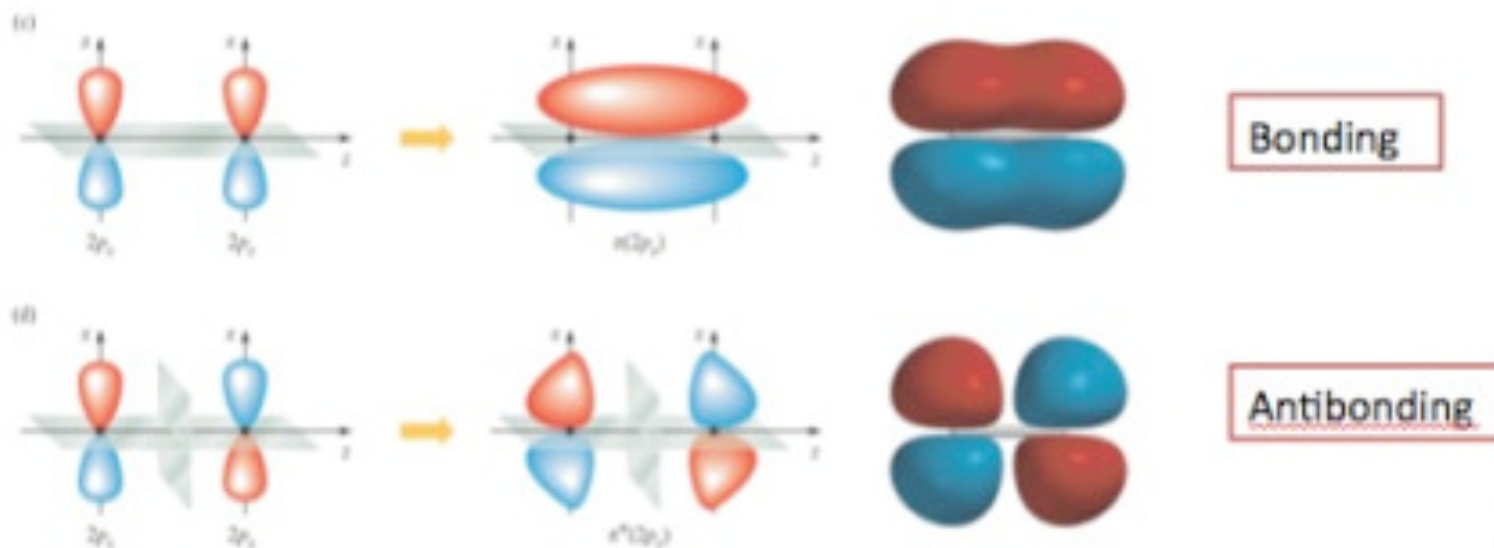


pp covalent bonding

σ

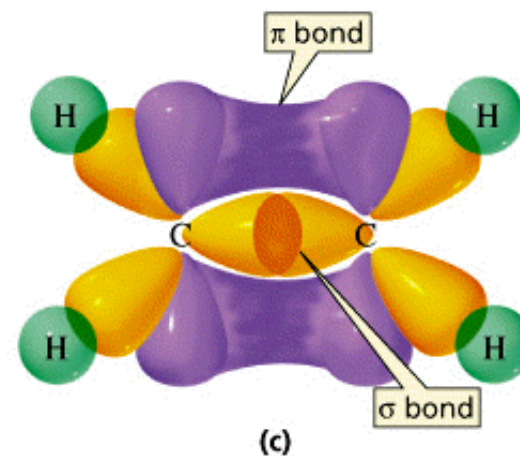
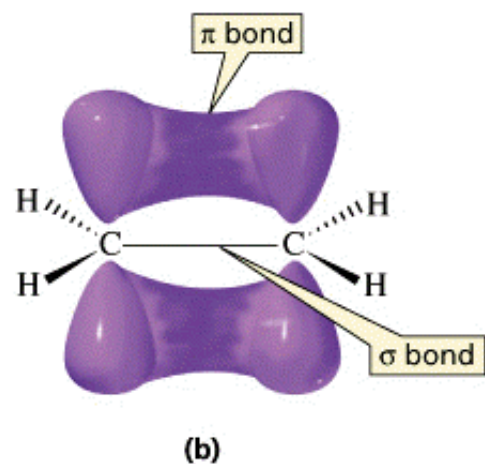
