林盈廷

高雄醫學大學
生命科學院
生物科技學系 助理教授

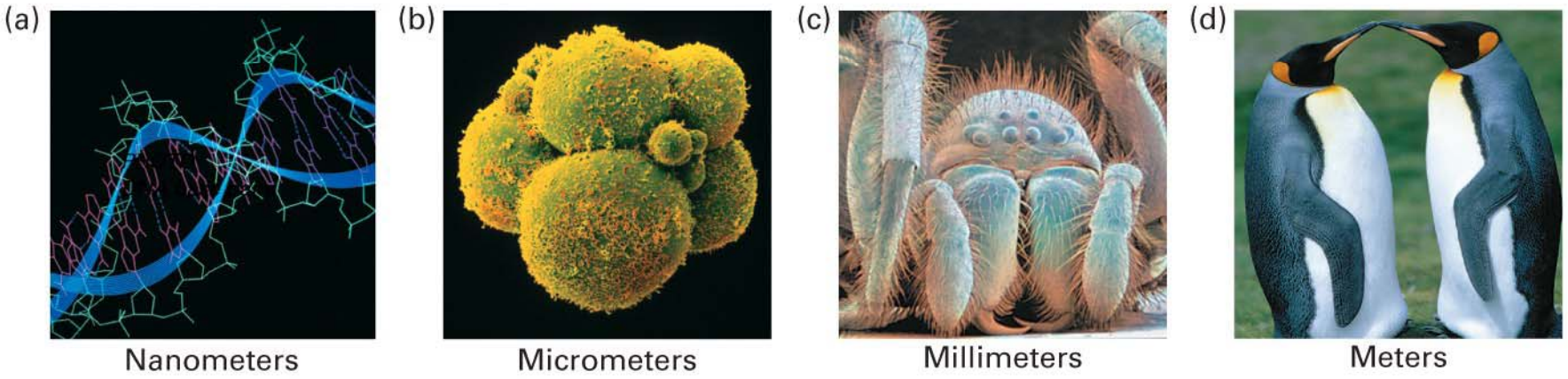
第一教學大樓 N1038 室
校內分機：2792
ytlin@kmu.edu.tw

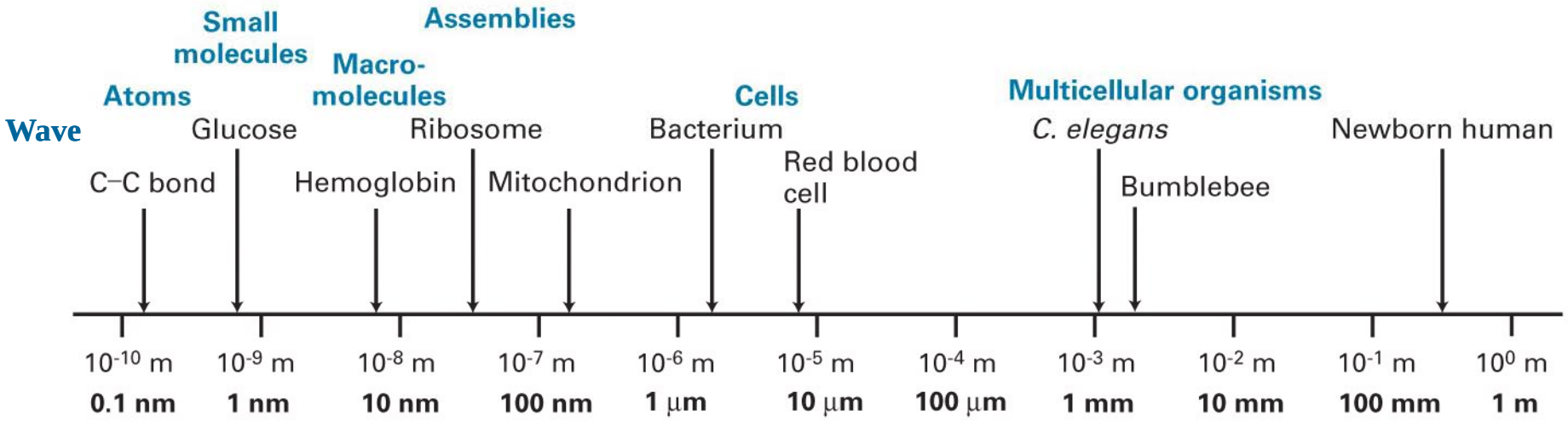
Y.T Lin's Presentation

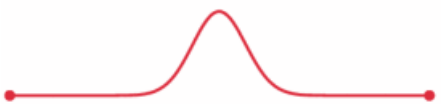
Reference Books

- Physical Chemistry for the Life Sciences
  (Engel, Drobny and Reid)
- Biophysical Chemistry
  (James P. Allen)

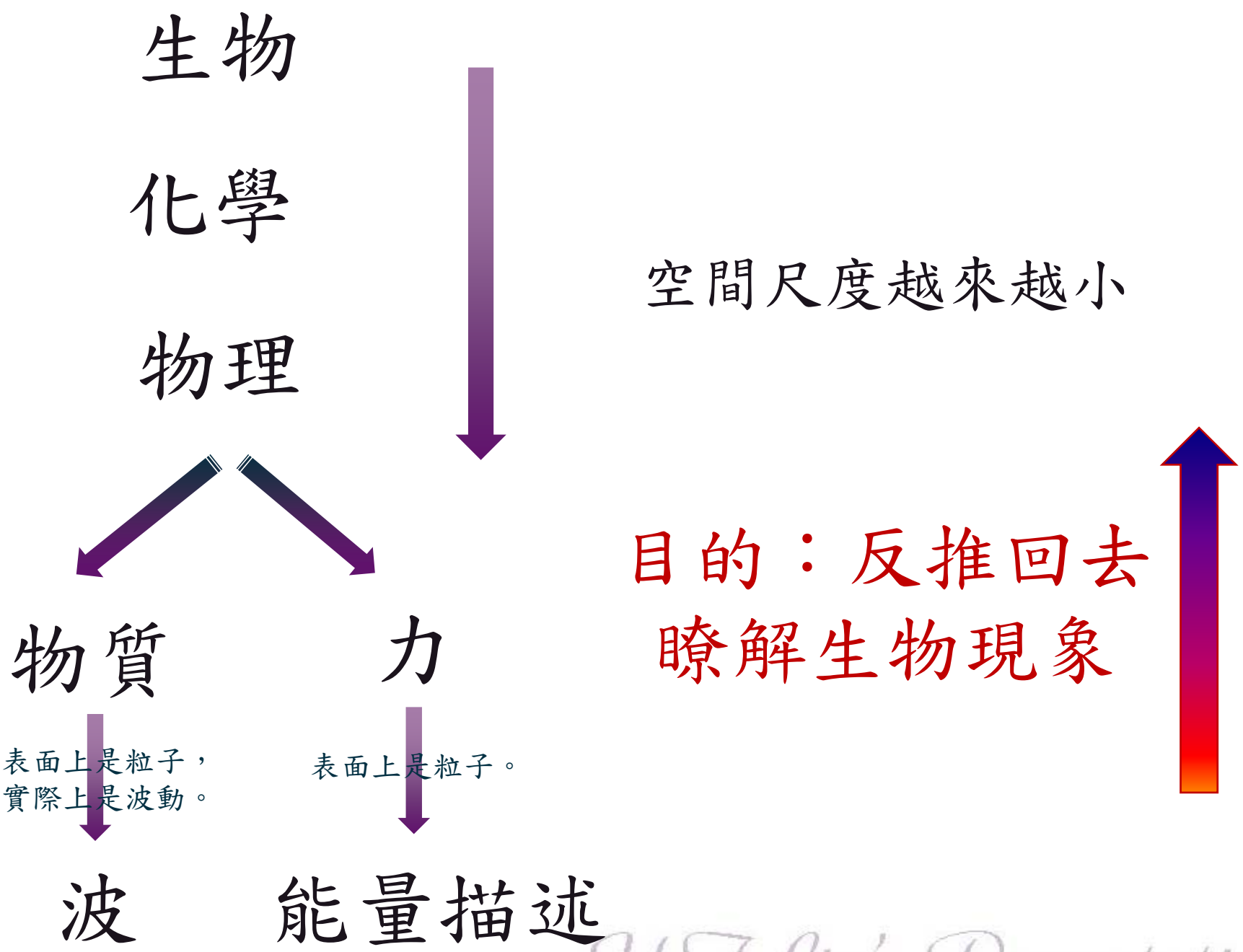
Y.T Lin's Presentation







Y.T.Lin's Presentation



Y.T.Lin's Presentation

物質

把物質切到最小，我們知道：
它表面上是粒子，實際上是波動。

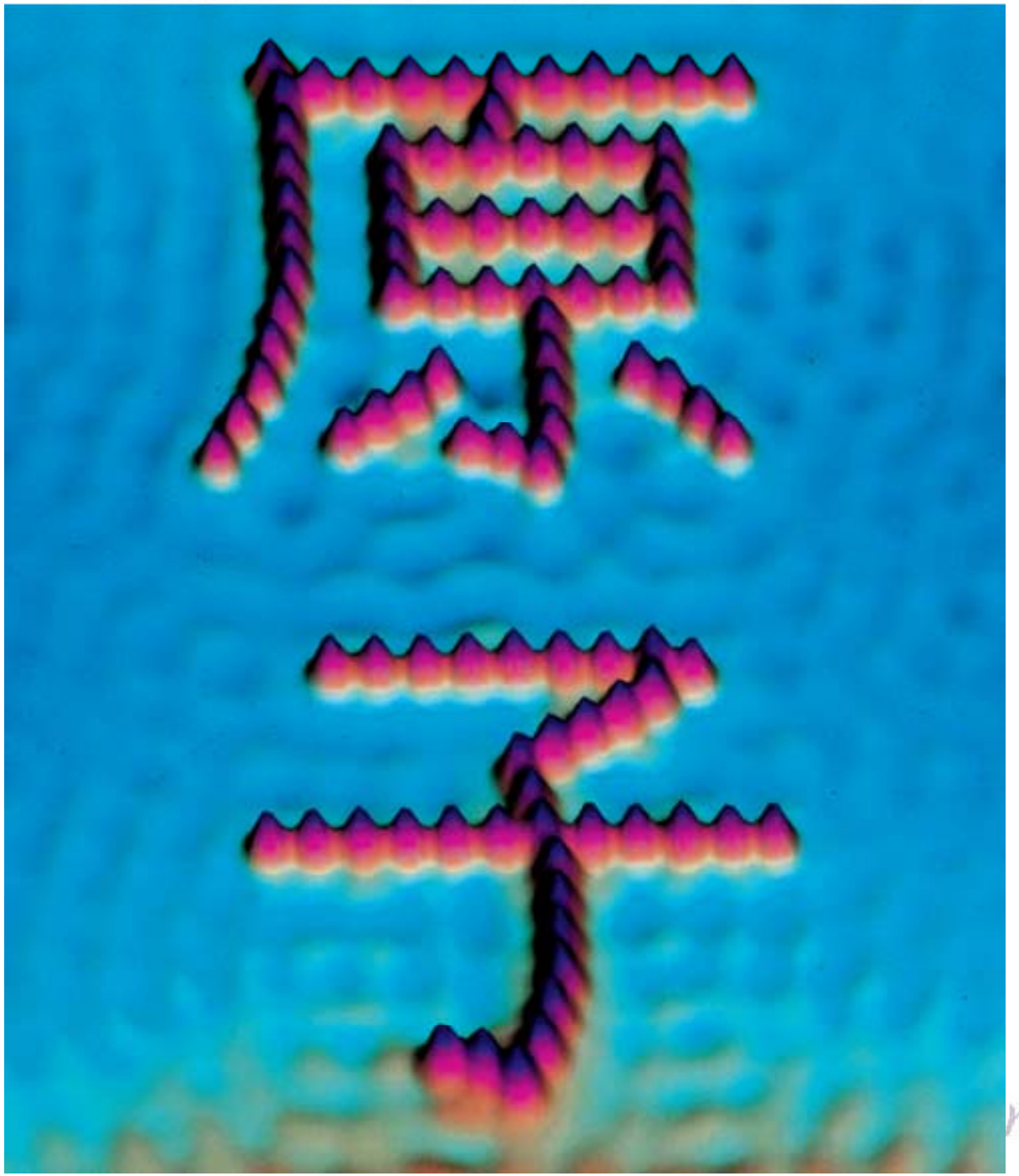
Y.T Lin's Presentation

Lecture

Quantum Chemistry (I)

表面上是粒子

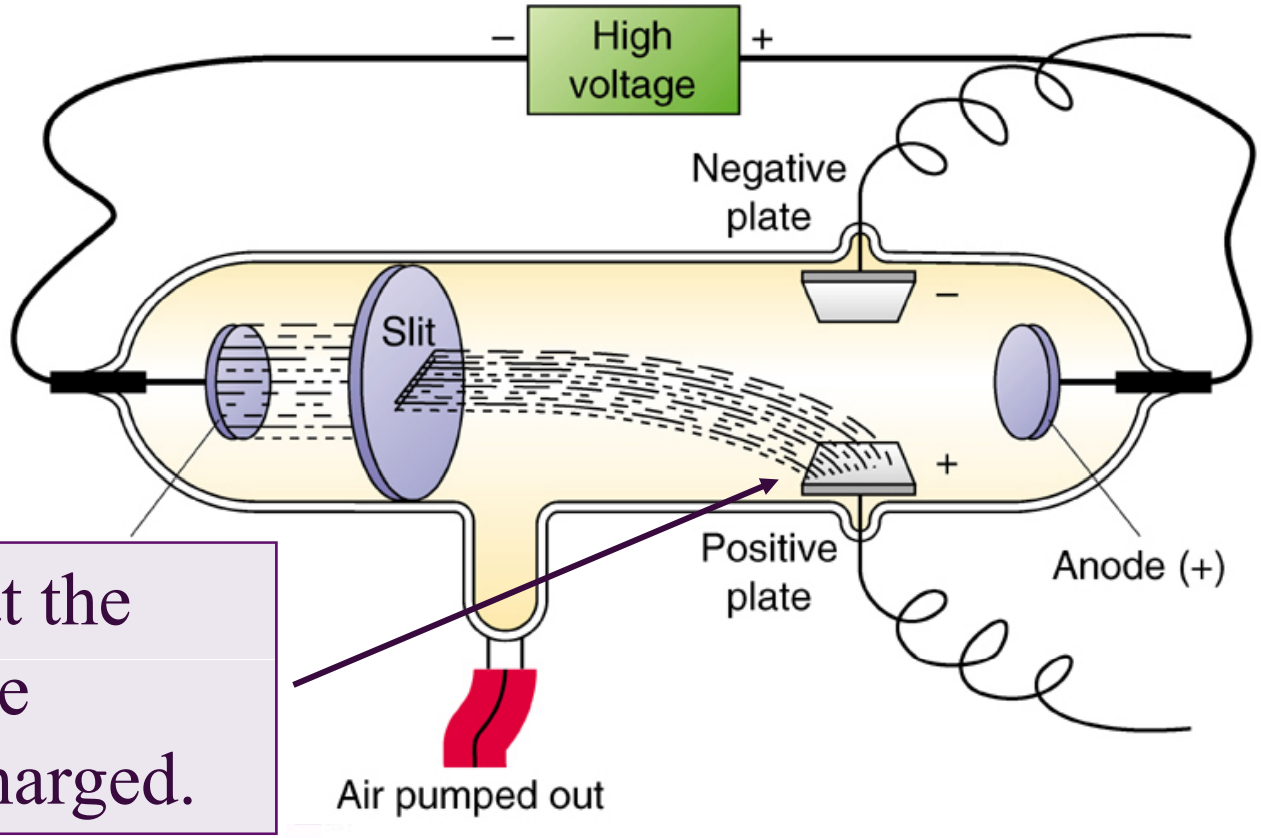
Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



表面上是粒子

Subatomic Particles: Electrons, Protons, and Neutrons

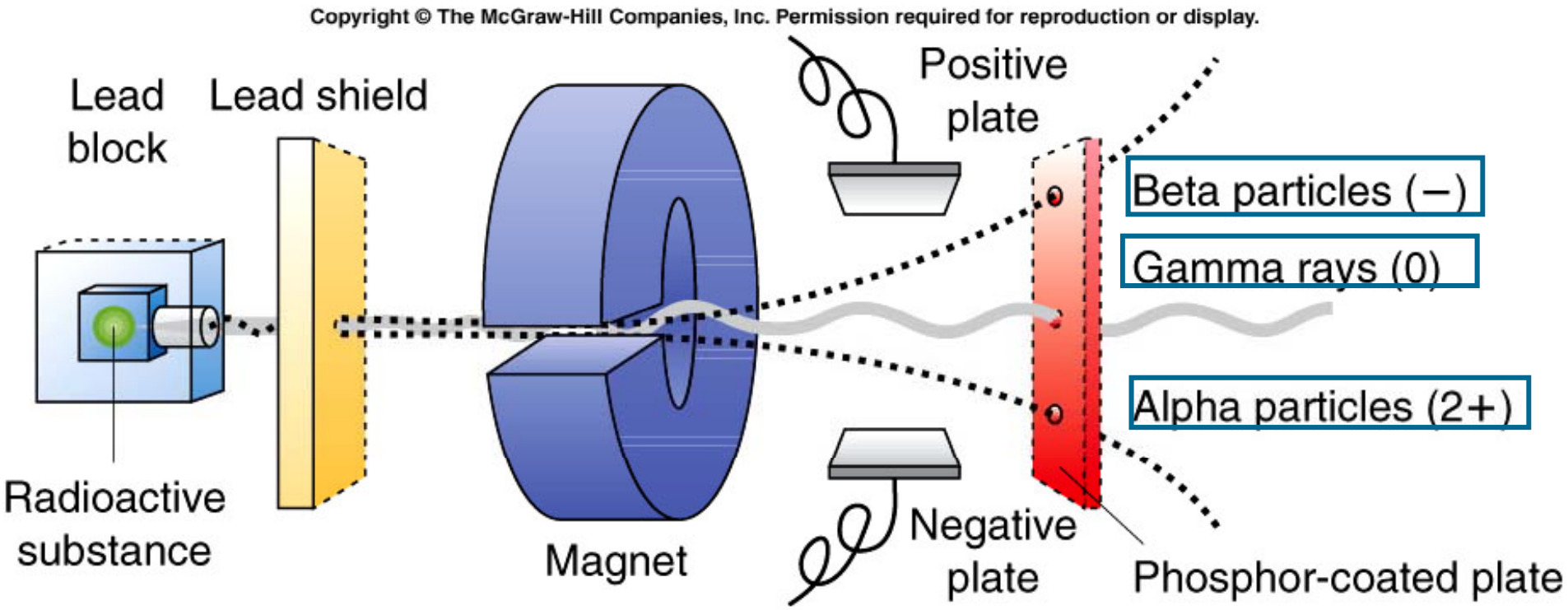
- Electrons were the first subatomic particles to be discovered using the cathode ray tube.



Indicated that the particles were negatively charged.

