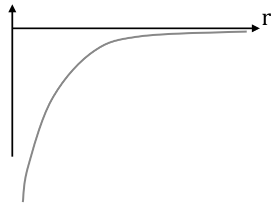
3.7 Hydrogenic atom

Schrodinger's Solutions for Hydrogen

For Hydrogen (-like):

$$V(r) = -\frac{Zke^2}{r}$$



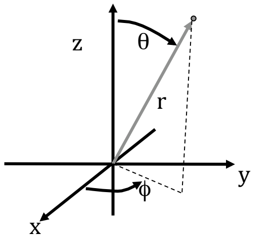
$$V(r) = -\frac{Zke^2}{r}$$

Does the potential above depend on

(1) time, (2) x, y, z, (3) r or (4) r, θ, ϕ ?

A) yes, yes, yes, yes
B) no, yes, yes, yes
C) no, no, yes, yes
[✓ D) no, yes, yes, no]

Use spherical coordinates



(x, y, z) = (r sinθ cosϕ, r sinθ sinϕ, r cosθ)

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)-\frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]+V(r)\psi = E\psi$$

What are the boundary conditions?

A. Ψ must go to 0 at r = 0
B. Ψ must go to 0 at r = ∞
C. Ψ at infinity must equal Ψ at 0
D. A and B
E. there are no boundary conditions

What are the boundary conditions?
A. Ψ must go to 0 at r=0
B. Ψ must go to 0 at r=infinity
C. Ψ at infinity must equal Ψ at 0
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Ψ must be normalizable, so it needs to go to zero.

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} |\Psi|^2 dr\, d\theta\, d\phi = 1$$

Also physically makes sense: no probably of finding electron at ∞.

n : principal quantum number (shell), n = 1, 2, 3,…

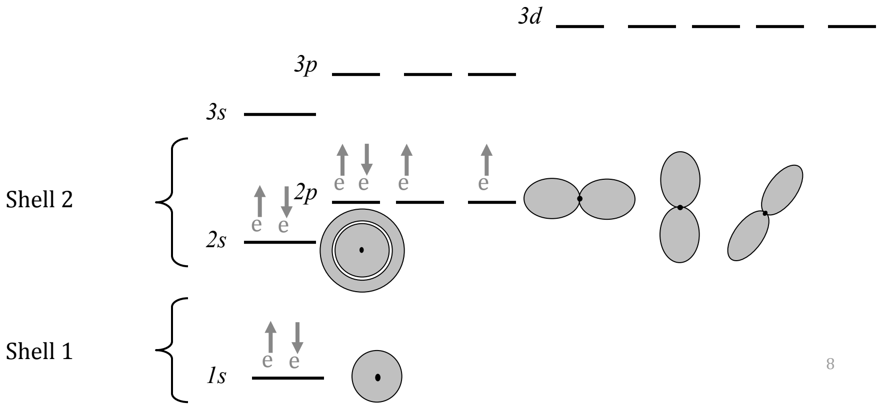
l : subshell (shape), l = 0, 1, 2, 3,…, n-1