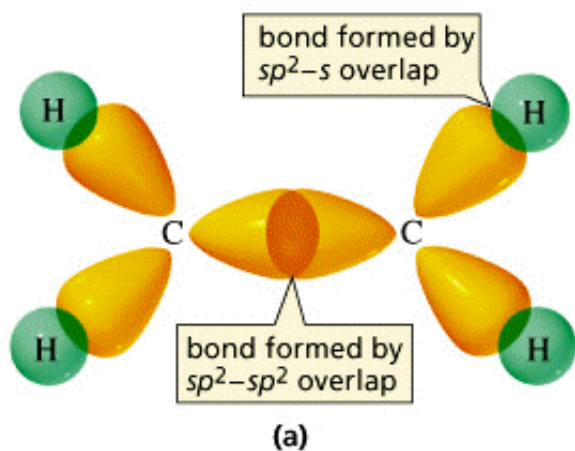
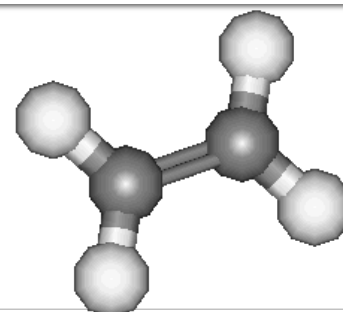
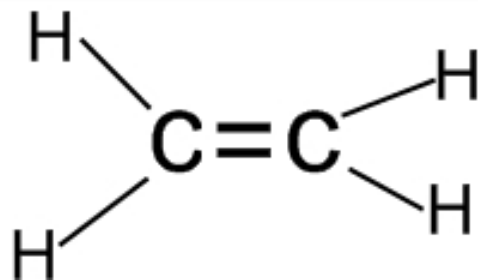