表面上是粒子

Radioactive Emissions

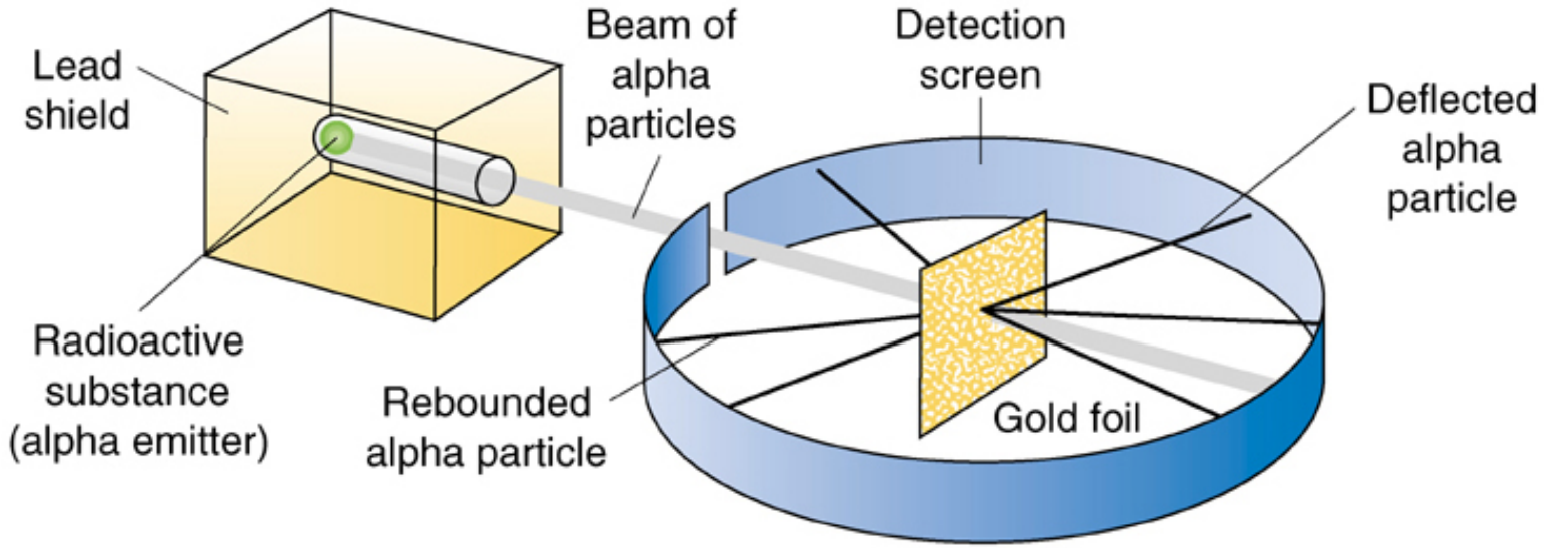


The direction taken by the radioactive emissions indicates the presence of 3 types of emissions

Y.T.Lin's Presentation

表面上是粒子

Rutherford's Gold Foil Experiment



- Most of the atom is empty space
- The majority of the mass is located in a small, dense region

Y.T Lin's Presentation

表面上是粒子

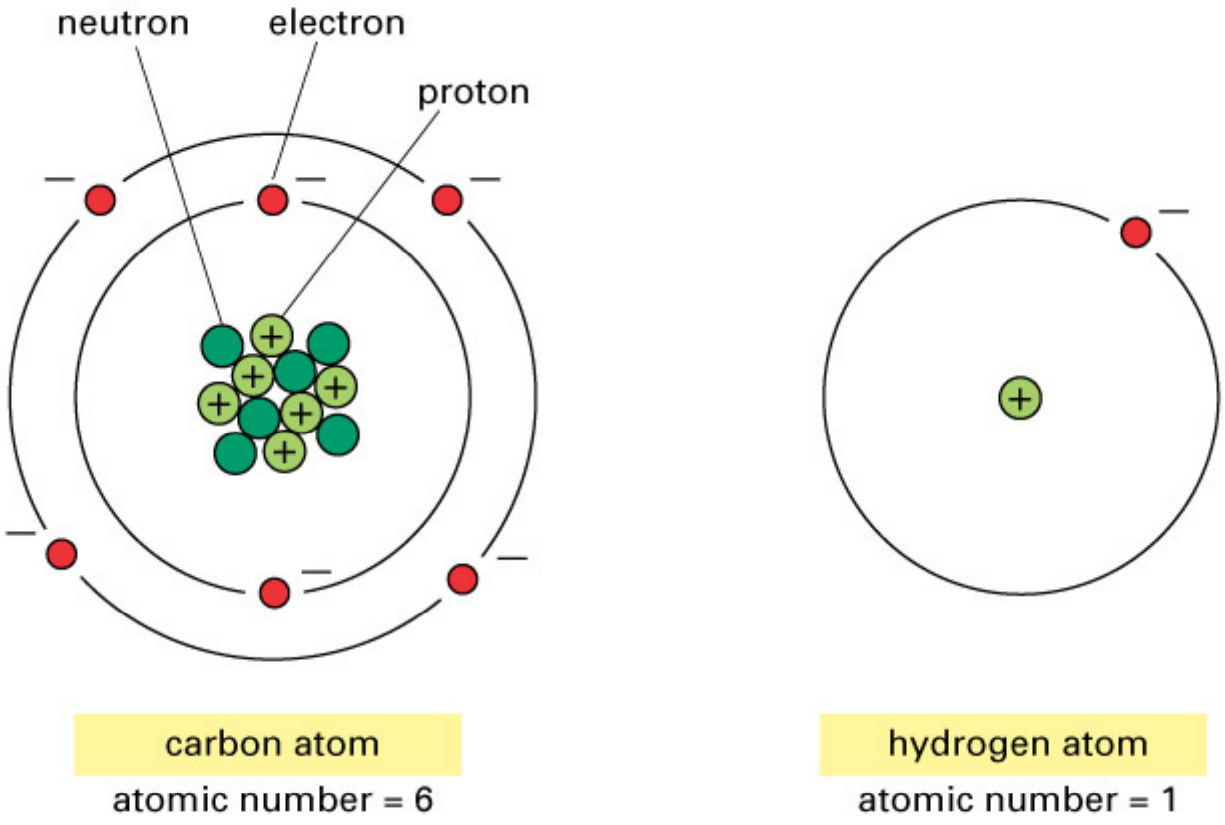


Figure 2-2 Essential Cell Biology, 2/e. (© 2004 Garland Science)

Y.T Lin's Presentation

表面上是粒子

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

TABLE 2.1 Selected Properties of the Three Basic Subatomic Particles

Name	Charge	Mass (amu)	Mass (grams)
Electron (e)	–1	5.4×10^{-4}	9.1095×10^{-28}
Proton (p)	+1	1.00	1.6725×10^{-24}
Neutron (n)	0	1.00	1.6750×10^{-24}

Y.T Lin's Presentation

Electron Arrangement by Energy Level

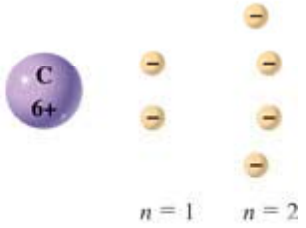
表面上是粒子的組合

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

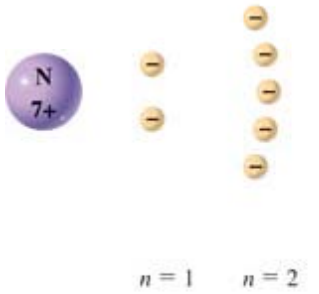
Lithium: Three-electron atom, one valence electron

Beryllium: Four-electron atom, two valence electrons

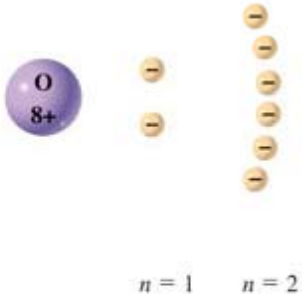
Boron: Five-electron atom, three valence electrons



Carbon: Six-electron atom, four valence electro



Nitrogen: Seven-electron atom, five valence electrons

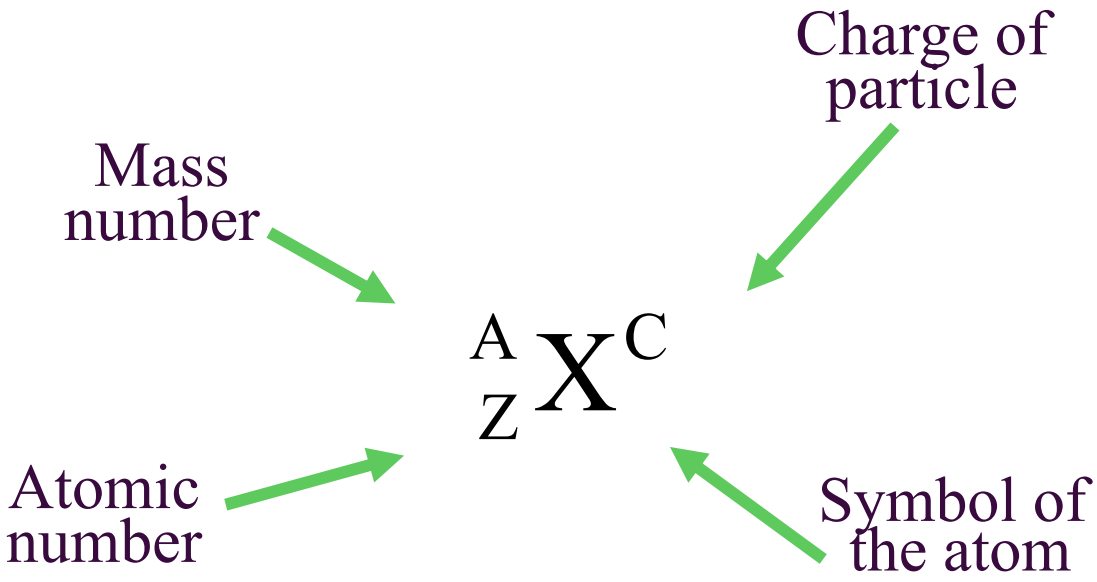


Oxygen: Eight-electron atom, six valence electrons

Y.T Lin's Presentation

Symbolic Representation of an Element

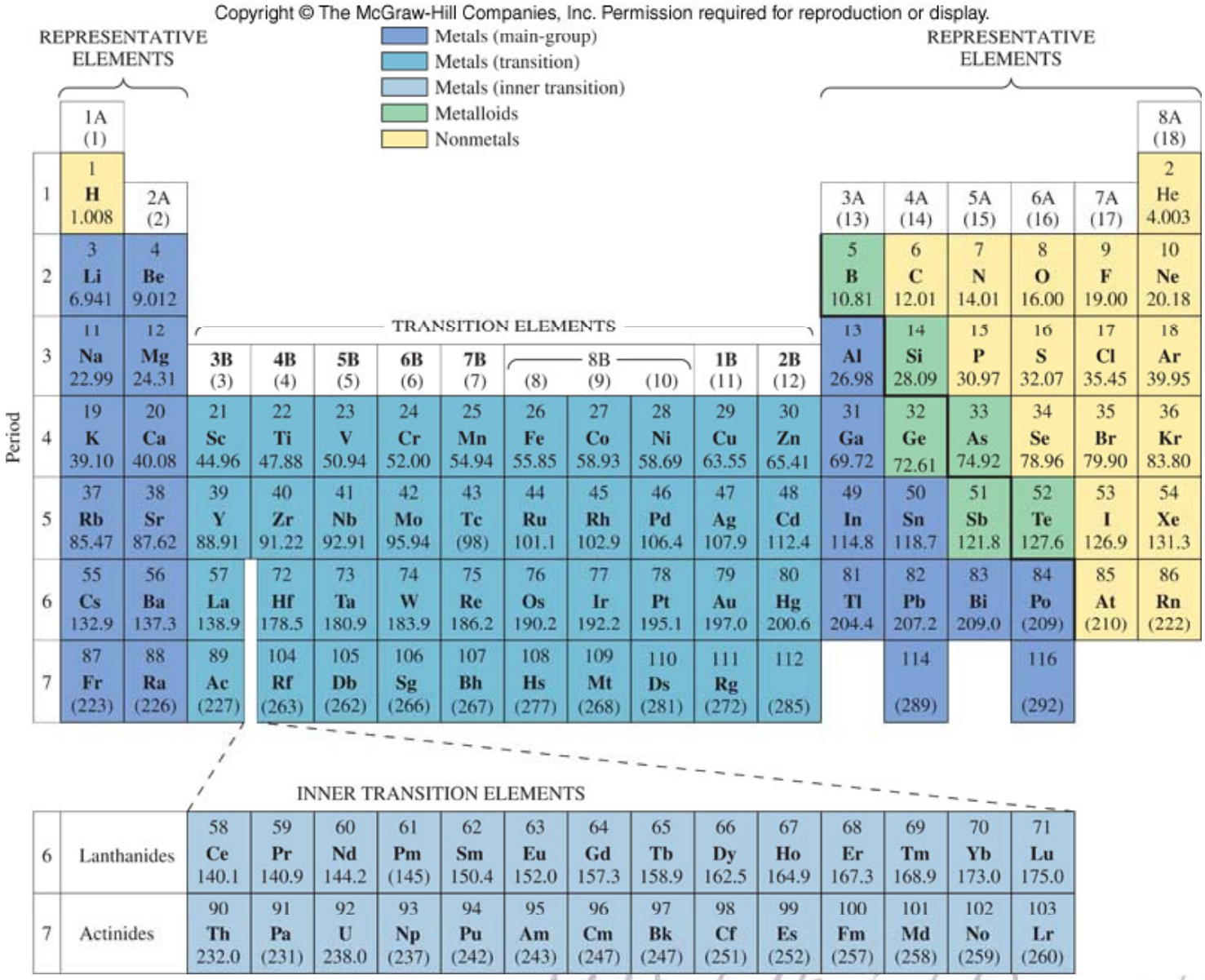
表面上是粒子的組合



- **Atomic number** (Z) - the number of protons in the atom
- **Mass number** (A) - sum of the number of protons and neutrons

Y. T Lin's Presentation

表面上是粒子的組合

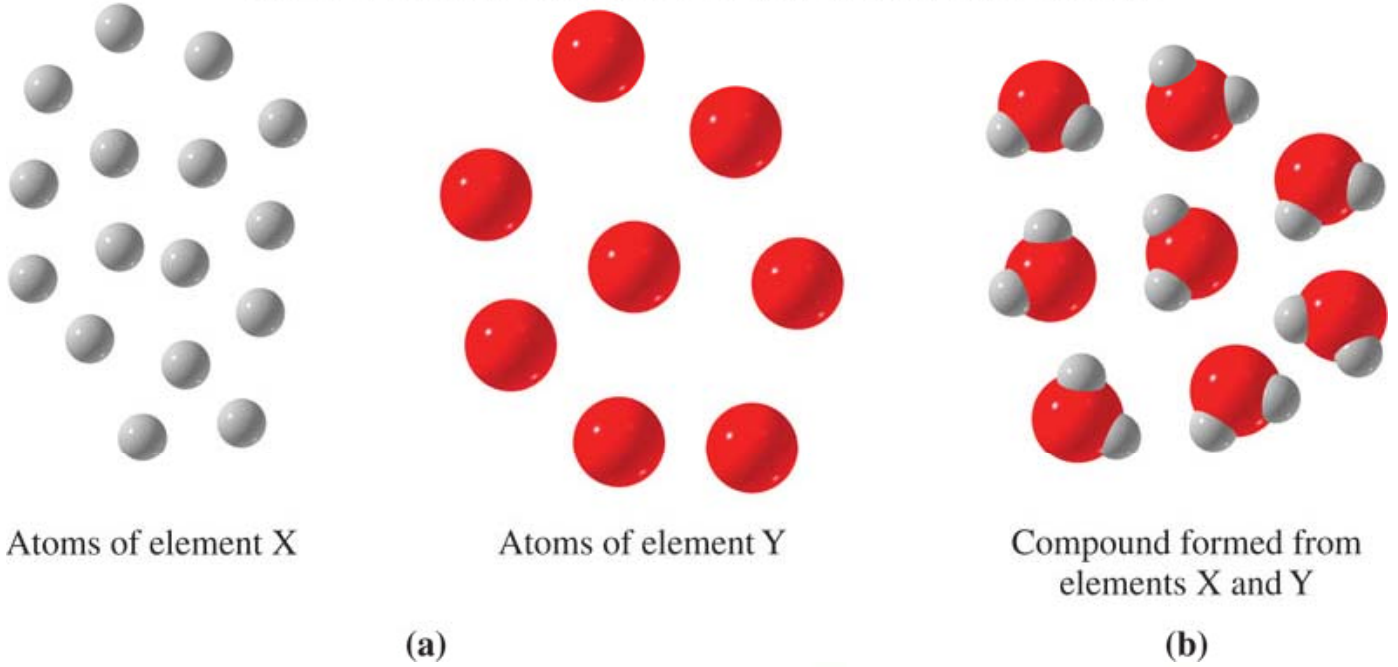


Y. T. Lin's Presentation

表面上是粒子的組合

- **Dalton's Atomic Theory** - the first experimentally based theory of atomic structure of the atom

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



Y.T Lin's Presentation

Important Biological Elements

表面上是粒子的組合

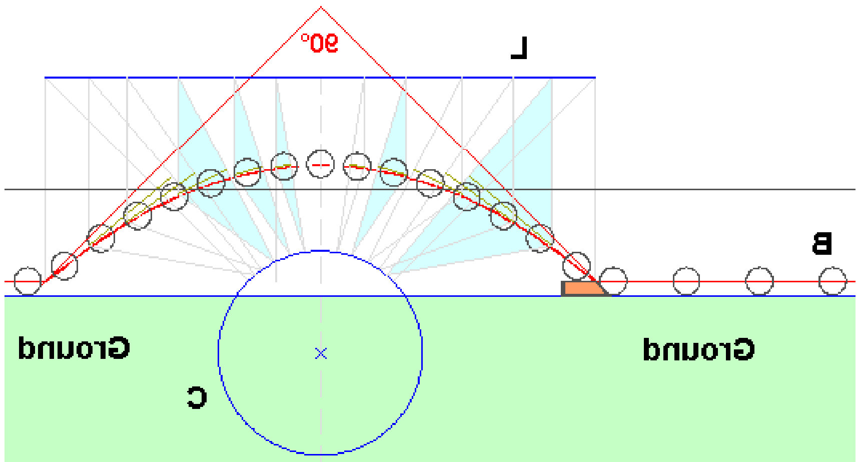
Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

TABLE 2.3 Summary of the Most Important Elements in Biological Systems

Element	Symbol	Significance
Hydrogen	H	Components of major biological molecules
Carbon	C	
Oxygen	O	
Nitrogen	N	
Phosphorus	P	
Sulfur	S	
Potassium	K	Produce electrolytes responsible for fluid balance and nerve transmission
Sodium	Na	
Chlorine	Cl	
Calcium	Ca	Bones, nerve function
Magnesium	Mg	
Zinc	Zn	Essential trace metals in human metabolism
Strontium	Sr	
Iron	Fe	
Copper	Cu	
Cobalt	Co	
Manganese	Mn	
Cadmium	Cd	"Heavy metals" toxic to living systems
Mercury	Hg	
Lead	Pb	

如何描述粒子？

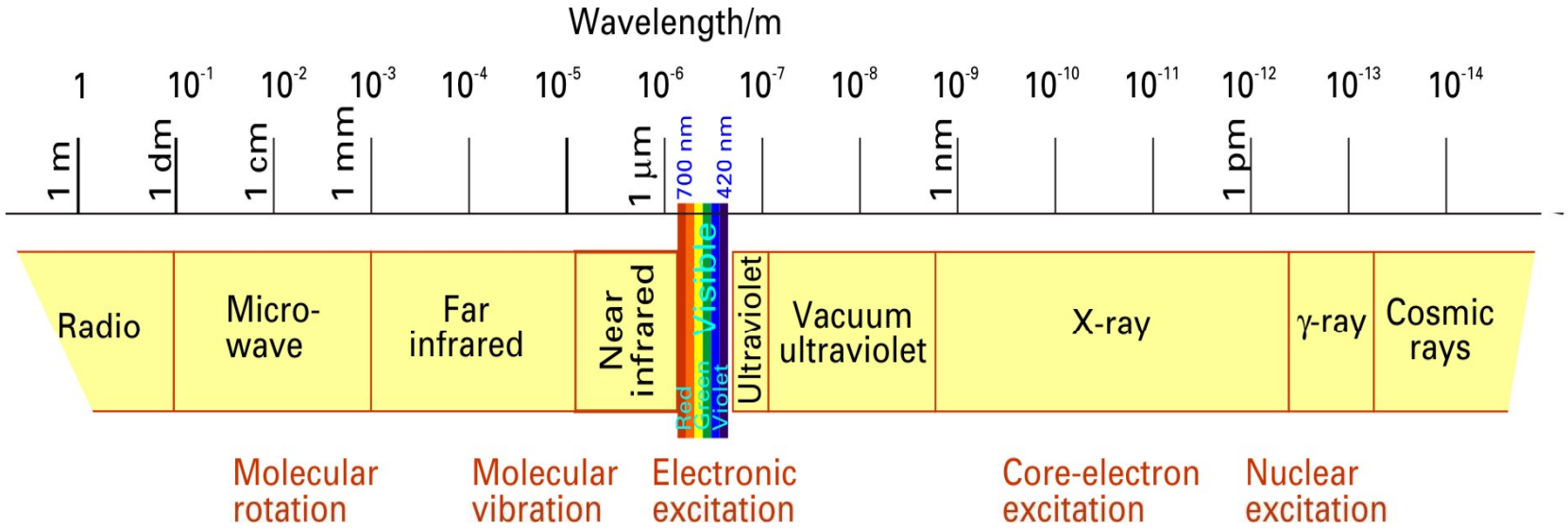
描述其動能及位能



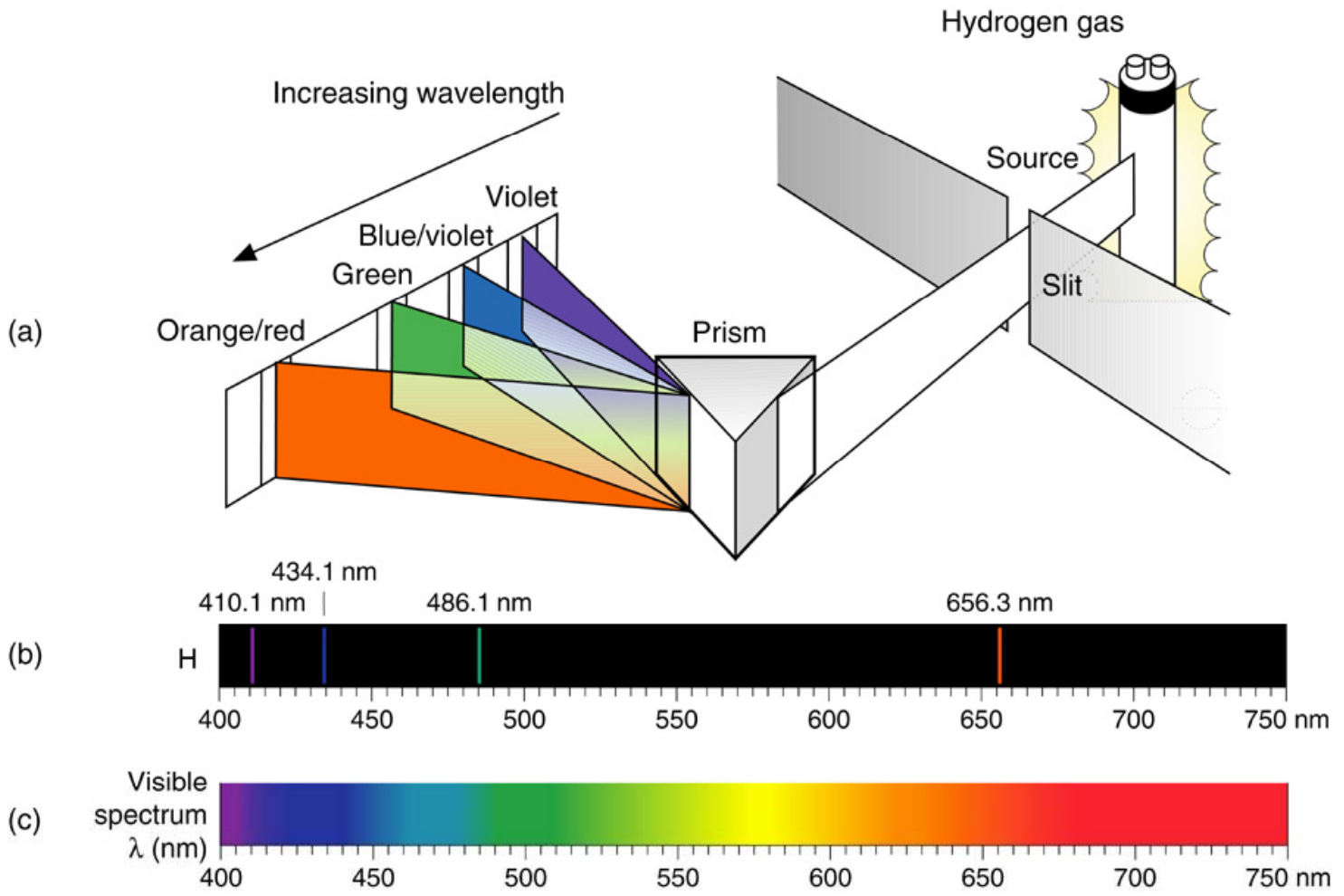
Y.T.Lin's Presentation

光也是粒子

Y.T Lin's Presentation



Y.T Lin's Presentation



The emission spectrum of hydrogen lead to the modern understanding of the electronic structure of the atom