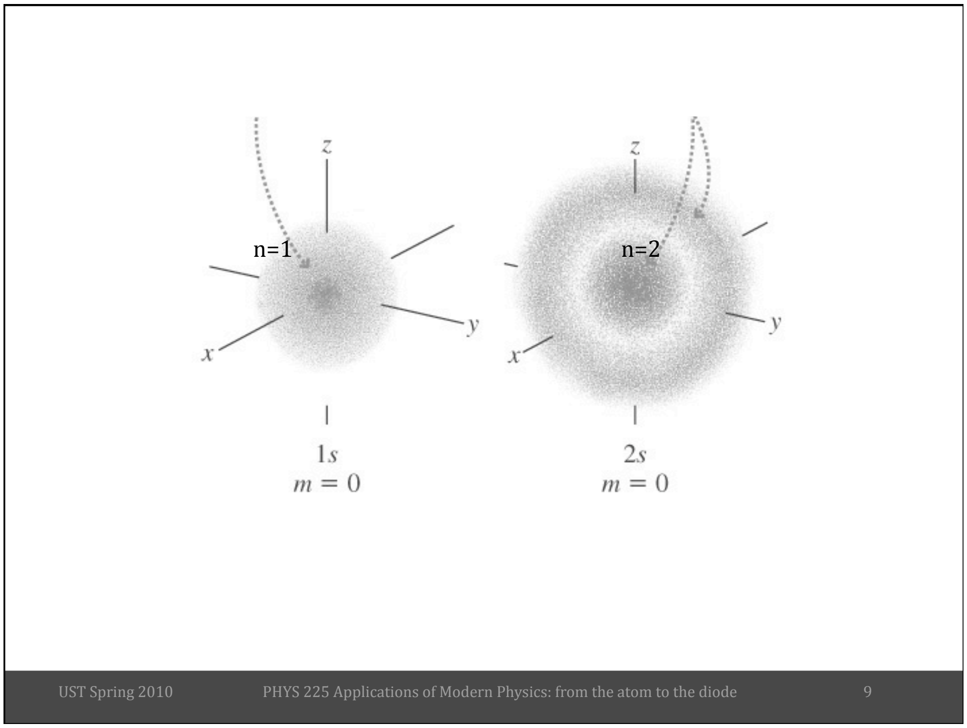
↑ ↑ ↑ ↑

s p d f

m_l: number of energy states in each subshell,

$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$





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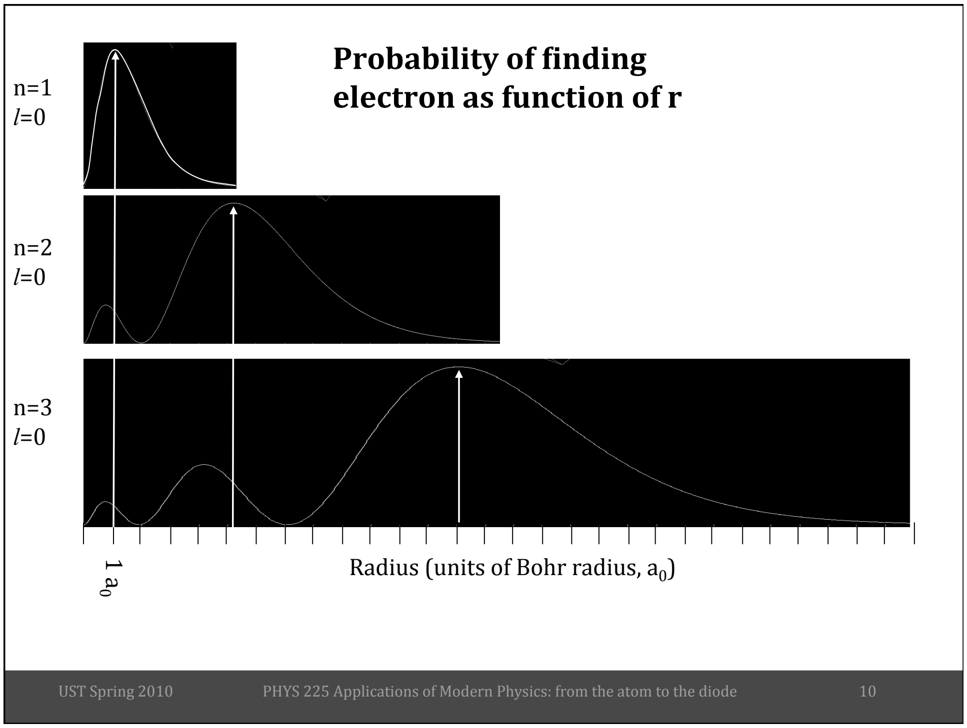