π



Multiple Bonds

Ethene

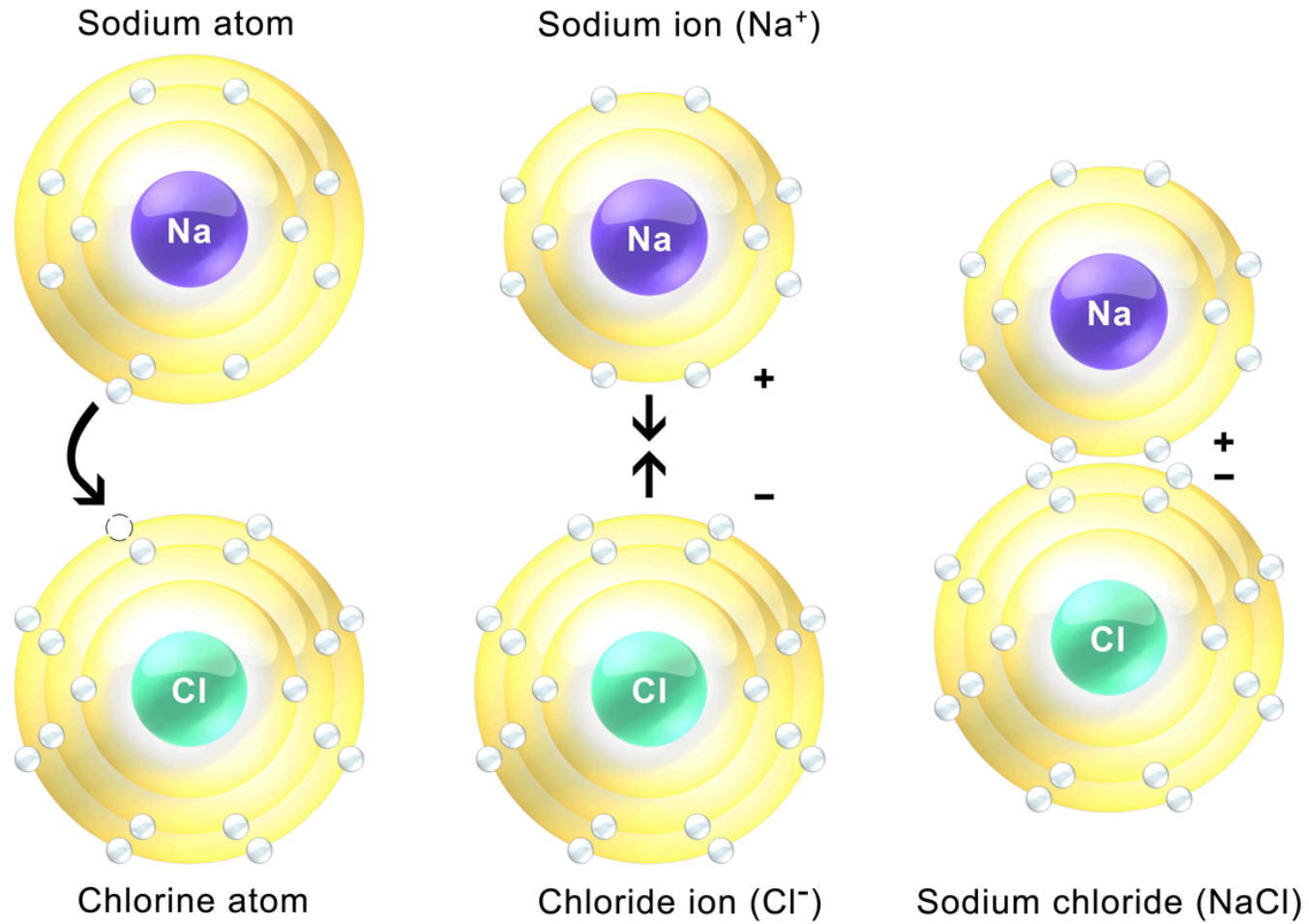


Molecule Shapes

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

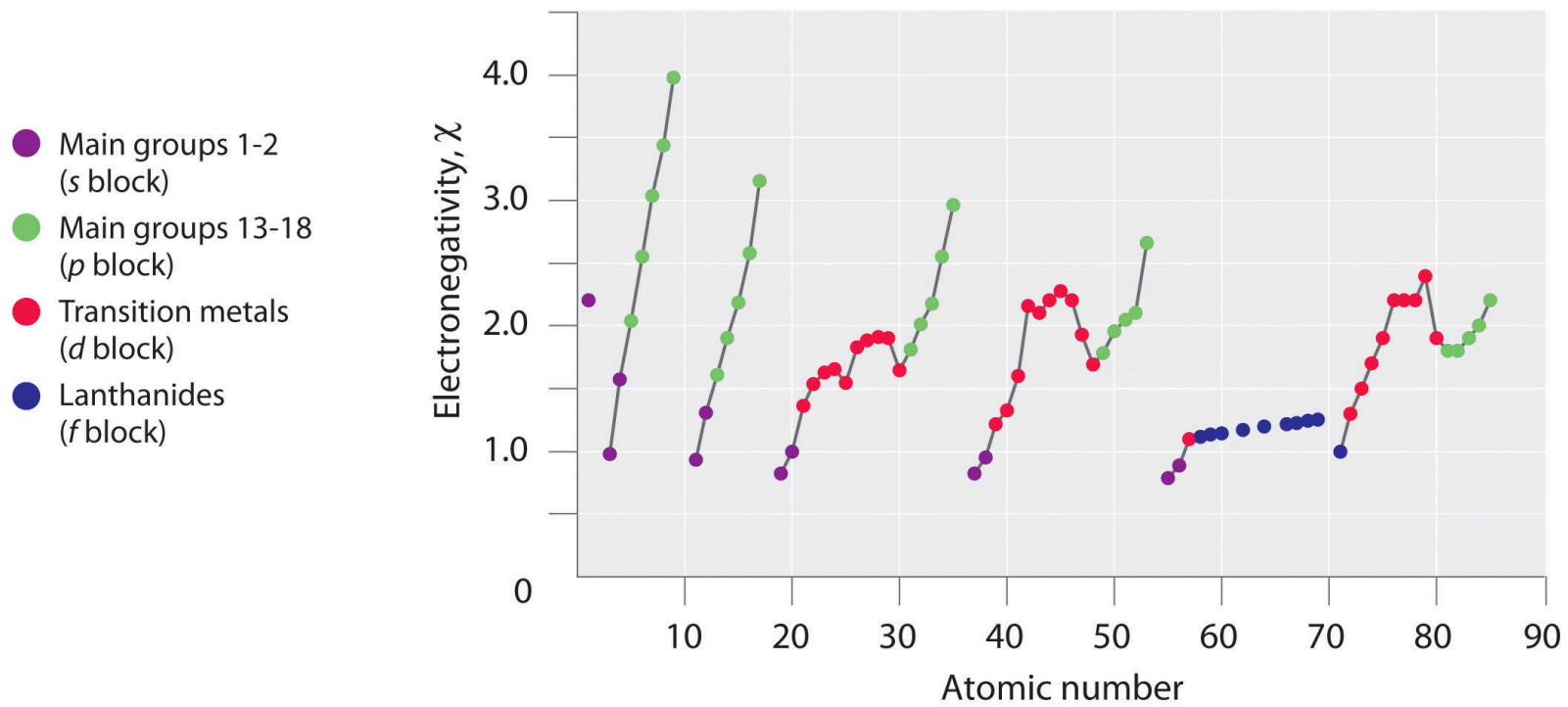
The screenshot displays the PhET Molecule Shapes simulation interface. At the top, there are radio buttons for 'Real' (selected) and 'Model'. To the right, a 'Molecule' dropdown menu is set to 'H₂O'. Below this, an 'Options' panel contains two checked checkboxes: 'Show Lone Pairs' and 'Show Bond Angles'. The central area shows a 3D ball-and-stick model of a water molecule (H₂O) with a bond angle of 104.5°. The oxygen atom is represented by a red sphere, and the hydrogen atoms by white spheres. Lone pairs are shown as yellow dots on the oxygen atom. At the bottom left, a 'Name' panel shows 'Molecule Geometry' as 'Bent' and 'Electron Geometry' as 'Tetrahedral'. A 'Refresh' button is located at the bottom right. The PhET logo and navigation icons are visible at the very bottom of the interface.