重要區分

光的頻率 vs 光的亮度

光的頻率 = 單一光子的能量
光的亮度 = 所有光子的數量

Y.T Lin's Presentation

Electromagnetic Spectrum

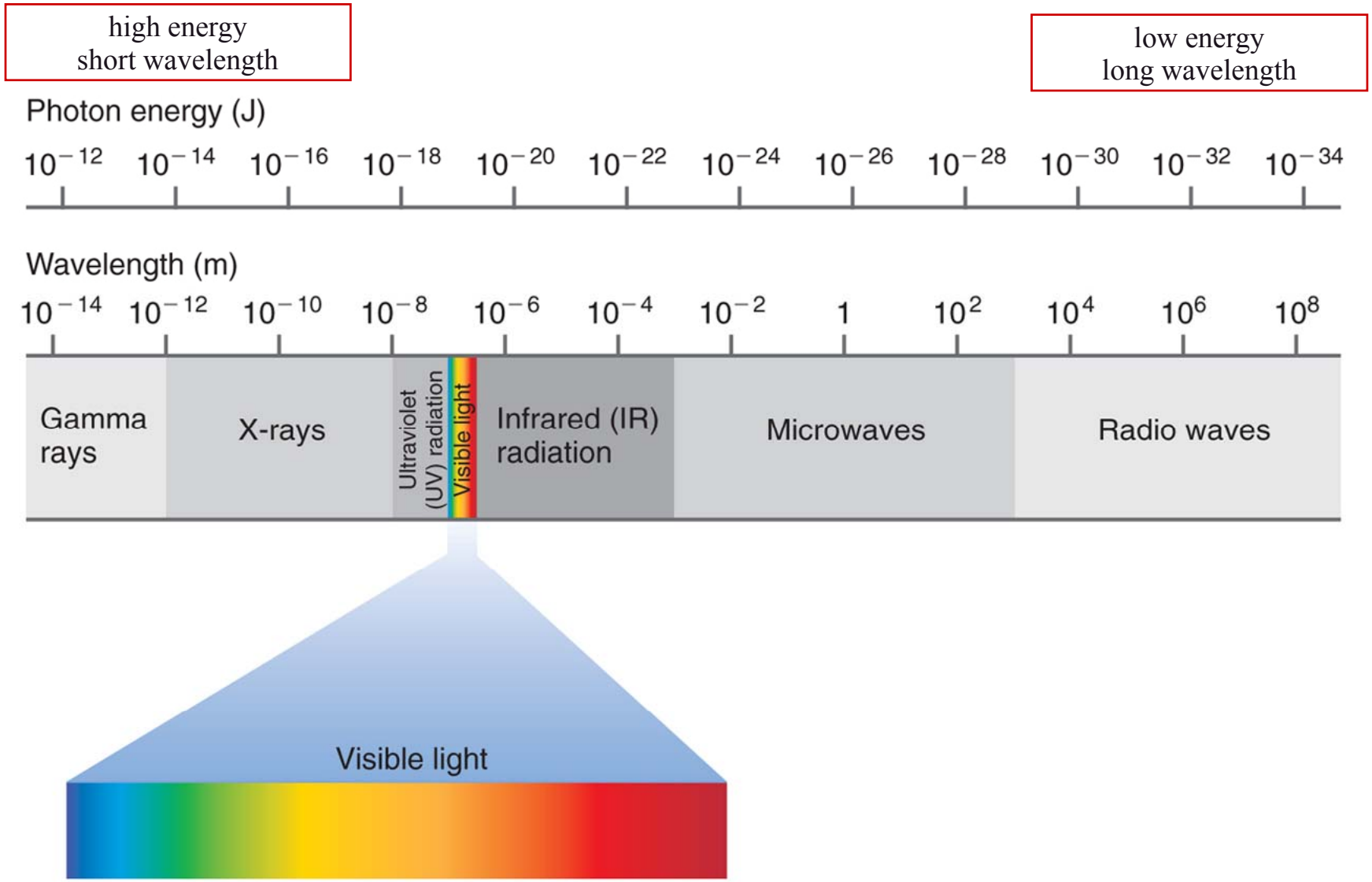
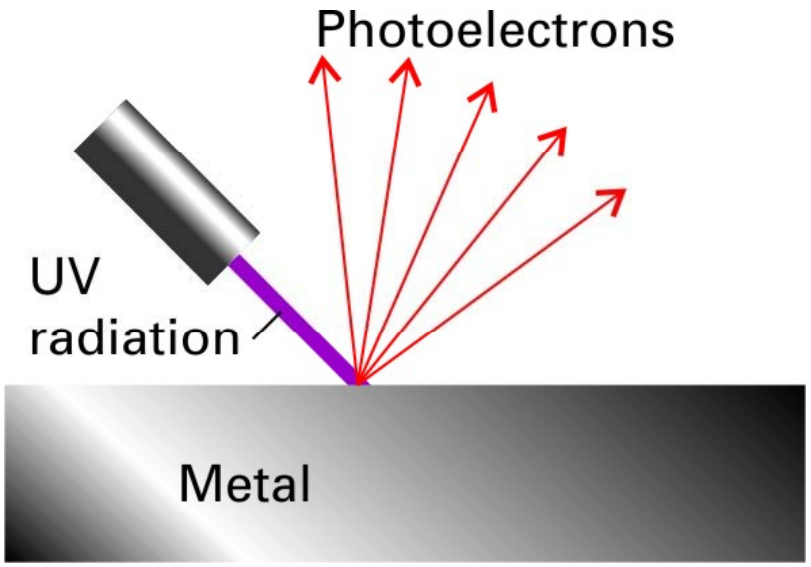


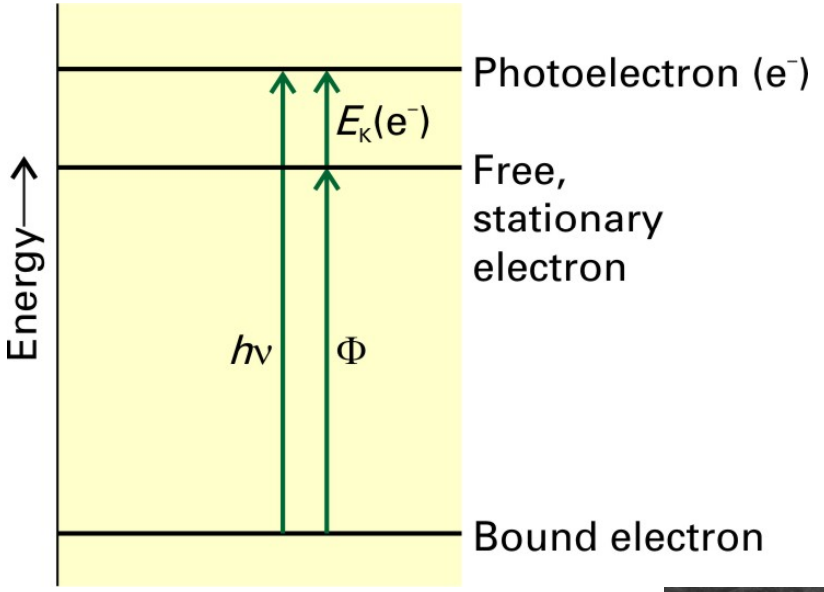
Figure: 18-01

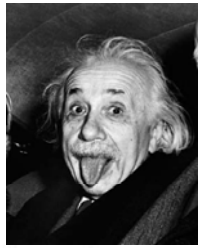
Copyright © 2008 Pearson Prentice Hall, Inc.

One photon $E = h\nu$ 光是光子。

h: plank's constant







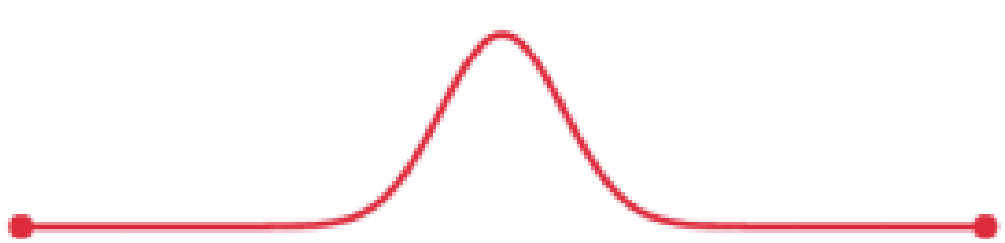
Y.T.Lin's Presentation

把物質切到最小，我們知道：

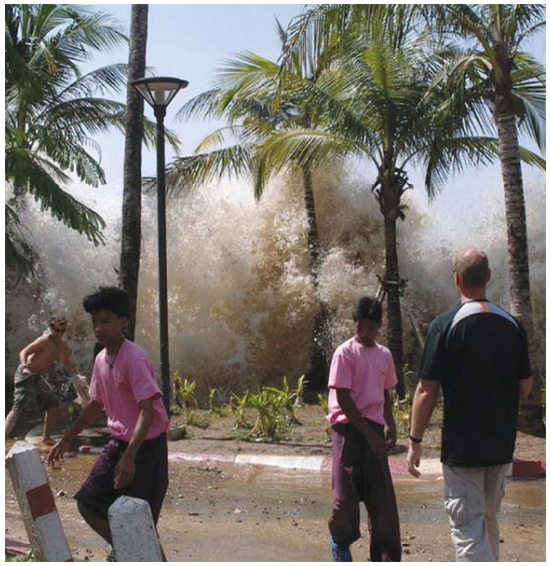
它表面上是粒子，實際上是?

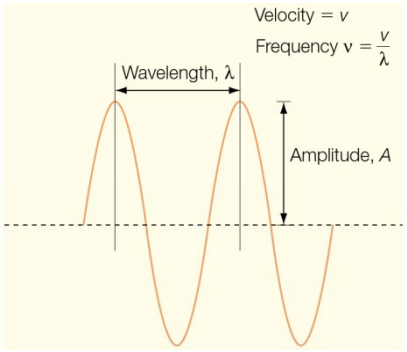
Y.T Lin's Presentation

Wave



Y.T Lin's Presentation





波的特性

Y.T Lin's Presentation

波
有建設性干涉及破壞性干涉

Y.T Lin's Presentation

波
可以共振

Y.T Lin's Presentation

波
可以相加减

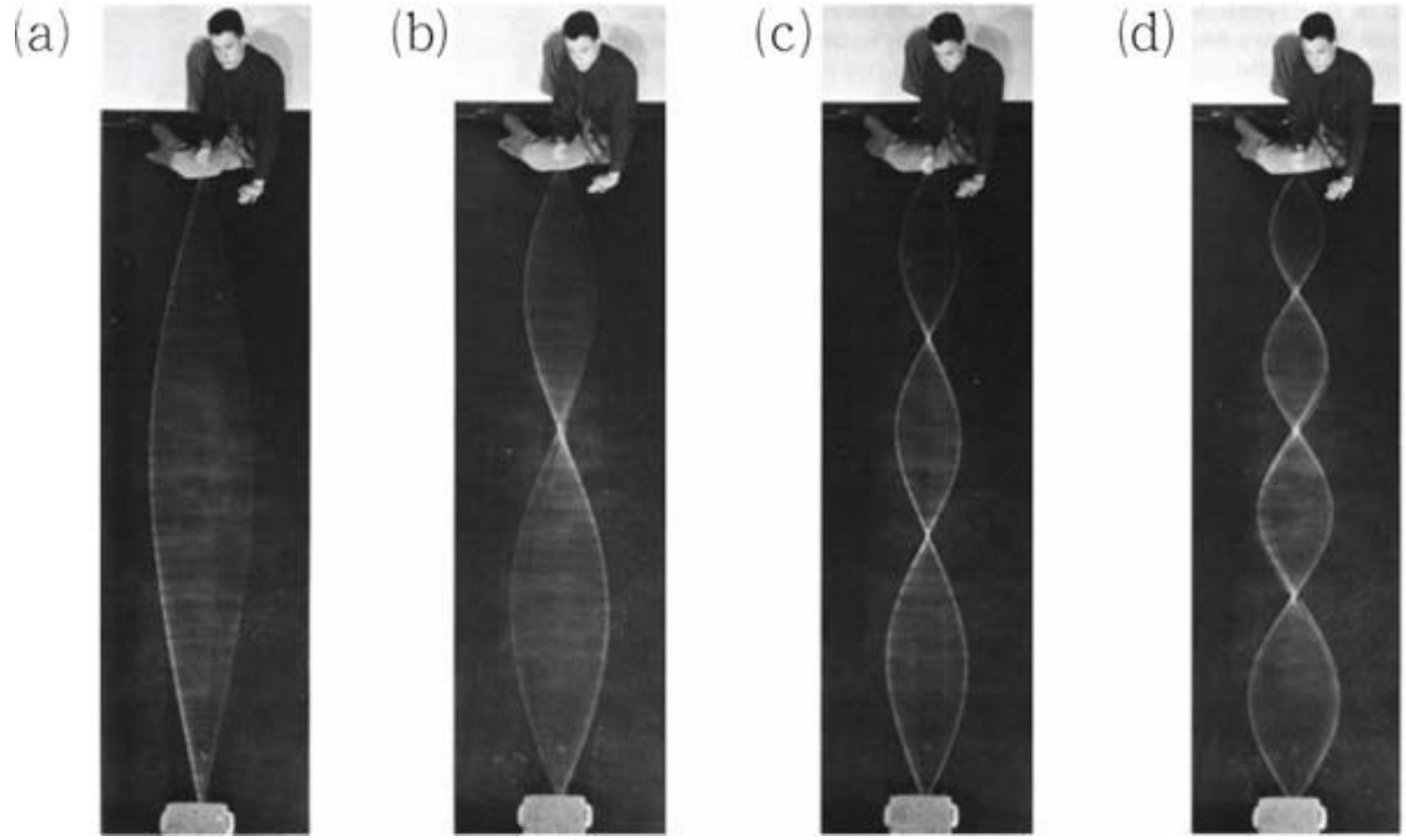
Y.T Lin's Presentation

特定條件下，

波

形成駐波

Y.T Lin's Presentation



Y.T Lin's Presentation

波
有波動方程式

描述波如何波動。

To describe how wave is waving.

Y.T Lin's Presentation

Wave equation

- Wind wave
- Airy wave theory
- Wave equation
- Acoustic wave equation
- Vibrations of a circular drum
- Standing wave
- Electromagnetic wave equation
- Schrödinger equation

Y.T Lin's Presentation

光子(Photon)也是波

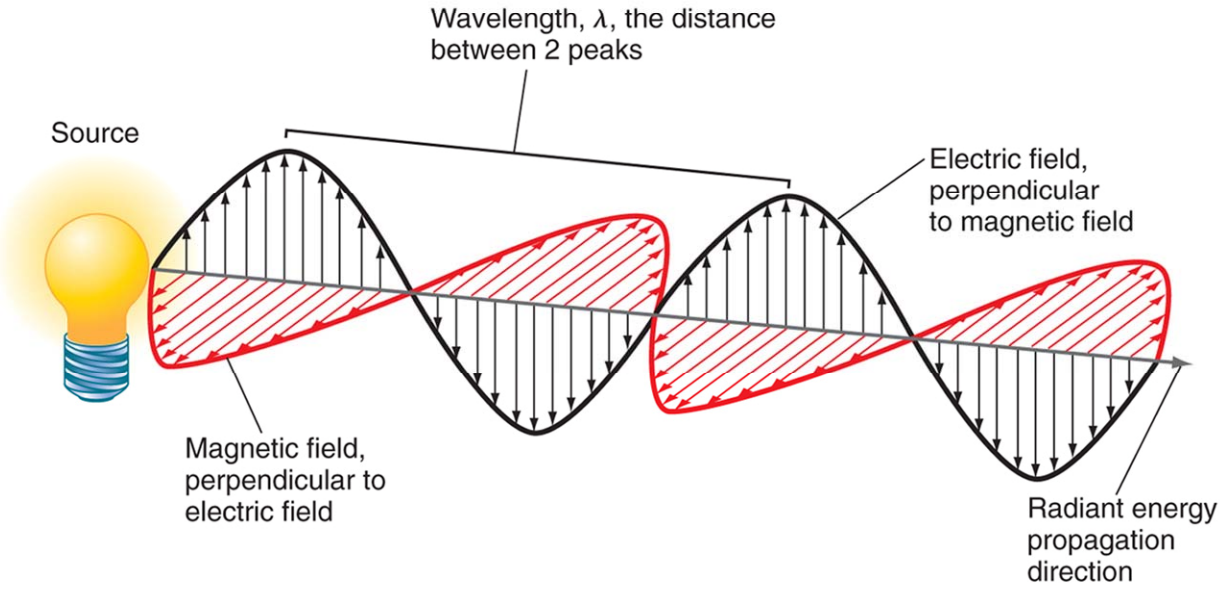


Figure: 18-02

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

Tiny Particle Wave equation

- Wind wave
- Airy wave theory
- Wave equation
- Acoustic wave equation
- Vibrations of a circular drum
- Standing wave
- Electromagnetic wave equation
- **Schrödinger equation**

Y.T Lin's Presentation

Schröedinger equation

CORBIS-Bettmann

Figure 10.4 Erwin Schrödinger (1887–1961). Schrödinger proposed an expression of quantum mechanics that was different from but equivalent to Heisenberg's. His expression is useful because it expresses the behavior of electrons in terms of something we understand—waves. The Schrödinger equation is the central equation of quantum mechanics.