Probability of finding electron as function of r

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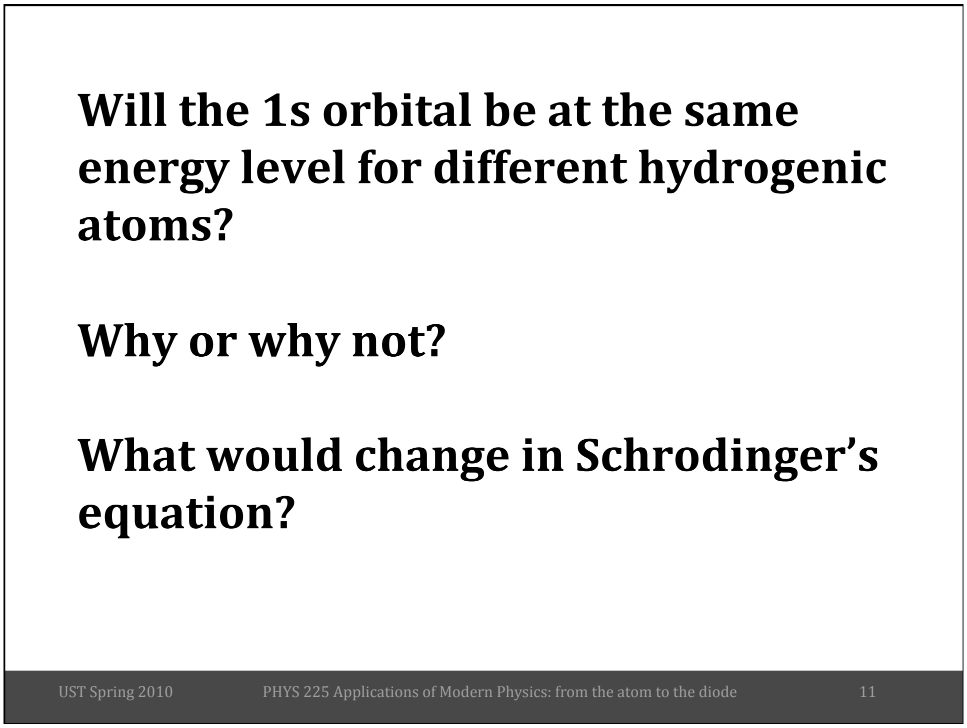
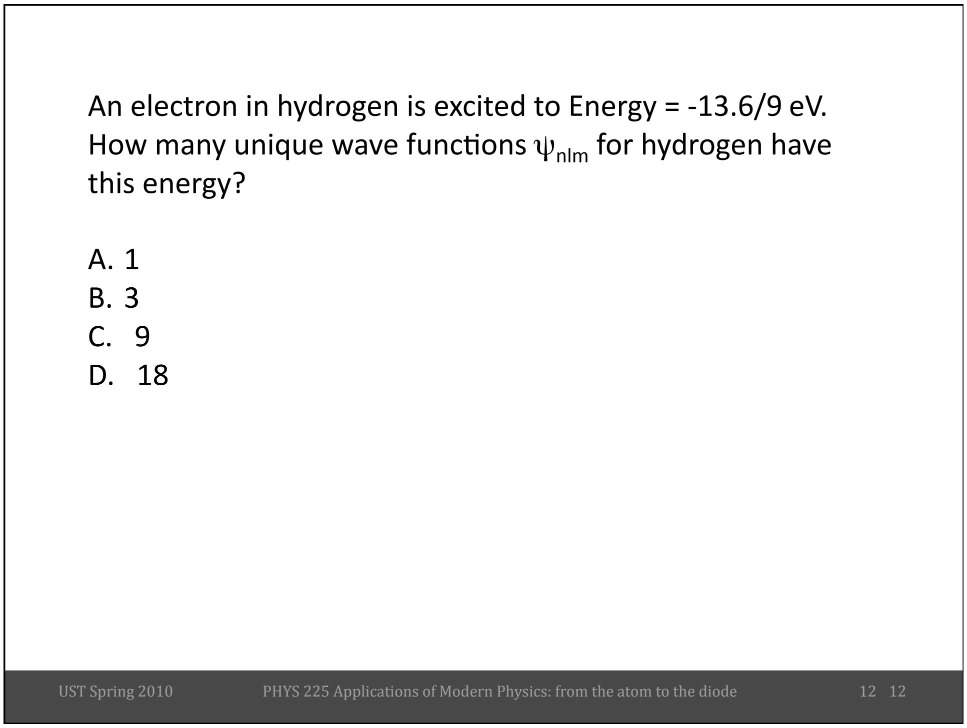


Will the 1s orbital be at the same energy level for different hydrogenic atoms?

Why or why not?

What would change in Schrodinger's equation?