Ionic Bonds



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



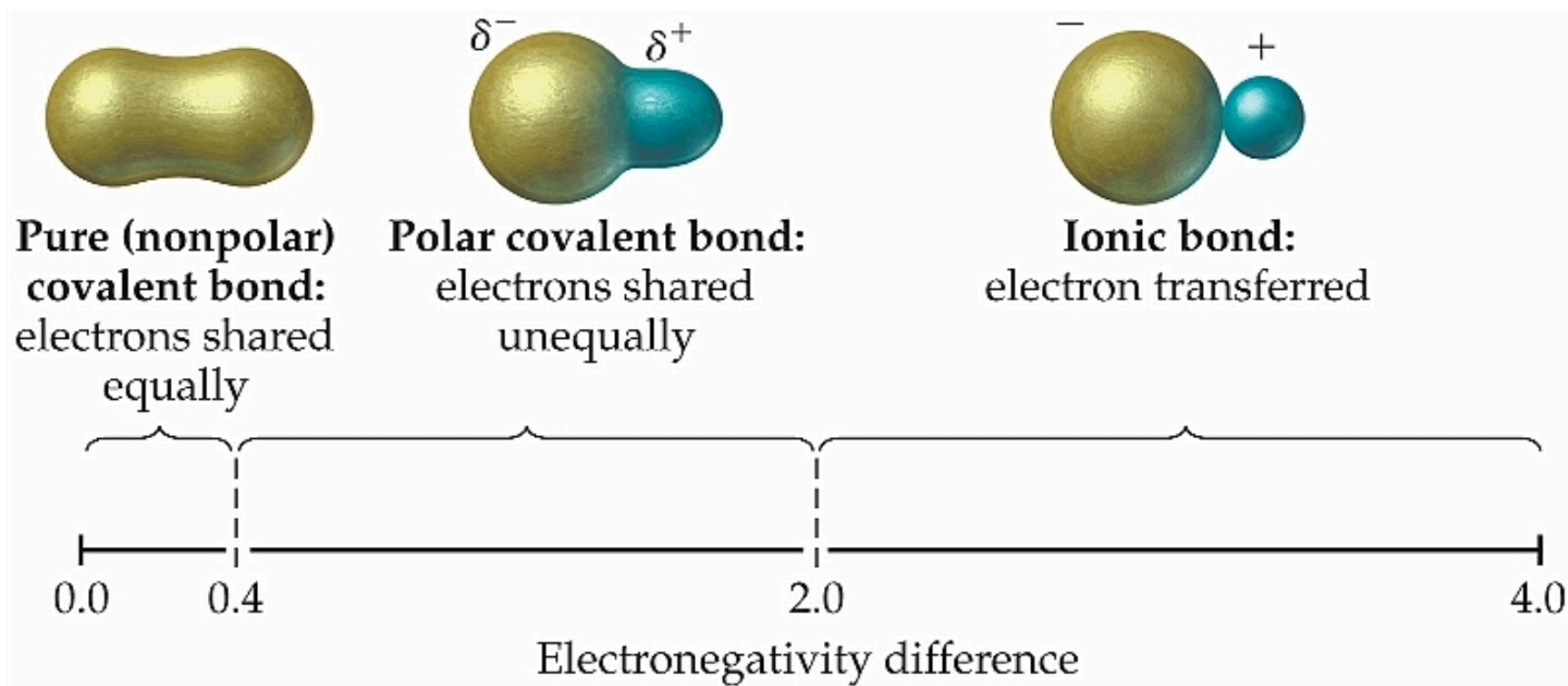
Electronegativity

Electronegativity

0.5-0.9	2.5-2.9
1.0-1.4	3.0-3.5
1.5-1.9	3.6-3.9
2.0-2.4	4.0+

	1	2											3	4	5	6	7	8
													(13)	(14)	(15)	(16)	(17)	(18)
H	Li	Be											B	C	N	O	F	He
2.1	1.0	1.6											2.0	2.5	3.0	3.5	4.0	--
Na	Mg		(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	Al	Si	P	S	Cl	Ar
0.9	1.3												1.6	1.9	2.2	2.5	3.0	--
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
0.8	1.3	1.4	1.5	1.6	1.7	1.6	1.8	1.9	1.9	1.9	1.7	1.6	2.0	2.2	2.6	2.8	--	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
0.8	1.0	1.2	1.3	1.6	2.2	2.1	2.2	2.3	2.2	1.9	1.7	1.8	2.0	2.1	2.1	2.7	2.6	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
0.8	0.9	1.1	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	2.0	2.3	2.0	2.0	2.2	--	
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub		Uuq					
0.7	0.9	1.1	--	--	--	--	--	--	--	--	--							
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Covalent Vs Ionic Bonding



Covalent Vs. Ionic Bonds

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