Y.T Lin's Presentation

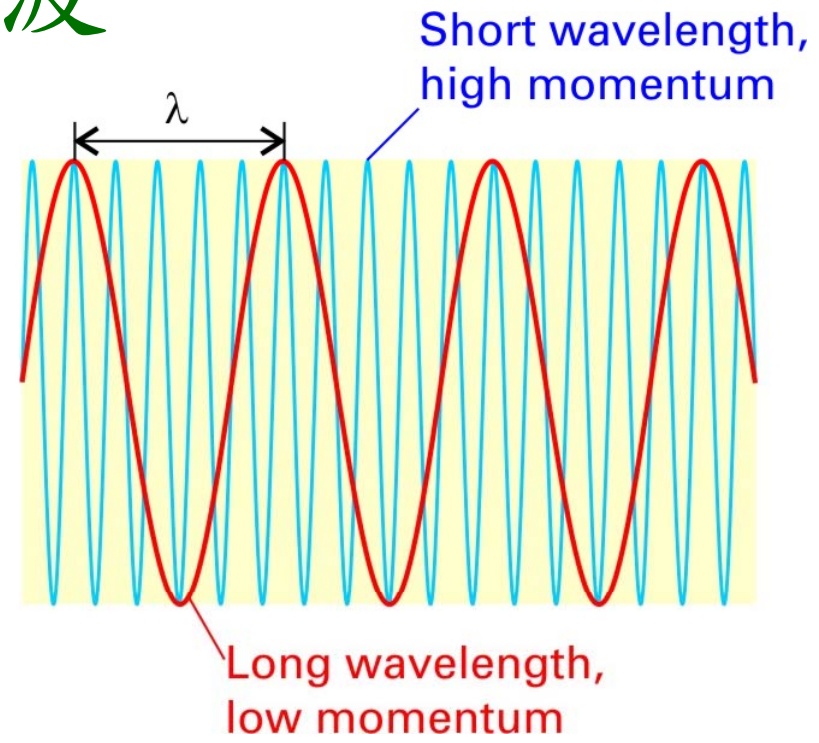
The wave nature of the electrons

電子是波。

$E = h\nu = mc^2$

$\lambda = c/\nu = h/mc = h/p$

(de Broglie relation)



p: momentum

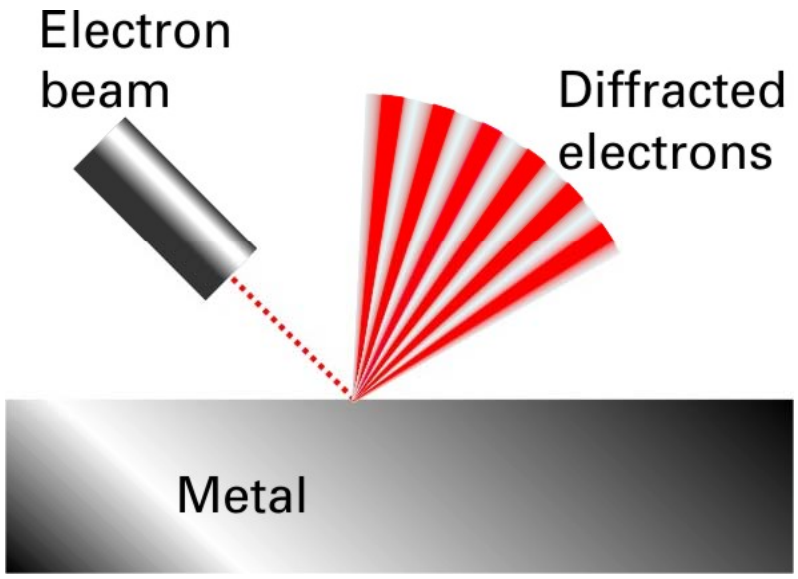
$p = mv$

m: mass

v: velocity

Y.T.Lin's Presentation

Davisson and Germer



電子是波。

$$\lambda = h / p$$

Y.T Lin's Presentation

Schröedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi$$

Total energy

Potential energy

Kinetic energy

$$\hbar=\frac{h}{2\pi}=1.054\times10^{-34}\ Js$$

Chapter 13, Physical Chemistry for the Life Sciences (Engel, Drobny and Reid)

Y.T Lin's Presentation

Quantum Chemistry 的七個法則

➔用來形成 Schröedinger equation

（也就是可用來描述電子的波動方程式）

Y.T Lin's Presentation

Quantum Mechanics 的七個法則

Table 10.2 The postulates of quantum mechanics

Postulate I. The state of a system of particles is given by a wavefunction Ψ, which is a function of the coordinates of the particles and the time. Ψ contains all information that can be determined about the state of the system. Ψ must be single-valued, continuous, and bounded, and $|\Psi|^2$ must be integrable. (Discussed in section **10.2**)

Postulate II. For every physical observable or variable O, there exists a corresponding Hermitian operator $\hat{O}$. Operators are constructed by writing their classical expressions in terms of position and (linear) momentum, then replacing "x times" (that is, $x\,\cdot$) for each x variable and $-i\hbar(\partial/\partial x)$ for each p_x variable in the expression. Similar substitutions must be made for y and z coordinates and momenta. (Section **10.3**)

Postulate III. The only values of observables that can be obtained in a single measurement are the eigenvalues of the eigenvalue equation constructed from the corresponding operator and the wavefunction Ψ:

$$\hat{O}\Psi = K \cdot \Psi$$

where K is a constant. (Section **10.3**)

Postulate IV. Wavefunctions must satisfy the time-dependent Schrödinger equation:

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

(Section **10.14**) (If it is assumed that Ψ is separable into functions of time and position, we find that this expression can be rewritten to get the time-independent Schrödinger equation, $\hat{H}\Psi = E\Psi$.) (section **10.7**)

Postulate V. The average value of an observable, $\langle O\rangle$, is given by the expression

$$\langle O\rangle = \int_{\substack{\text{all}\\\text{space}}} \Psi^{*}\hat{O}\Psi\, d\tau$$

for normalized wavefunctions. (Section **10.9**)

Postulate VI. The set of eigenfunctions for any quantum mechanical operator is a complete mathematical set of functions.

Postulate VII. If, for a given system, the wavefunction Ψ is a linear combination of nondegenerate wavefunctions Ψ_n which have eigenvalues a_n:

$$\Psi = \sum_n c_n\Psi_n \quad \text{and} \quad \hat{A}\Psi_n = a_n\Psi_n$$

then the probability that a_n will be the value of the corresponding measurement is $|c_n|^2$. The construction of Ψ as the combination of all possible Ψ_n's is called the *superposition principle.*

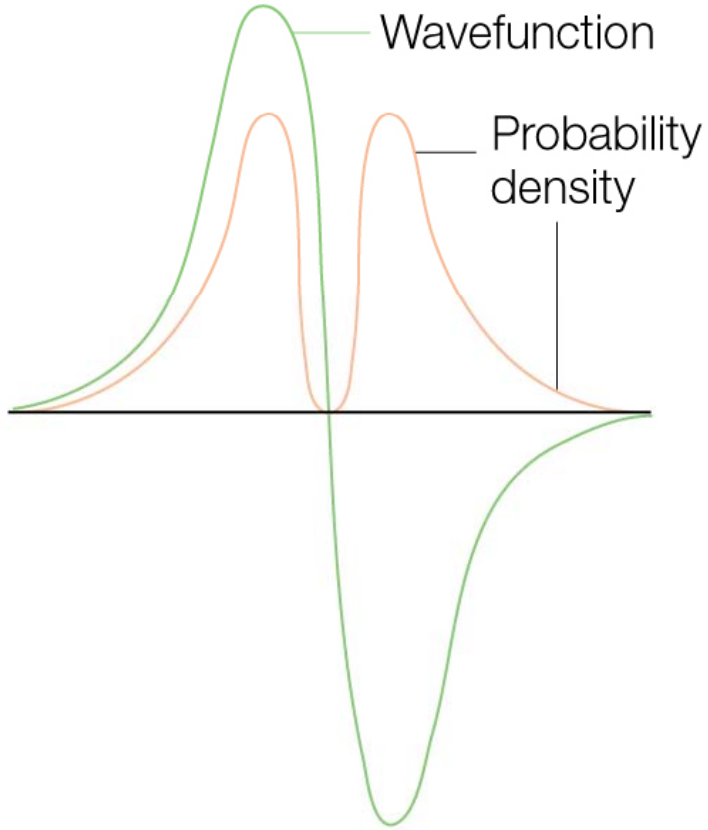
Y.T Lin's Presentation

Table 10.1 Operators for various observables and their classical counterparts[a]

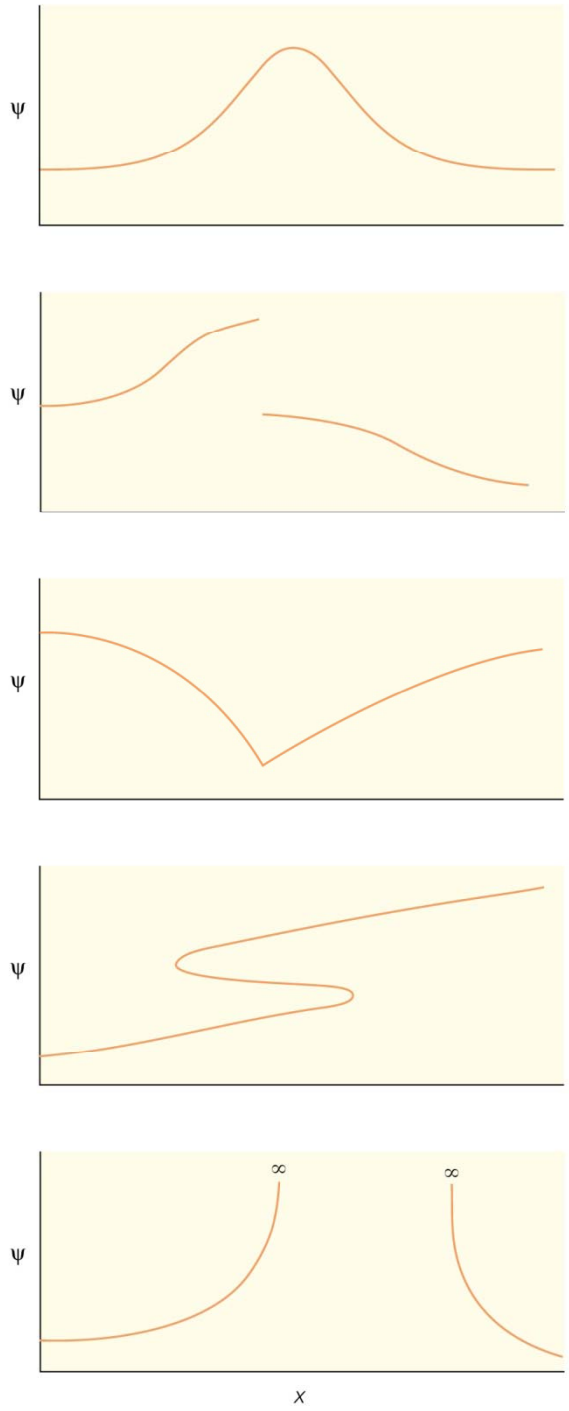
Observable	Operator	Classical counterpart
Position	$\hat{x} = x \cdot$	x
	And so forth for coordinates other than x	
Momentum (linear)	$\widehat{p_x} = -i\hbar\dfrac{\partial}{\partial x}$	$p_x = mv_x$
	And so forth for coordinates other than x	
Momentum (angular)	$\widehat{L_x} = -i\hbar\left(\hat{y}\dfrac{\partial}{\partial z} - \hat{z}\dfrac{\partial}{\partial y}\right)$	$L_x = yp_z - zp_y$
Kinetic energy, 1-D[b]	$\hat{K} = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$	$K = \dfrac{1}{2}mv_x^2 = \dfrac{p_x^2}{2m}$
Kinetic energy, 3-D[b]	$\hat{K} = -\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right)$	$K = \dfrac{1}{2}m(v_x^2 + v_y^2 + v_z^2)$ $= \dfrac{p_x^2 + p_y^2 + p_z^2}{2m}$
Potential energy:		
Harmonic oscillator	$\hat{V} = \dfrac{1}{2}kx^2 \cdot$	$V = \dfrac{1}{2}kx^2$
Coulombic	$\hat{V} = \dfrac{q_1 \cdot q_2}{4\pi\epsilon_0 r} \cdot$	$V = \dfrac{q_1 \cdot q_2}{4\pi\epsilon_0 r}$
Total energy	$\hat{H} = -\dfrac{\hbar^2}{2m}\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right) + \hat{V}$	$H = \dfrac{p^2}{2m} + V$

[a]Operators expressed in x, y, and/or z are Cartesian operators; operators expressed in r, θ, and/or ϕ are spherical polar operators.

[b]The kinetic energy operator is also symbolized by $\hat{T}$.



Y.T Lin's Presentation



Presentation

物理

物質

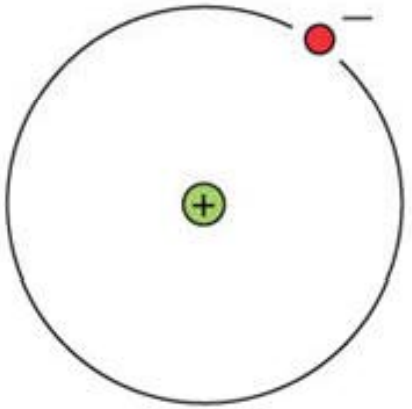
表面上是粒子，
實際上是波動。

波

力

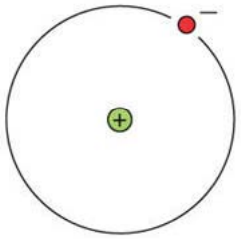
表面上是粒子。

能量描述



- 受到作用力
- 位能

Y.T Lin's Presentation



Schröedinger equation for hydrogen atom

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi$$

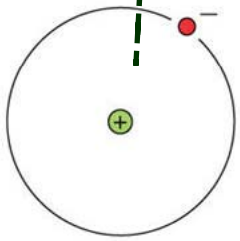
E

ψ

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.

TABLE 2.1 Selected Properties of the Three Basic Subatomic Particles

Name	Charge	Mass (amu)	Mass (grams)
Electron (e)	–1	5.4×10^{-4}	9.1095×10^{-28}
Proton (p)	+1	1.00	1.6725×10^{-24}
Neutron (n)	0	1.00	1.6750×10^{-24}