An electron in hydrogen is excited to Energy = -13.6/9 eV. How many unique wave functions ψ_{nlm} for hydrogen have this energy?

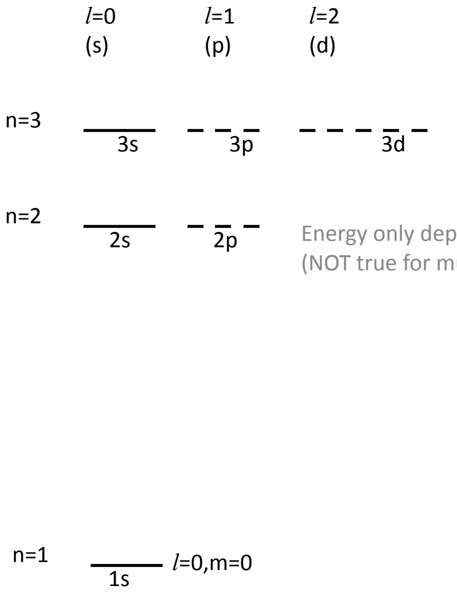
A. 1
B. 3
C. 9
D. 18

n	*l*	m	
3	0	0	3s state
3	1	-1	3p states (*l*=1)
3	1	0	
3	1	1	
3	2	-2	3d states (*l*=2)
3	2	-1	
3	2	0	
3	2	1	
3	2	2	

Answer is c:
9 states all with the same energy

In HYDROGEN, energy only depends on n
(NOT true for mulit-electron atoms).

Energy Diagram for Hydrogen



Energy only depends on n
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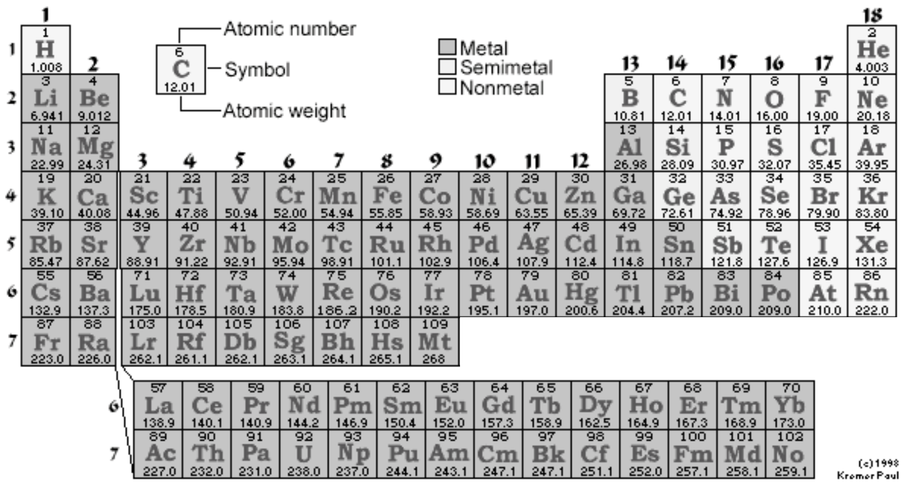
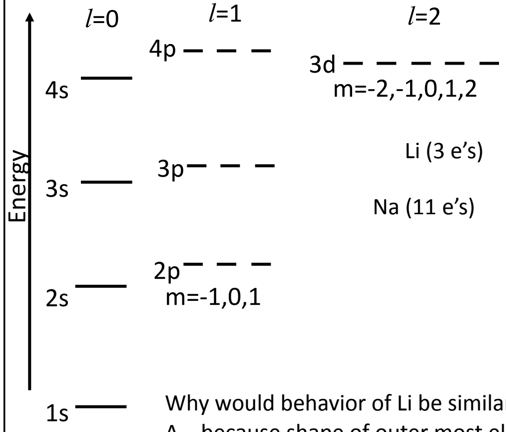
Can Schrodinger make sense of the periodic table?