Y. T. Lin's Presentation

Solution of Schröedinger equation for hydrogen atom

- n, l, m_l

  $n = 1, 2, 3, \ldots$

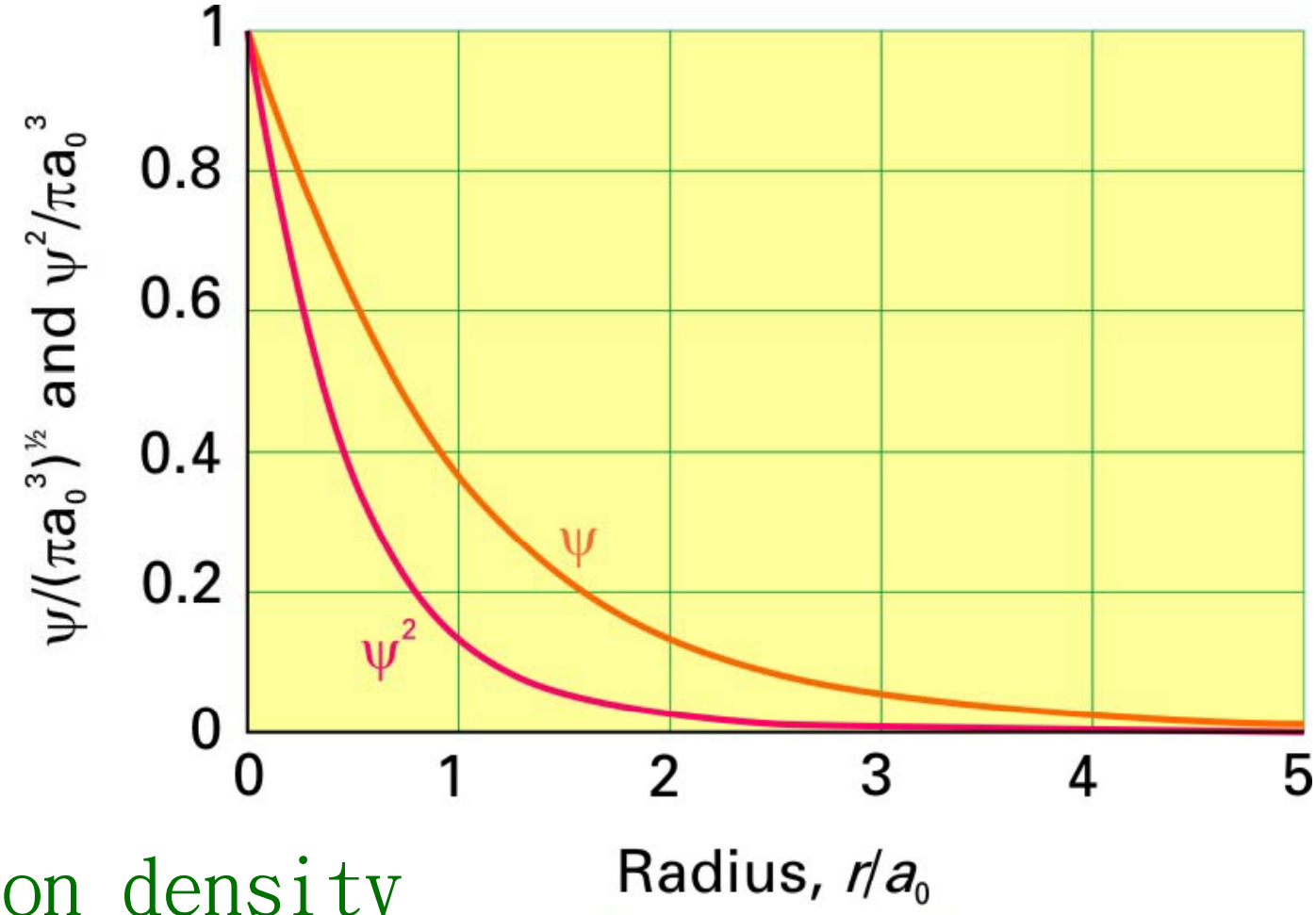
  $l = 0, 1, 2, 3, \ldots, n-1$

  $ml = 0, \pm1, \pm2, \pm3, \ldots, \pm l$
- E_n
- Ψ_{n,l,m_l}

Y.T Lin's Presentation

The shapes of atomic orbitals

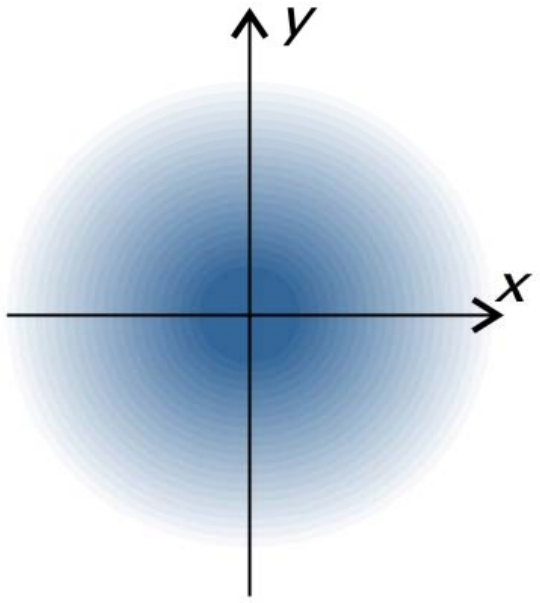
1s



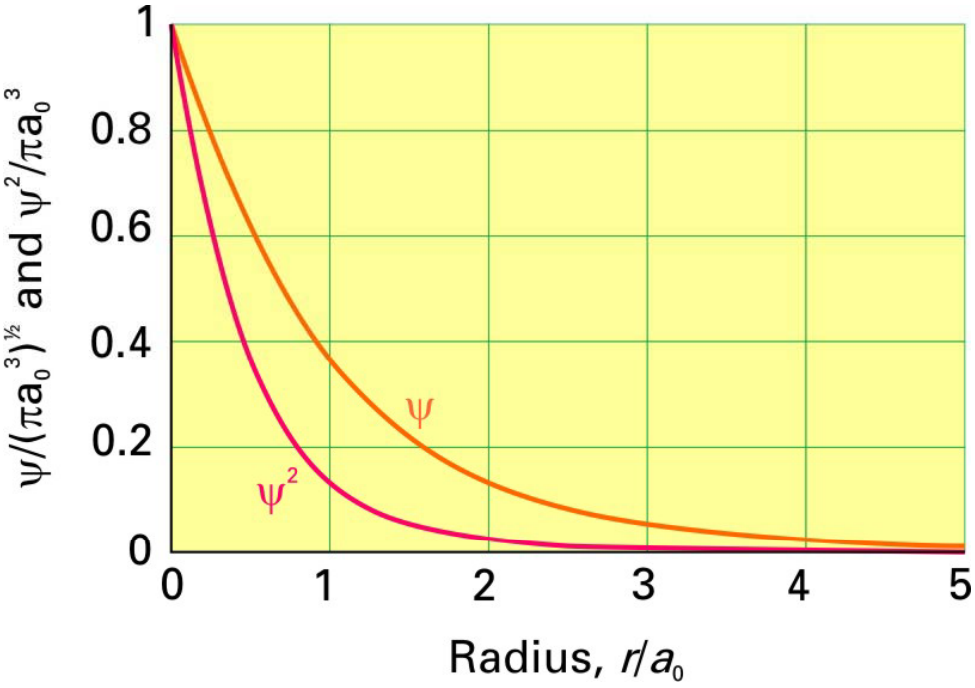
ψ^2: electron density

Y.T.Lin's Presentation

1s

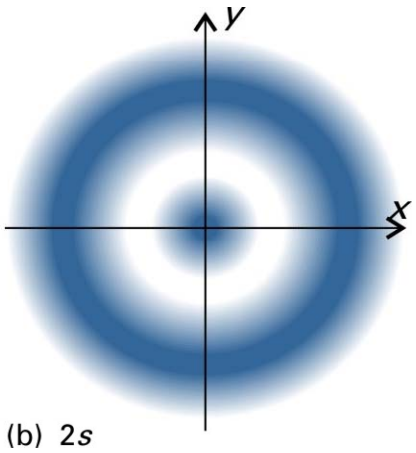


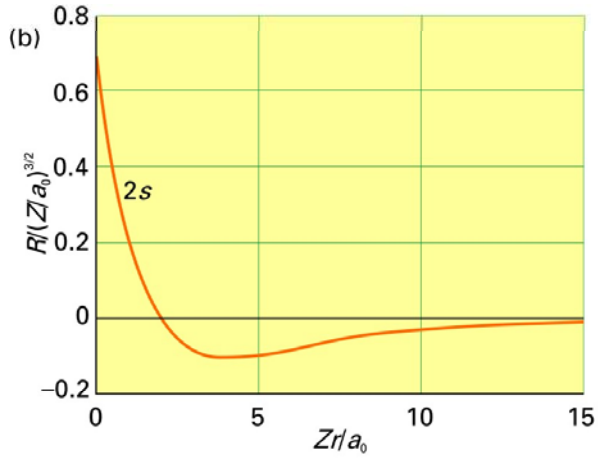
(a) 1*s*



Y.T Lin's Presentation

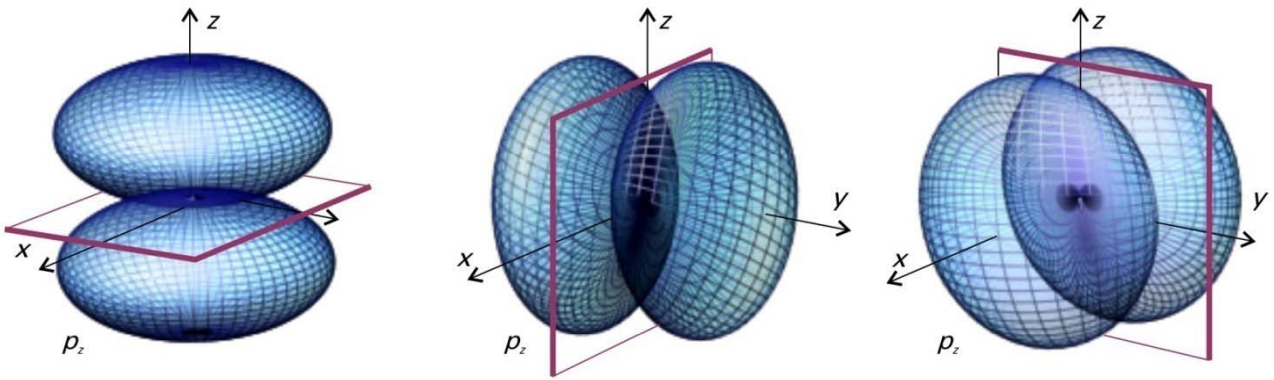
2s





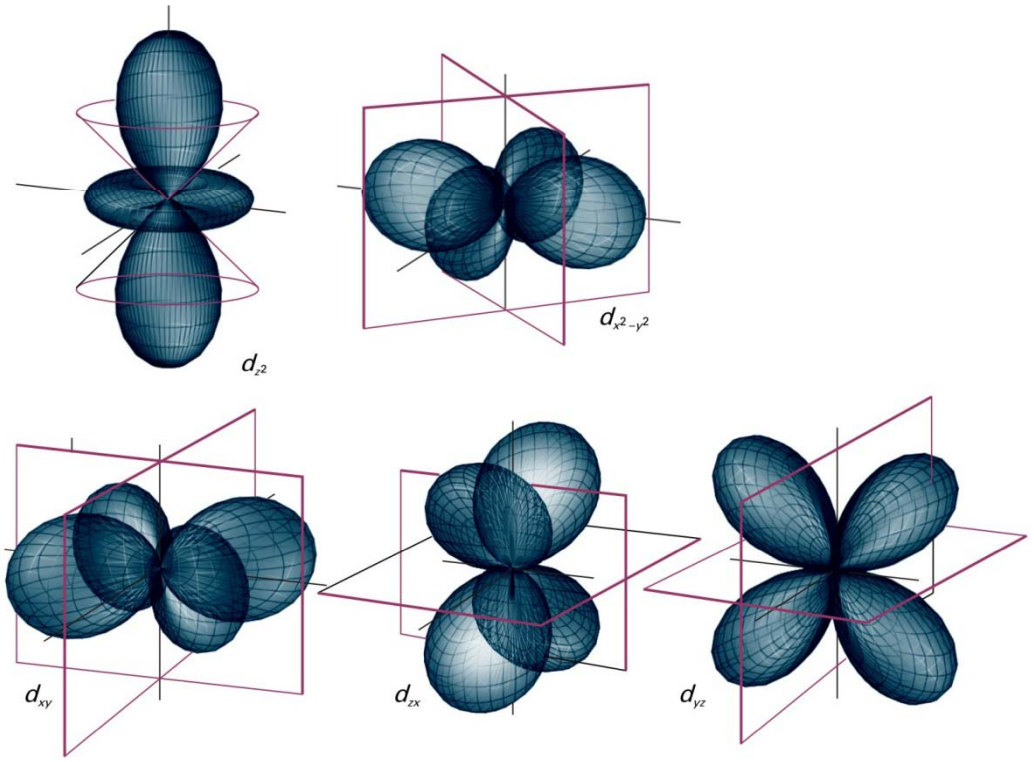
Y.T Lin's Presentation

2p



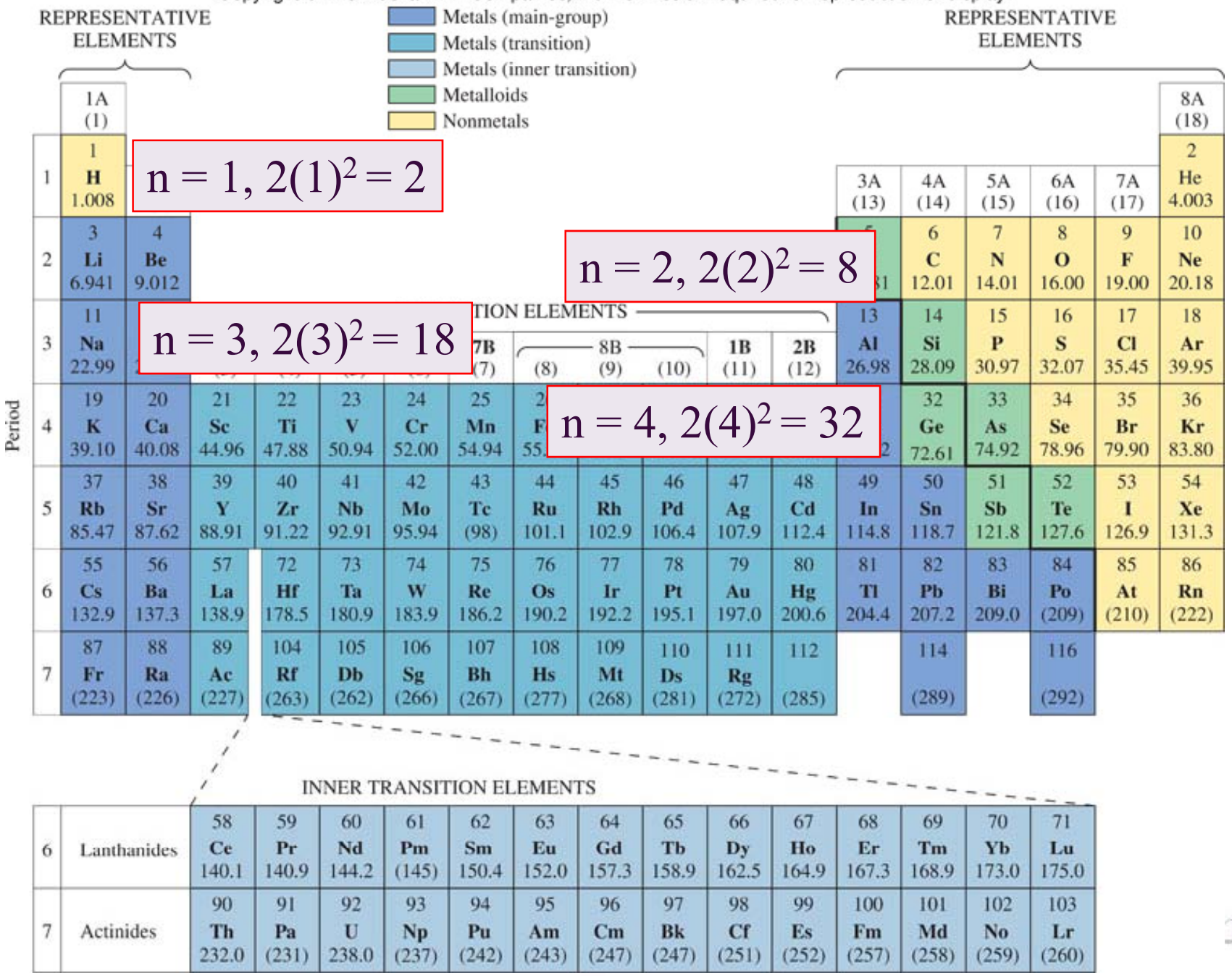
Y.T Lin's Presentation

3d



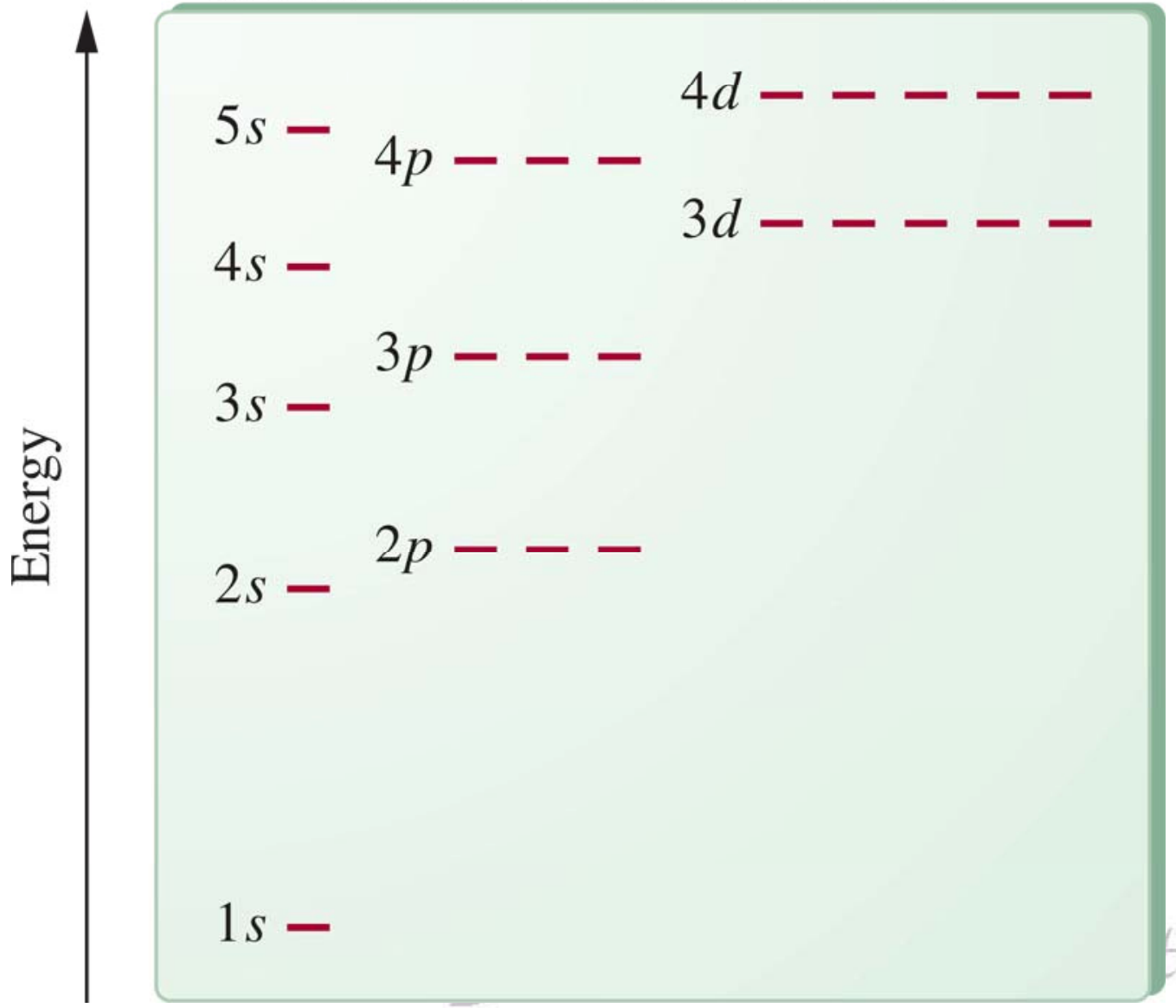
Y.T Lin's Presentation

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



Orbital Energy-level Diagram

Copyright © The McGraw-Hill Companies, Inc. Permission required for reproduction or display.



Different Systems

(Chapter 14 ~ Chapter 18)

- 不同的系統，
  有不同的 Schröedinger equation 的解

Y.T Lin's Presentation

Schröedinger equation 的解，是 Orthogonal。

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)dx = \begin{cases} 0, i \neq j \\ 1, i = j \end{cases} \qquad (13.21)$$

Y.T Lin's Presentation

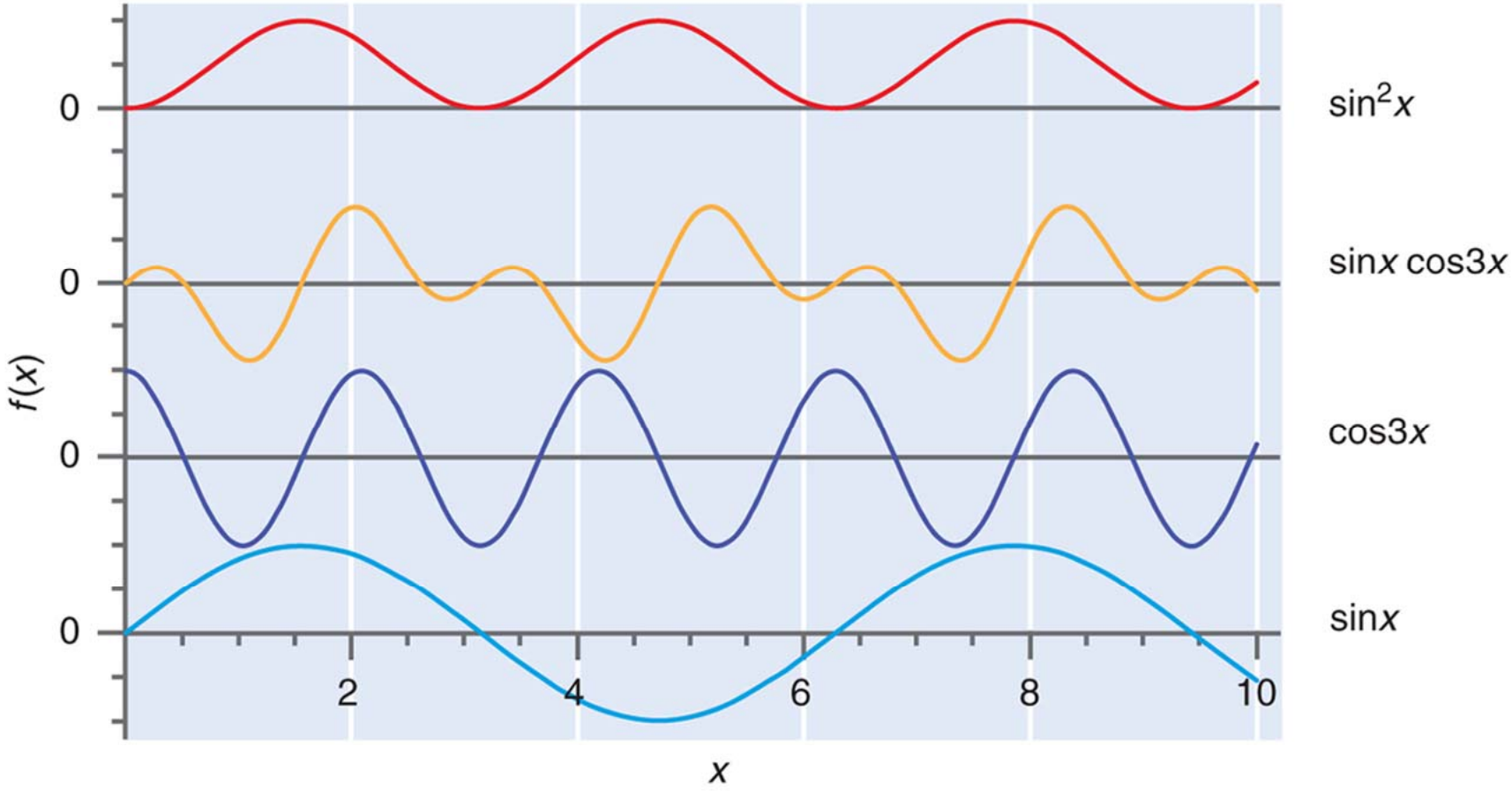


Figure: 13-02EP

Copyright © 2008 Pearson Prentice Hall, Inc.

'Y.' J Lin's Presentation

The Free Particle

Chapter 14.1, Physical Chemistry for the Life Sciences (Engel, Drobny and Reid)

Y.T Lin's Presentation

The Heisenberg Uncertainty Principle

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

Copyright © 2006 Pearson Education, Inc., publishing as Benjamin Cummings

Y.T Lin's Presentation

A ball in a box – what happened?

Potential of wall

$$V = \infty$$

Y.T Lin's Presentation

The Particle in a One-Dimensional Box

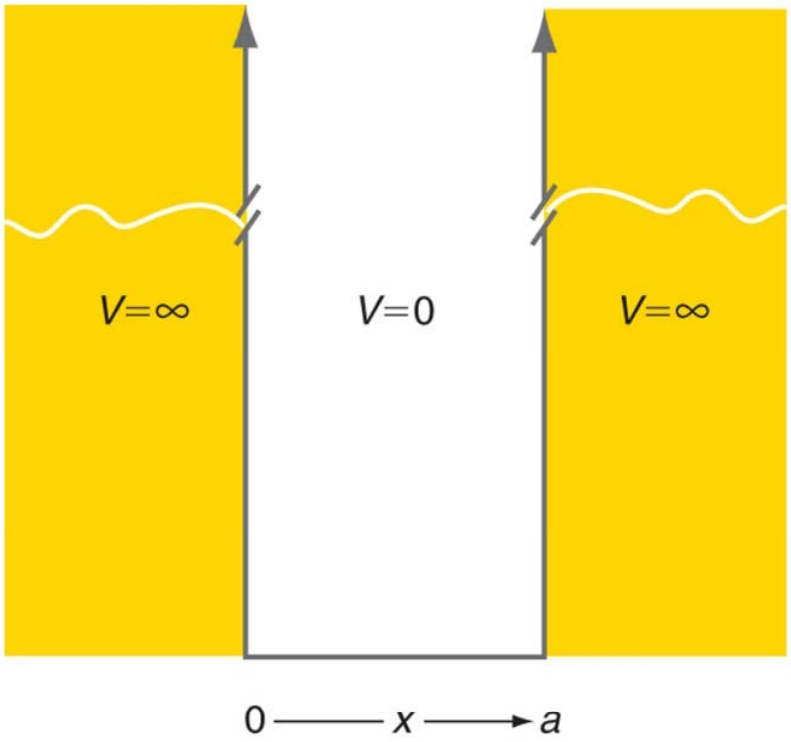
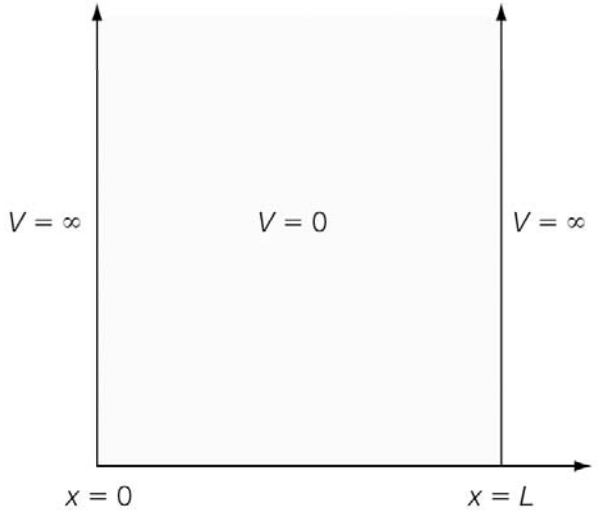


Figure: 14-01

Copyright © 2008 Pearson Prentice Hall, Inc.