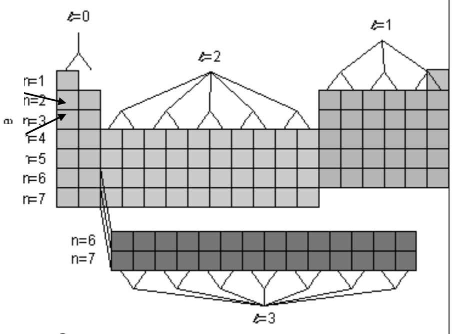


	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	71 Lu 175.0	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po 209.0	85 At 210.0	86 Rn 222.0
7	87 Fr 223.0	88 Ra 226.0	103 Lr 262.1	104 Rf 261.1	105 Db 262.1	106 Sg 263.1	107 Bh 264.1	108 Hs 265.1	109 Mt 268									

6	57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm 146.9	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0
7	89 Ac 227.0	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np 237.0	94 Pu 244.1	95 Am 243.1	96 Cm 247.1	97 Bk 247.1	98 Cf 251.1	99 Es 252.0	100 Fm 257.1	101 Md 258.1	102 No 259.1

For a given atom, Schrodinger predicts allowed wave functions and energies of these wave functions.

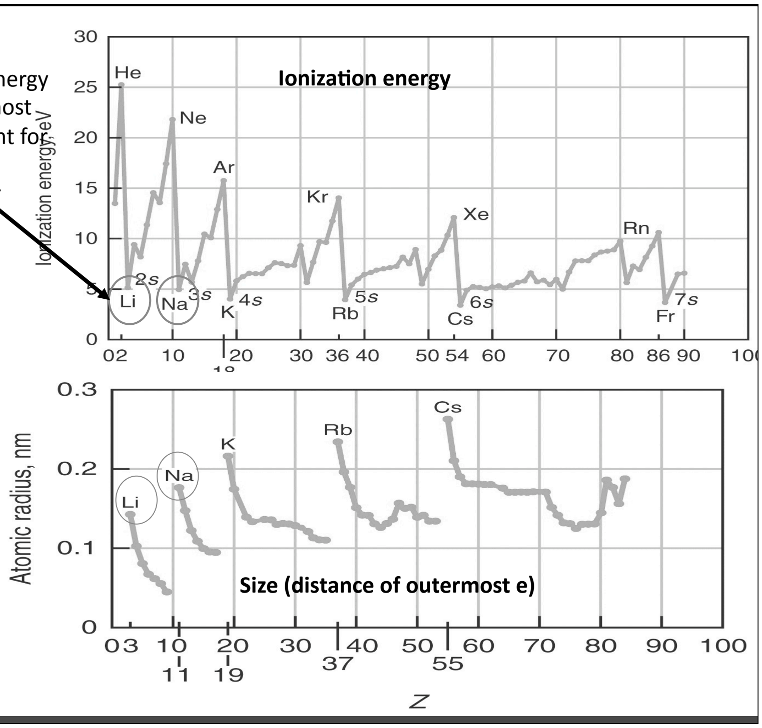




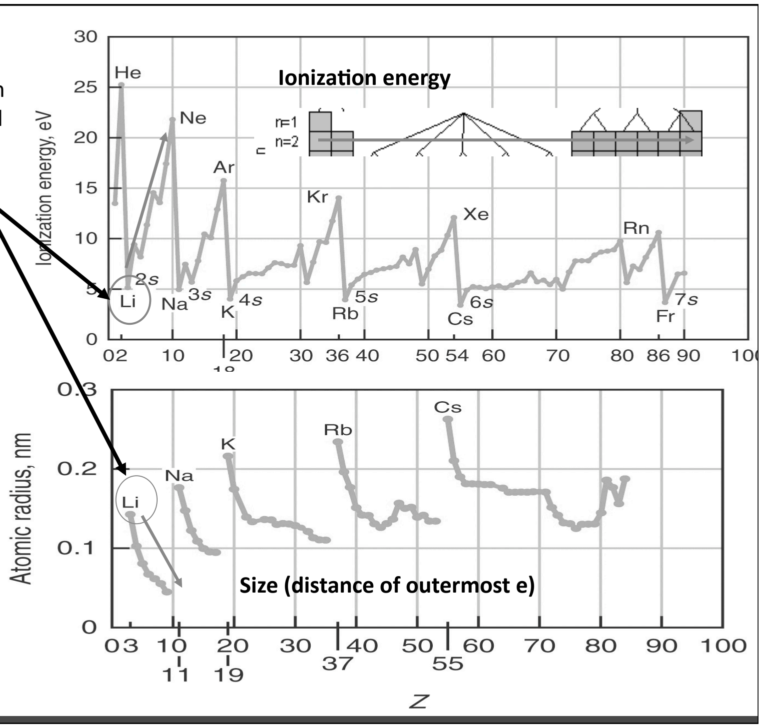
Why would behavior of Li be similar to Na?