Y.T Lin's Presentation

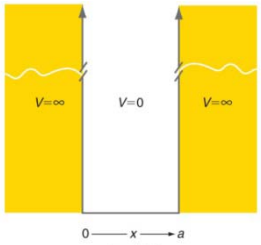


Figure: 14-01

Copyright © 2008 Pearson Prentice Hall, Inc.

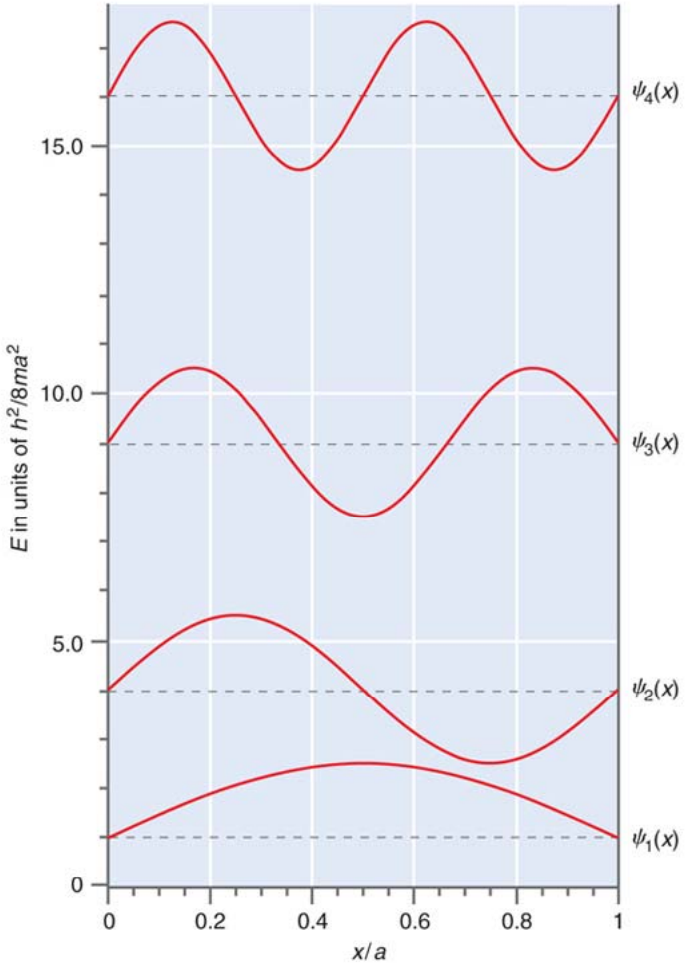


Figure: 14-02

Copyright © 2008 Pearson Prentice Hall, Inc.

Y. J Lin's Presentation

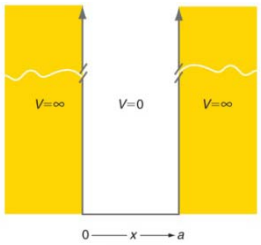


Figure: 14-01

Copyright © 2008 Pearson Prentice Hall, Inc.

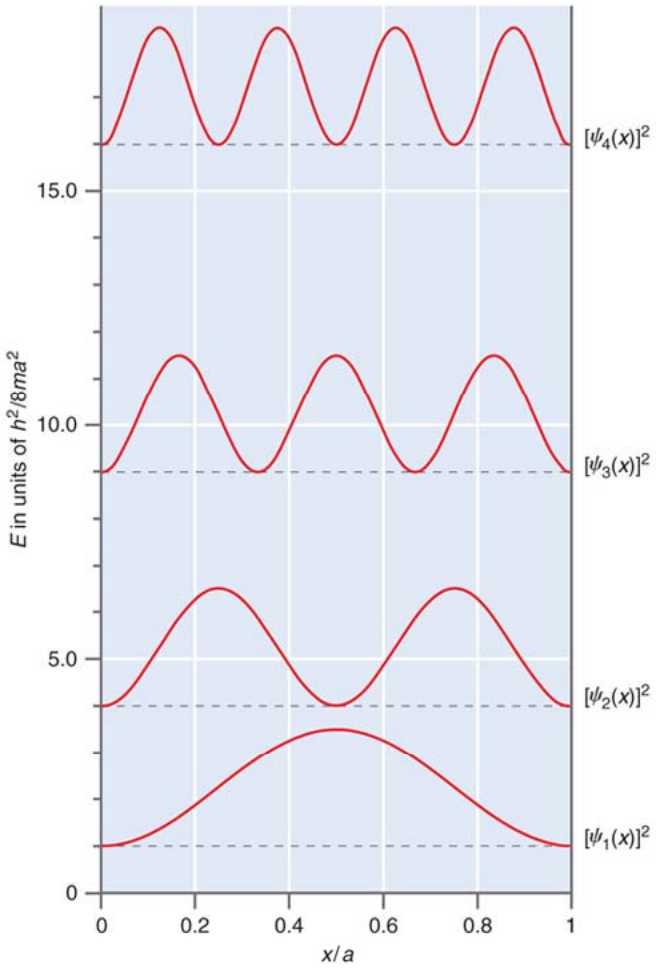


Figure: 14-03

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

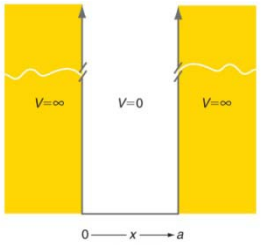
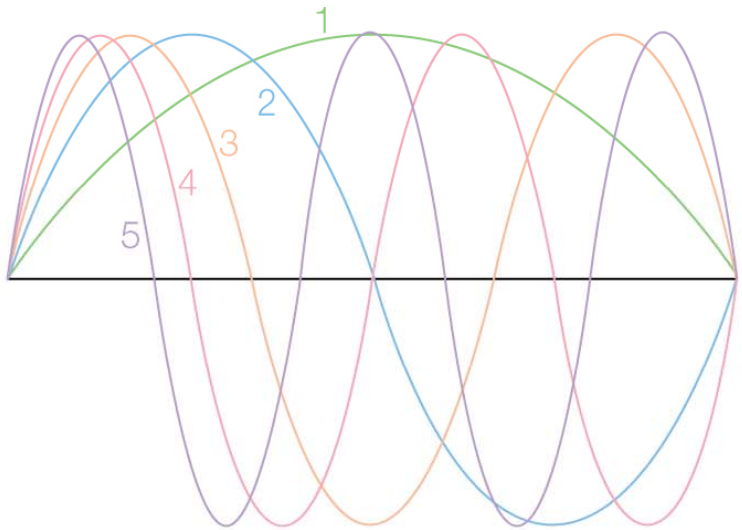
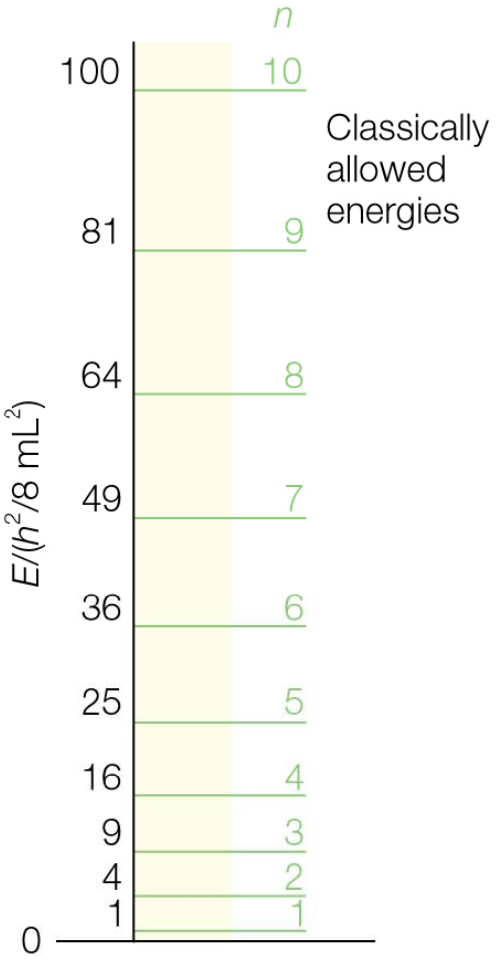


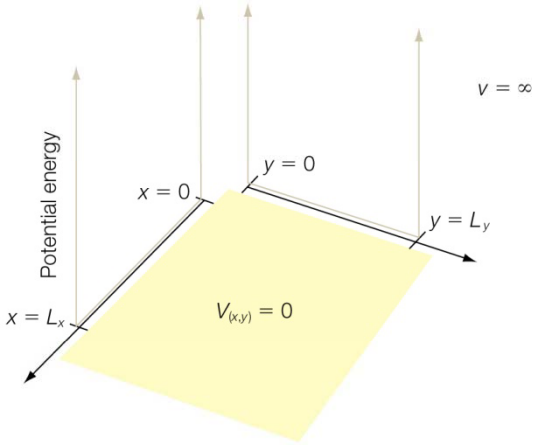
Figure: 14-01
Copyright © 2008 Pearson Prentice Hall, Inc.



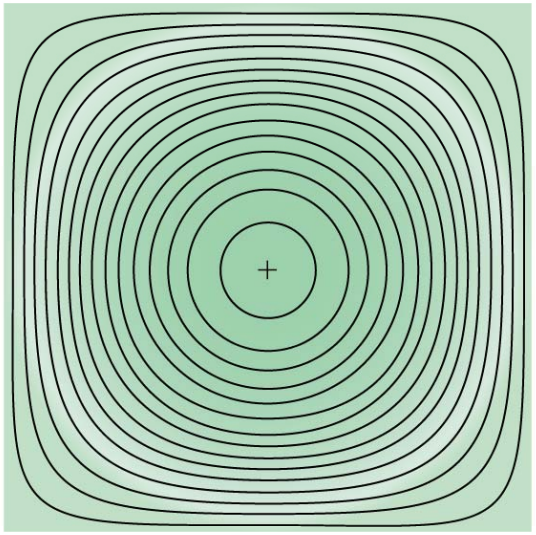


Y.T Lin's Presentation

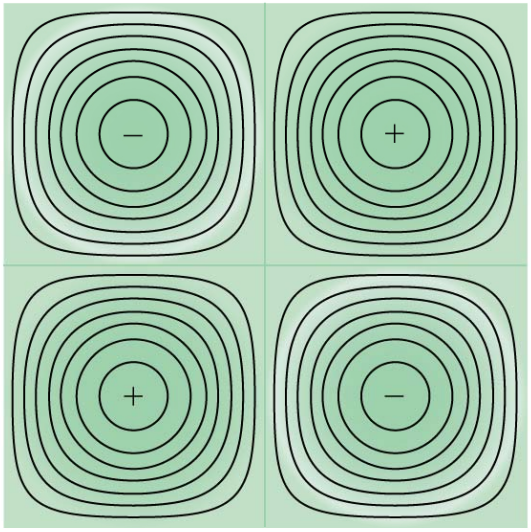
Two-Dimensional Box



$n_x = n_y = 1$



$n_x = n_y = 2$



Y.T Lin's Presentation

Three-Dimensional Box

Y.T Lin's Presentation

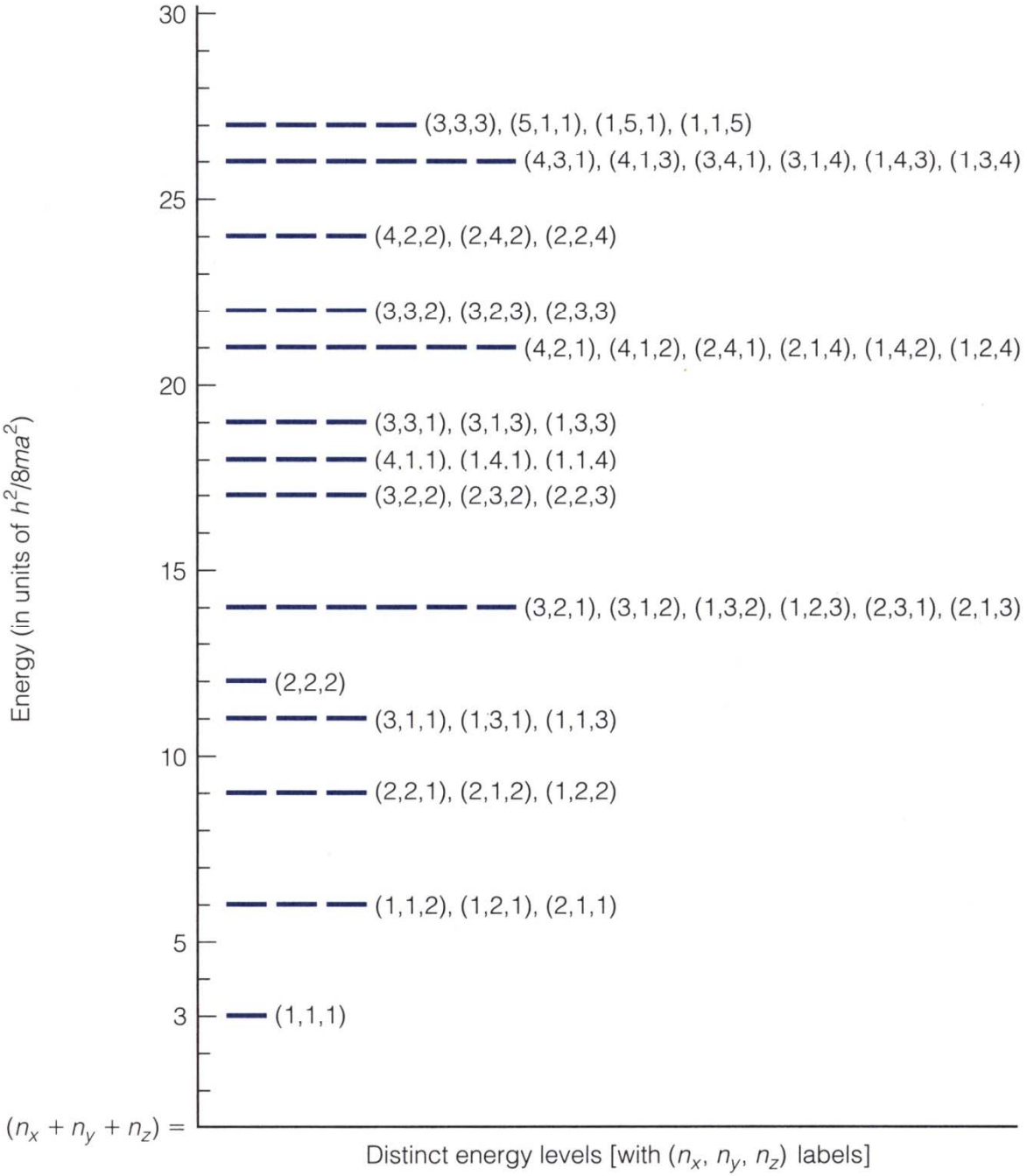


Figure 10.13 The energy levels of the 3-D particle-in-a-(cubical)-box. In this system, different wavefunctions can have the same energy. This is an example of degeneracy.

sentation

The Particle in the Finite Depth Box

Potential of wall

$$V = V_0$$

Y.T Lin's Presentation

The Particle in the Finite Depth Box

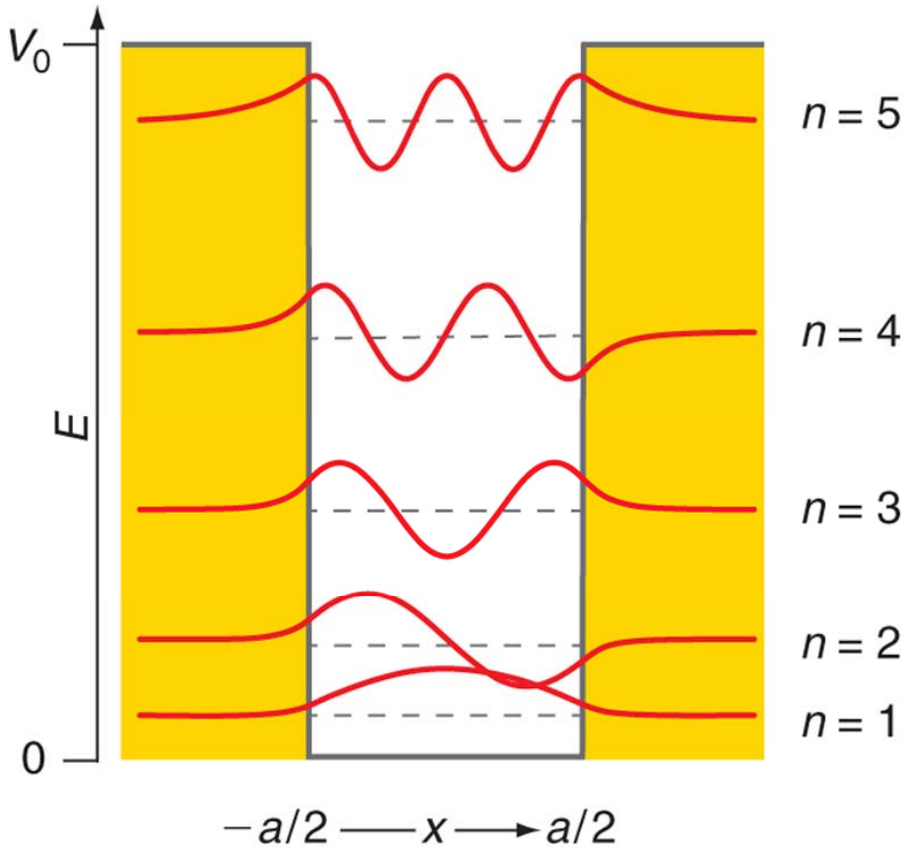


Figure: 14-04

Copyright © 2008 Pearson Prentice Hall, Inc.

Y. T. Lin's Presentation

Tunneling

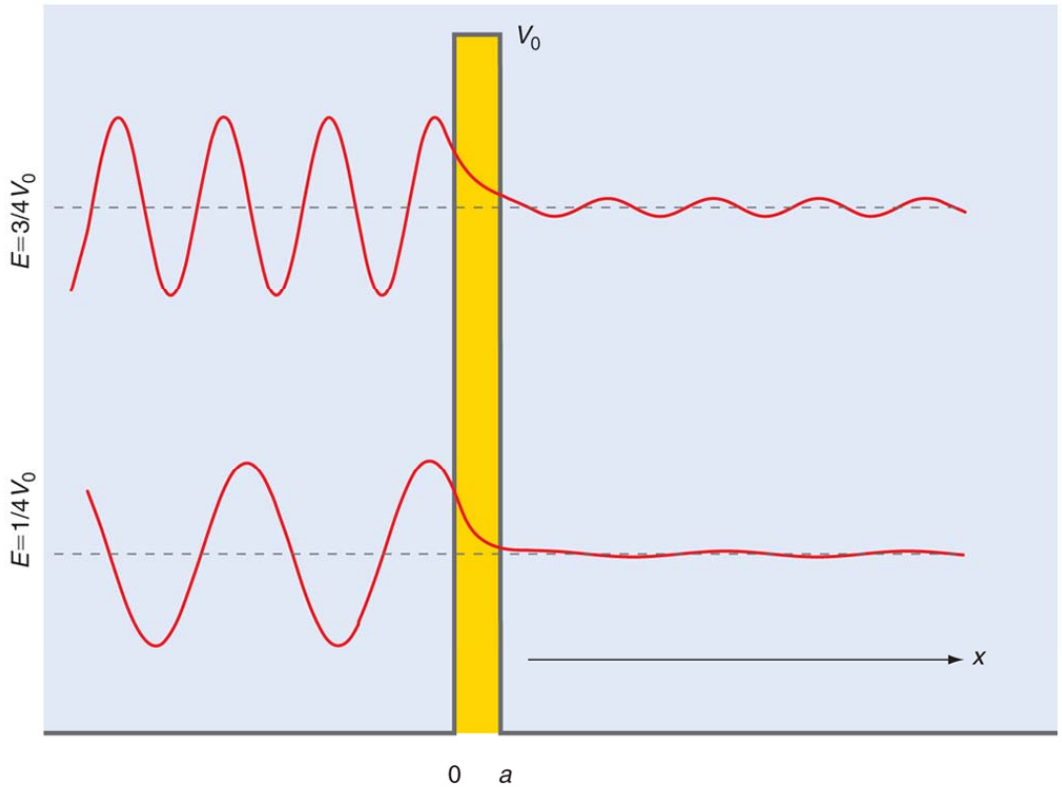
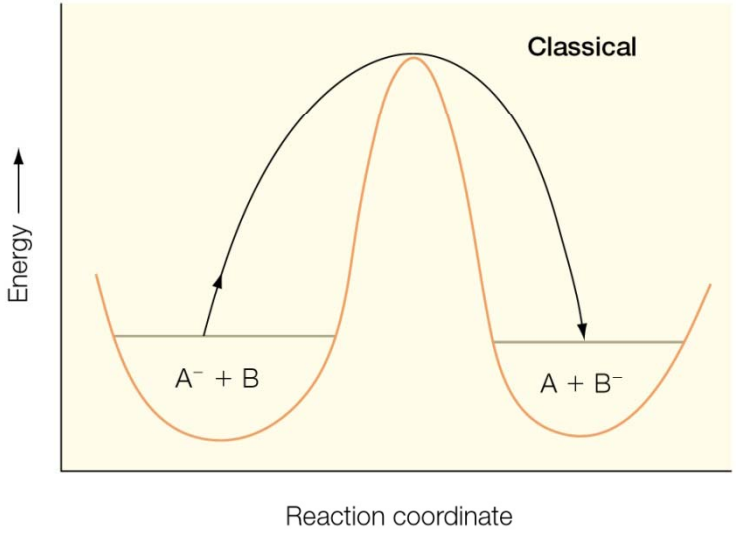


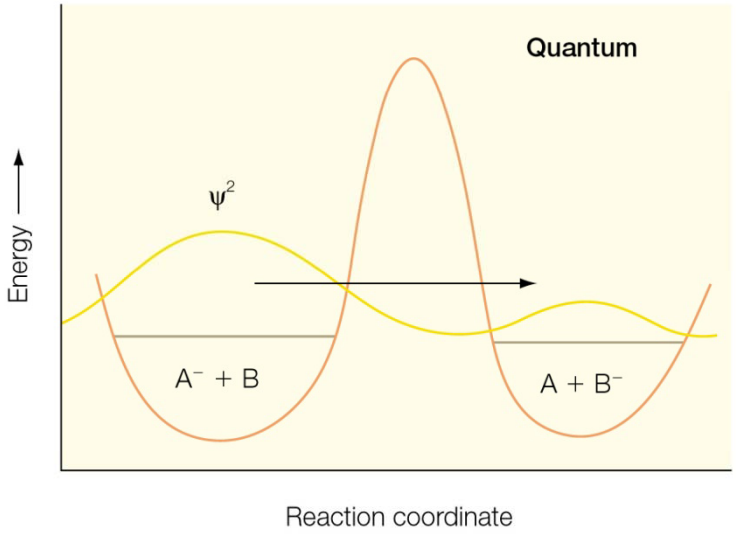
Figure: 14-09

Copyright © 2008 Pearson Prentice Hall, Inc.