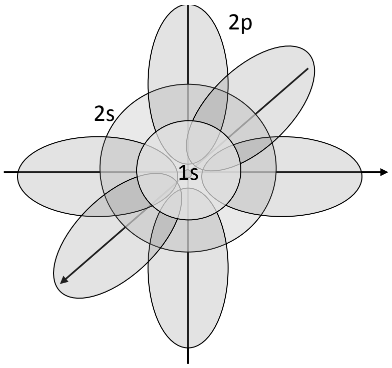
A. because shape of outer most electron orbital is similar.
B. because energy of outer most electron is similar.
C. both A and B
D. some other reason

Li, Na, K, Rb ..
about the same energy to remove outermost electron. Important for explaining similar chemical behavior

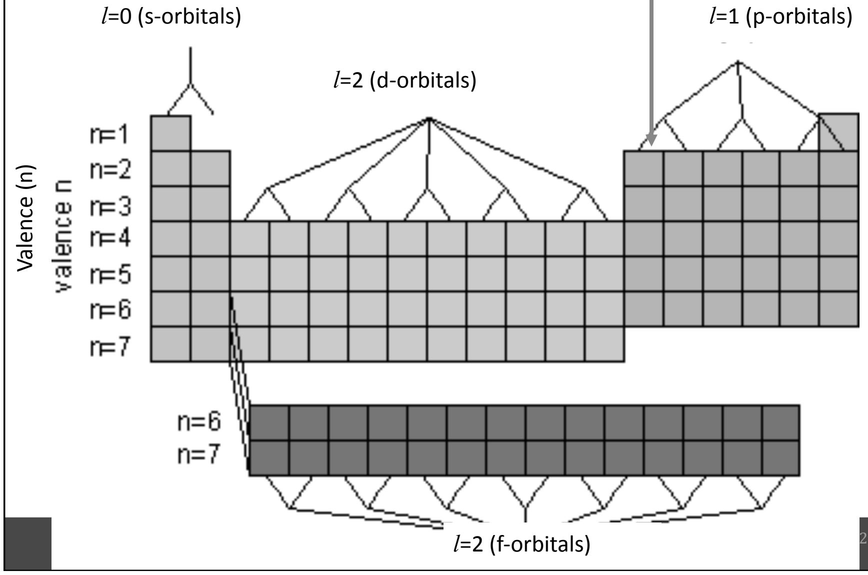


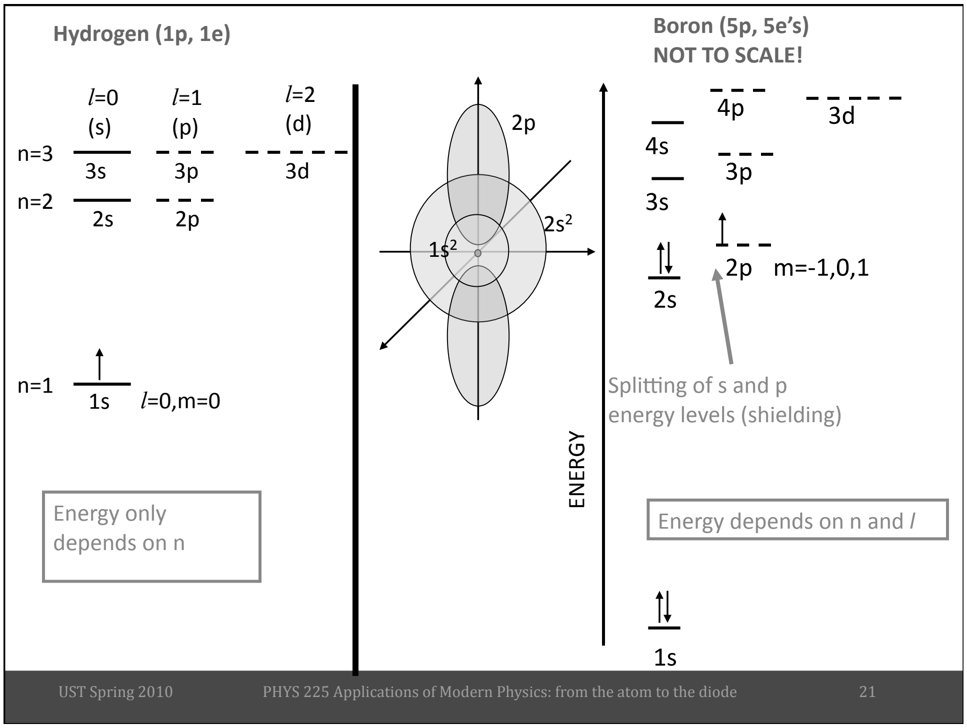
Why does ionization energy increase and size decrease as there are more electrons in p orbitals?





All atoms in this row have common filling of outer most shell (valence electrons), common shapes, similar energies … so similar behavior





Hydrogen (1p, 1e)

l=0 (s) | *l*=1 (p) | *l*=2 (d)

n=3 3s 3p 3d

n=2 2s 2p

n=1 ↑ 1s *l*=0,m=0

Energy only depends on n

Boron (5p, 5e's)
NOT TO SCALE!

ENERGY

4p 3d

4s

3p

3s

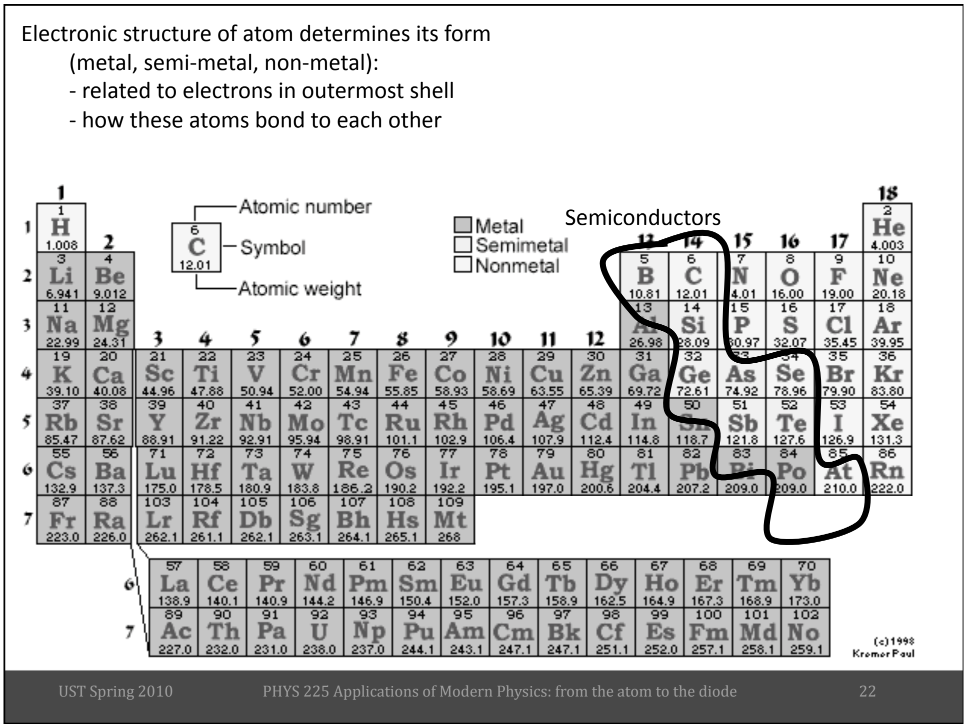
↑ 2p m=-1,0,1

↑↓ 2s

Splitting of s and p energy levels (shielding)

Energy depends on n and *l*

↑↓ 1s



Electronic structure of atom determines its form
(metal, semi-metal, non-metal):
- related to electrons in outermost shell
- how these atoms bond to each other

Semiconductors

▨ Metal
☐ Semimetal
☐ Nonmetal

Atomic number: 6 · Symbol: C · Atomic weight: 12.01

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