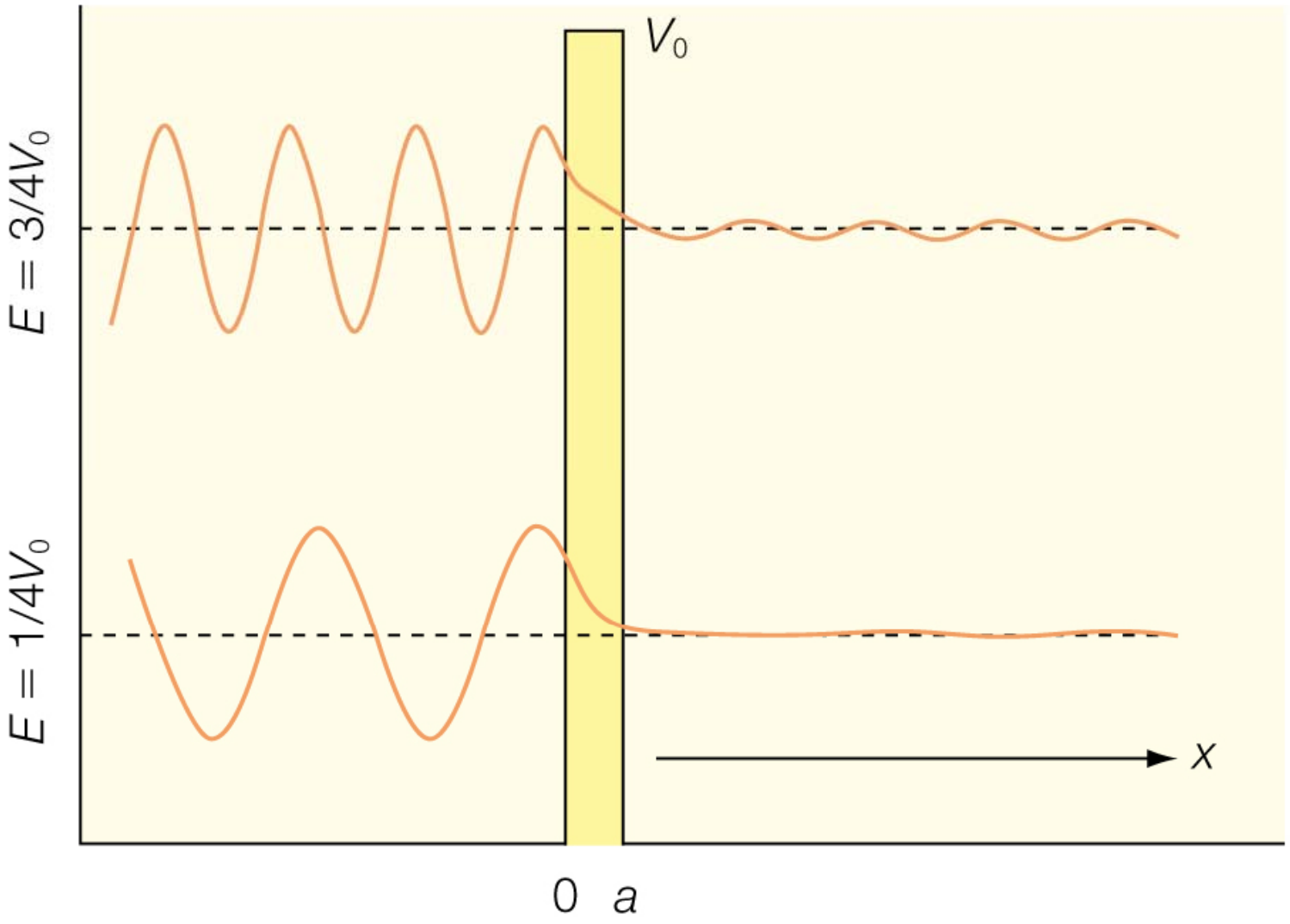
Y. J. Lin's Presentation

Tunneling



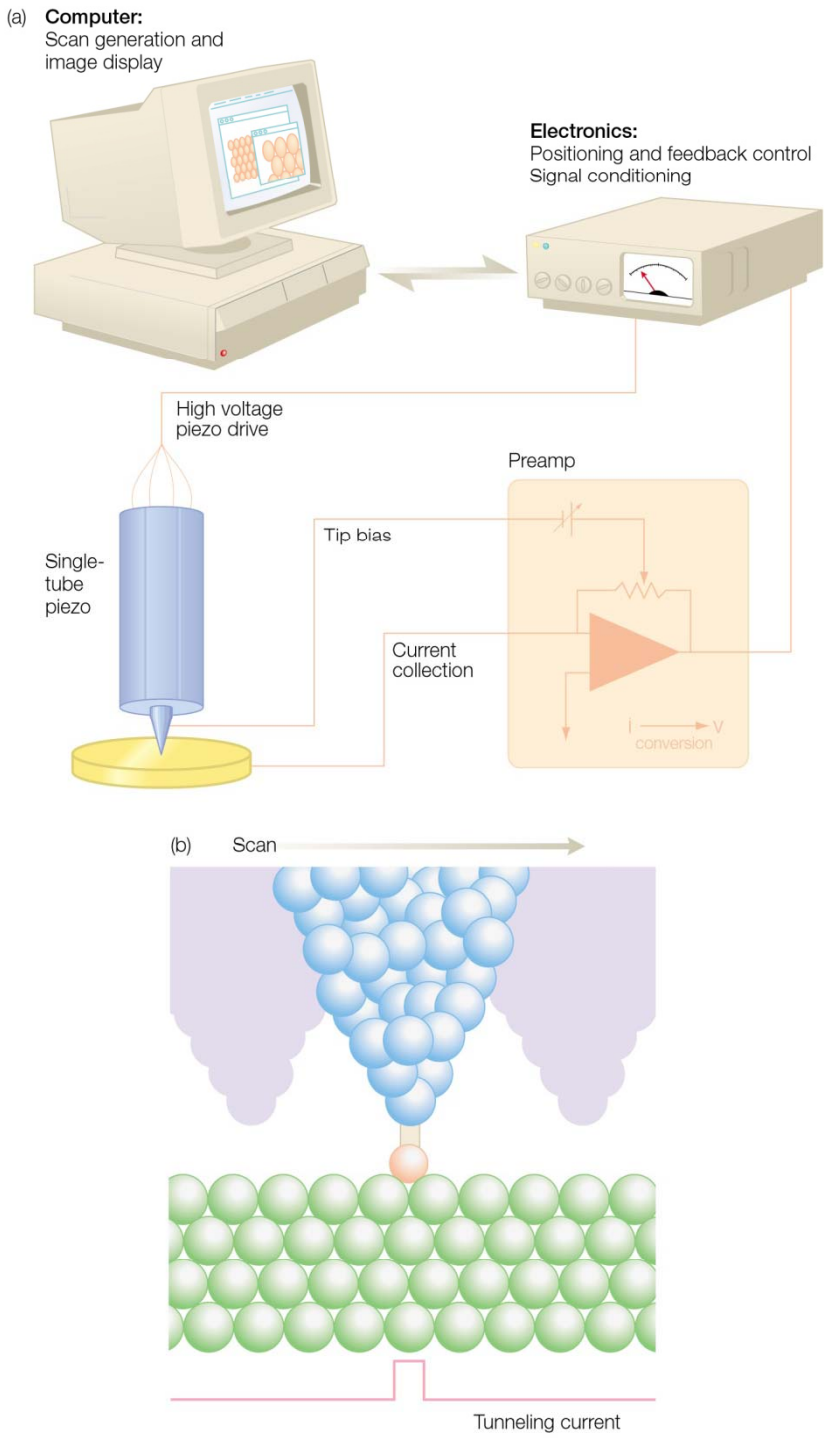


Y. Lin's Presentation



Y.T Lin's Presentation

Scanning Tunneling Microscopy (STM)



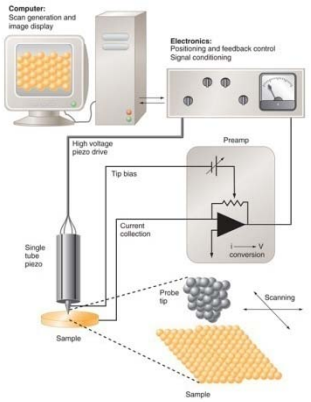


Figure: 14-11

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

Scanning Tunneling Microscopy

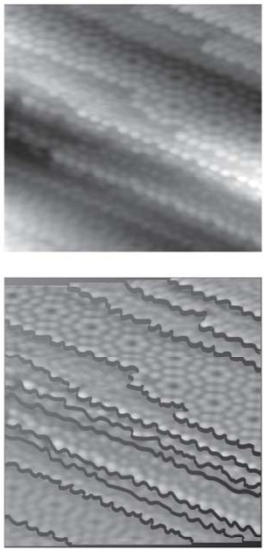


Figure: 14-12

Copyright © 2008 Pearson Prentice Hall, Inc.

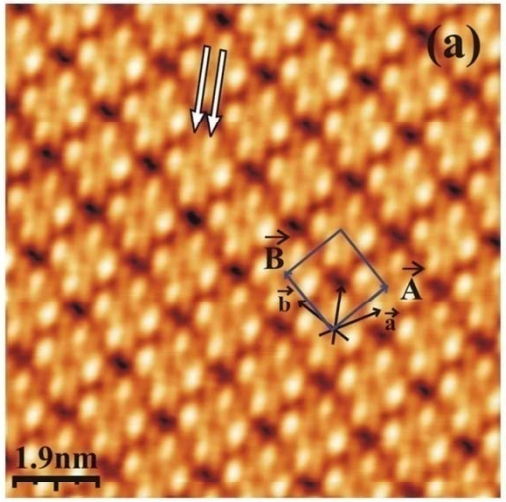


Figure: 14-13 TOP

Copyright © 2008 Pearson Prentice Hall, Inc.

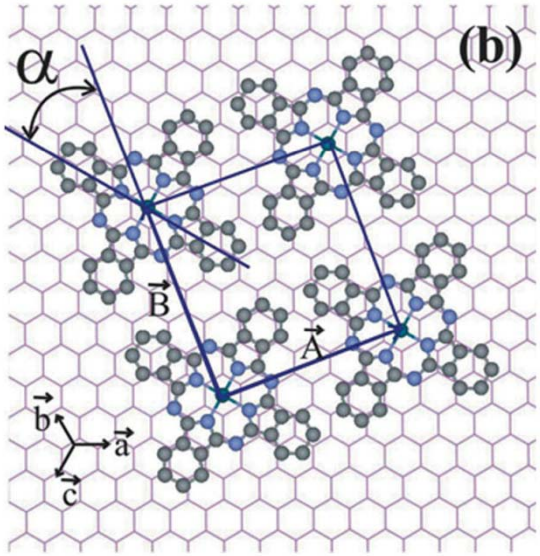


Figure: 14-13 BOTTOM

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T.Lin's Presentation

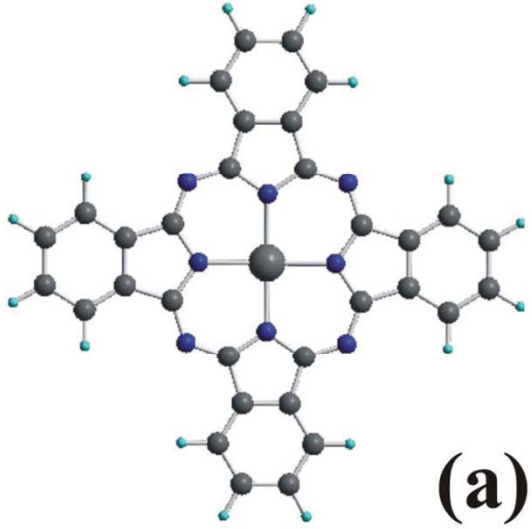


Figure: 14-14A

Copyright © 2008 Pearson Prentice Hall, Inc.

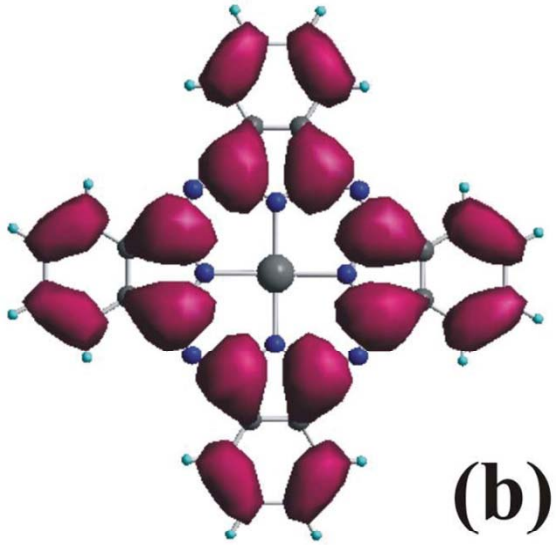


Figure: 14-14B

Copyright © 2008 Pearson Prentice Hall, Inc.

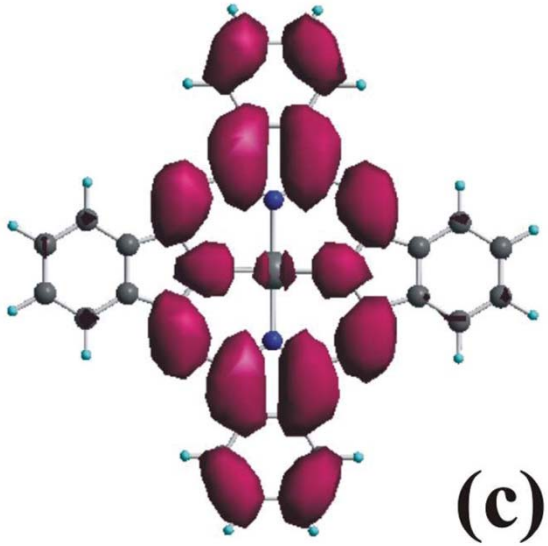


Figure: 14-14C

Copyright © 2008 Pearson Prentice Hall, Inc.

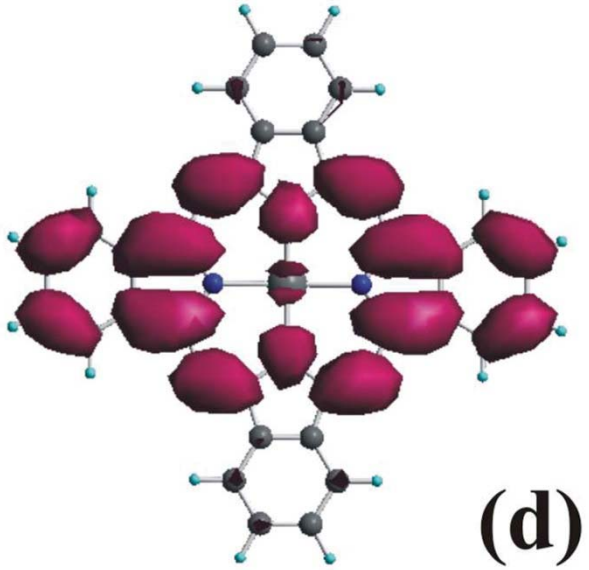


Figure: 14-14D

Copyright © 2008 Pearson Prentice Hall, Inc.

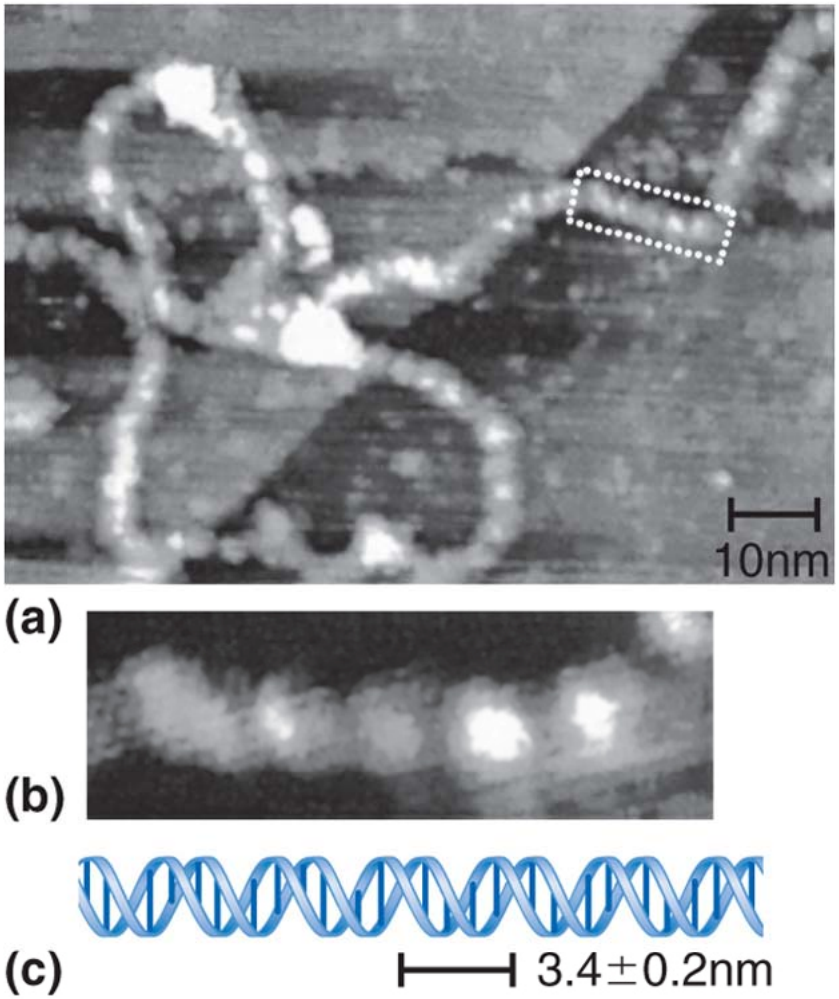


Figure: 14-15

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

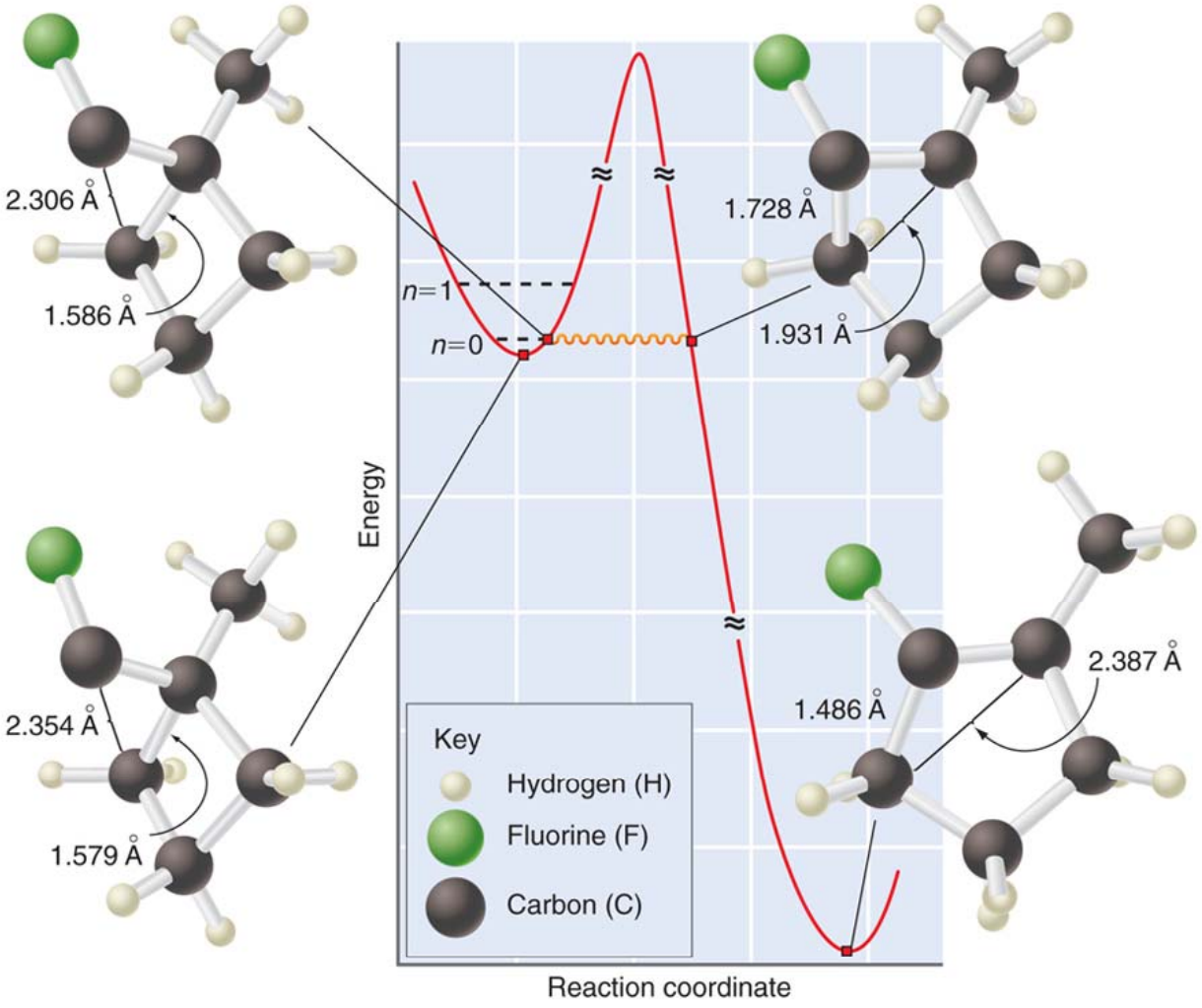
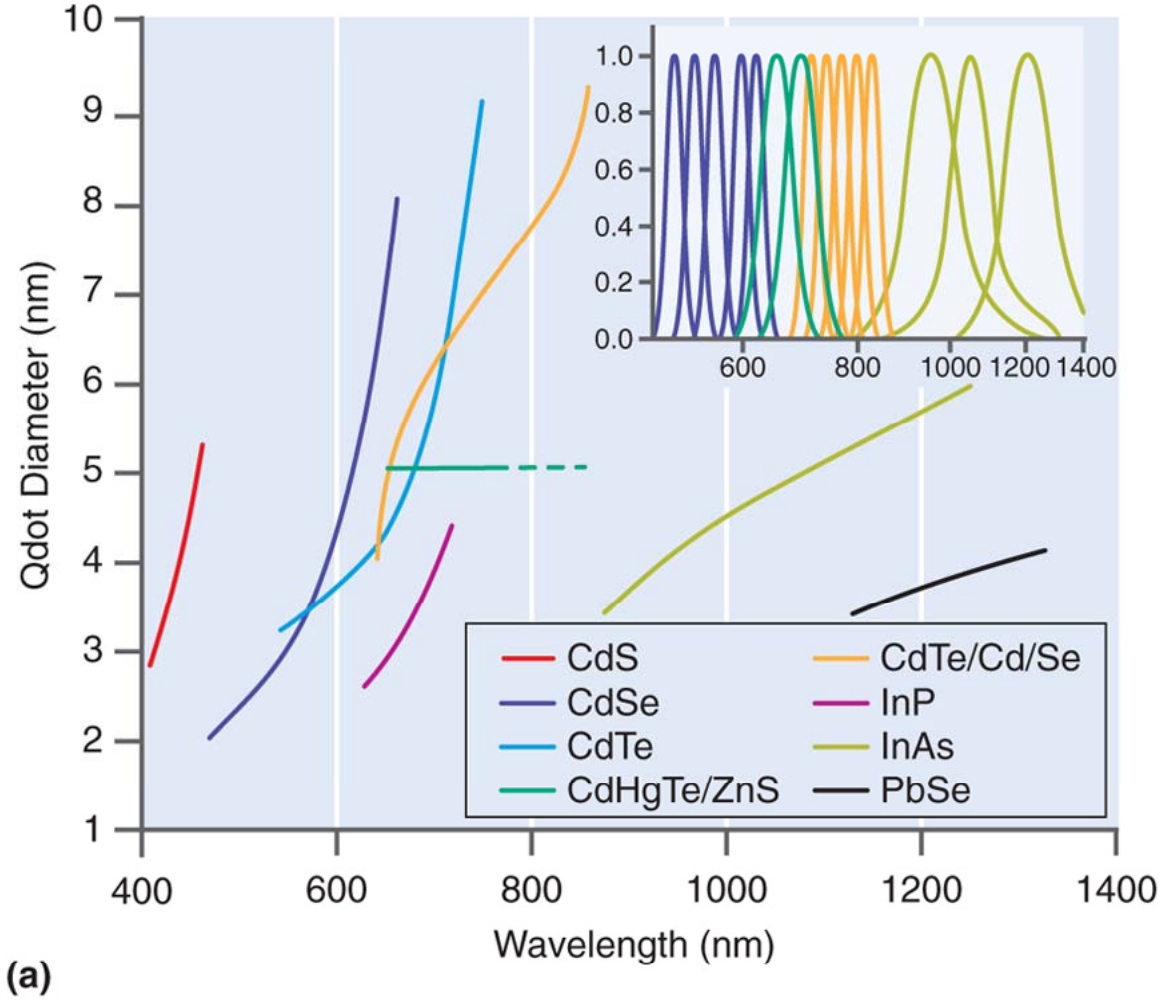


Figure: 14-16

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

Quantum dots

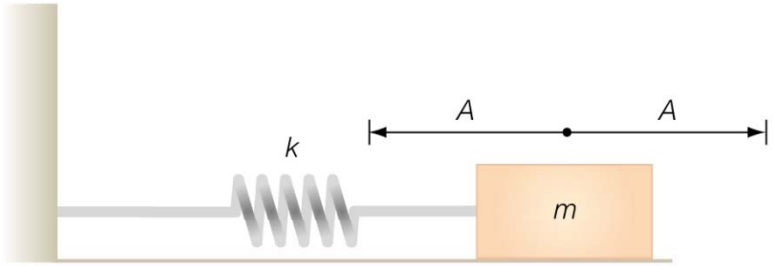


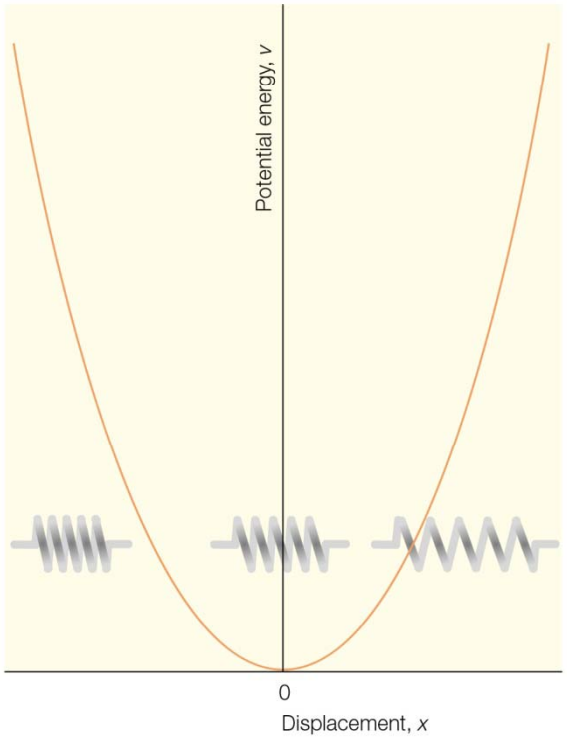
(a)

Figure: 14-17A

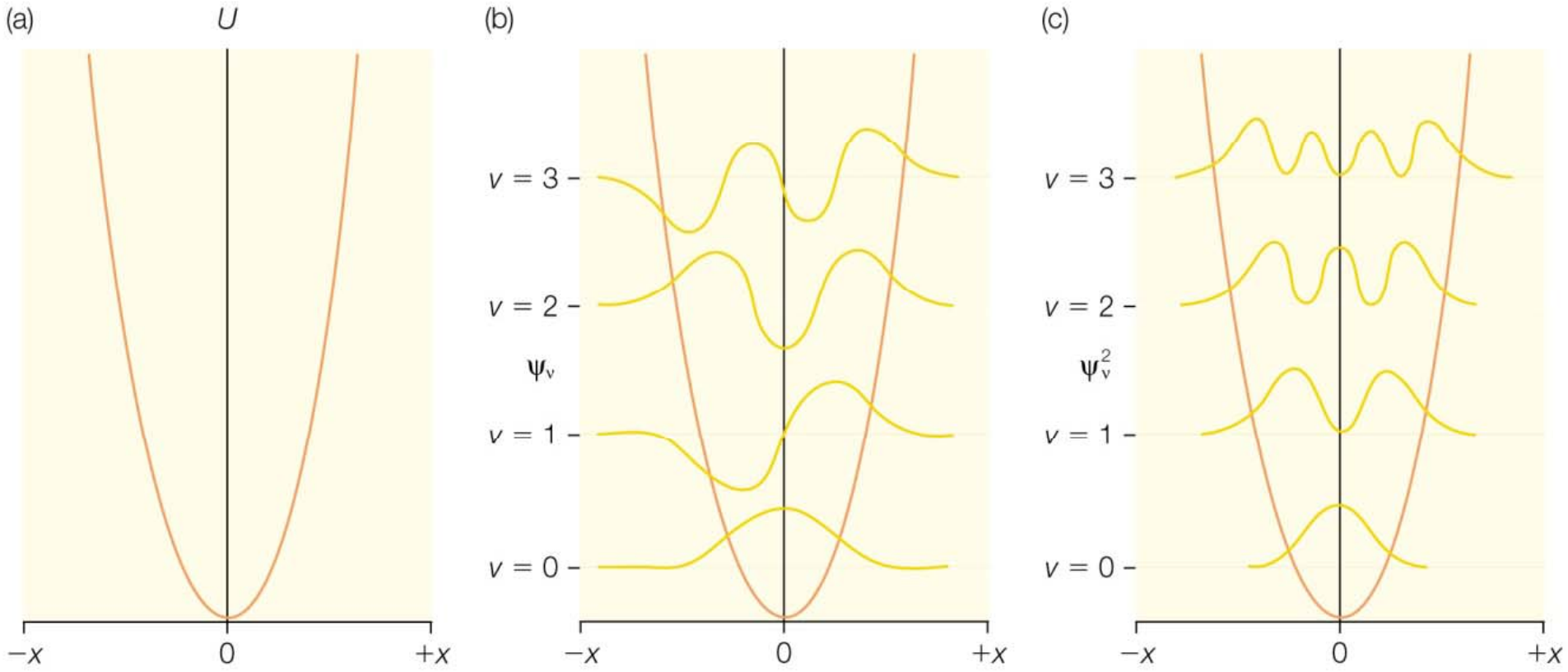
Copyright © 2008 Pearson Prentice Hall, Inc.

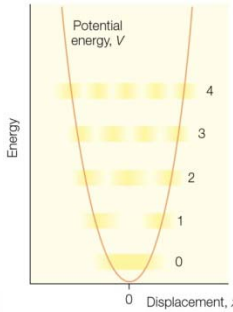
Harmonic Oscillator





Lin's Presentation





Y.T.Lin's Presentation

Rotational Energy Levels

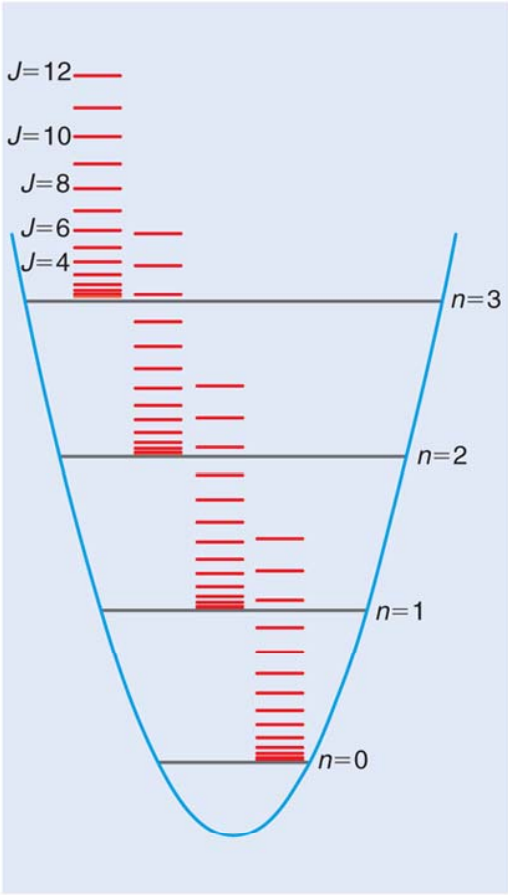
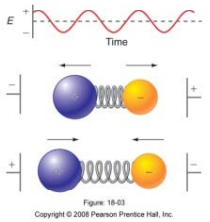


Figure: 18-08

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

CO_2



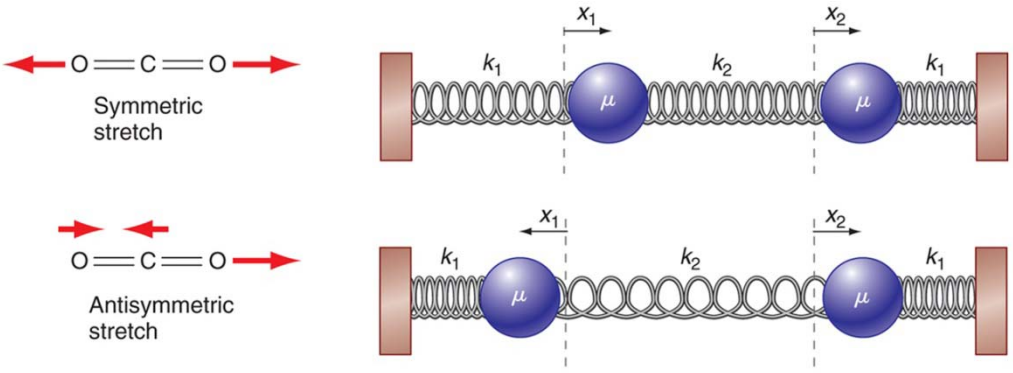
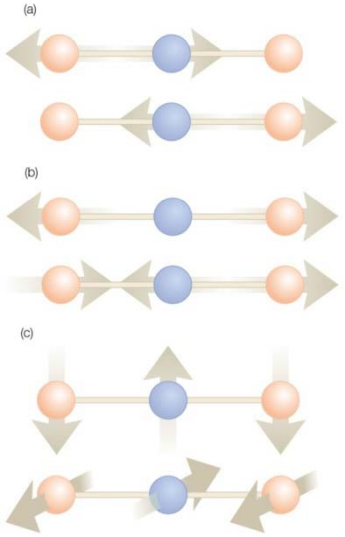


Figure: 18-11
Copyright © 2008 Pearson Prentice Hall, Inc.



Y.T Lin's Presentation

H_2O

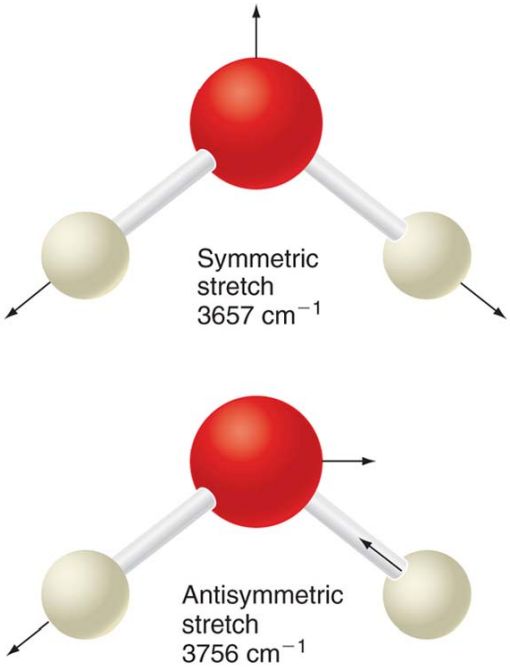


Figure: 18-12

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

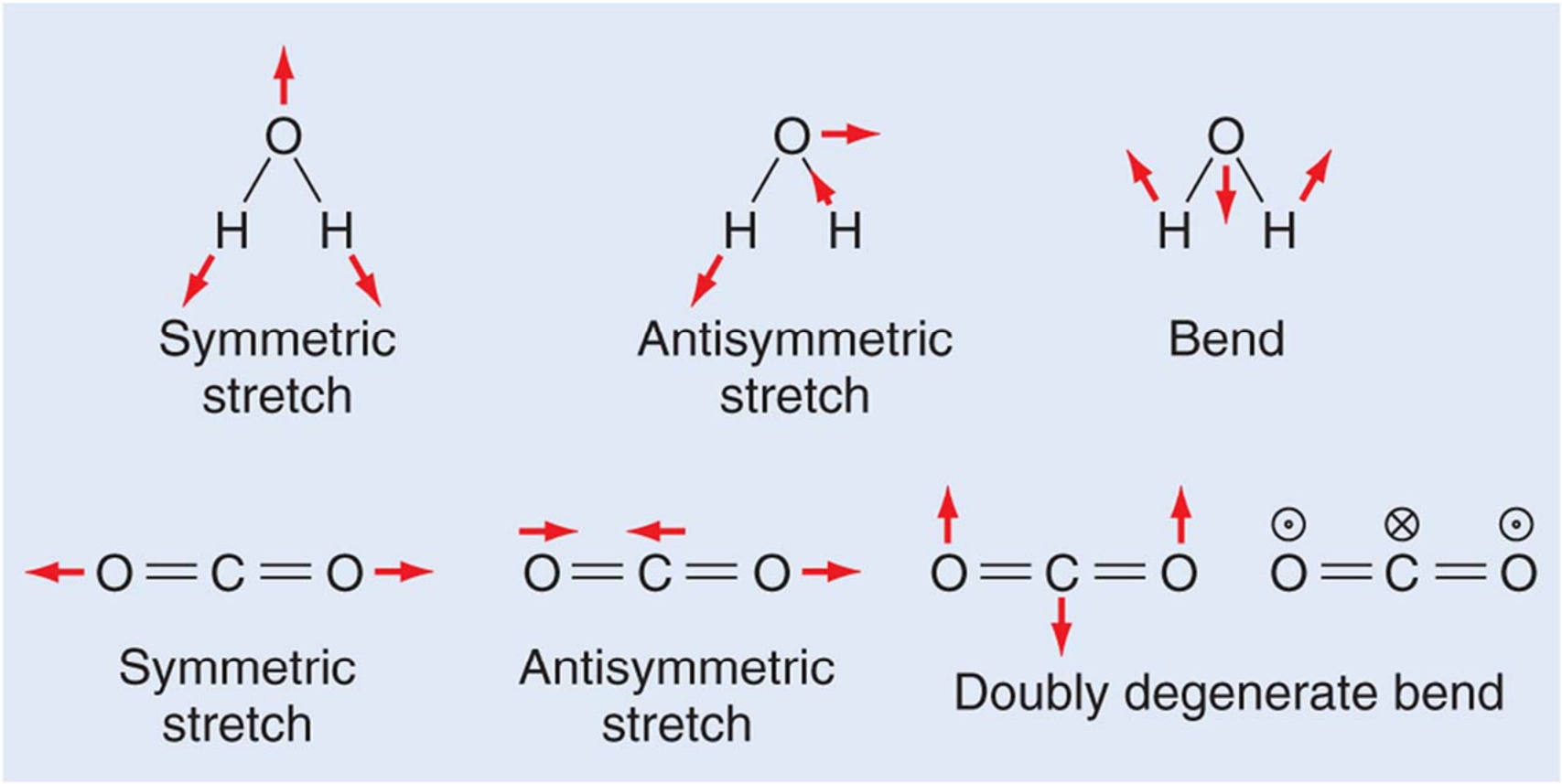


Figure: 18-14P

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

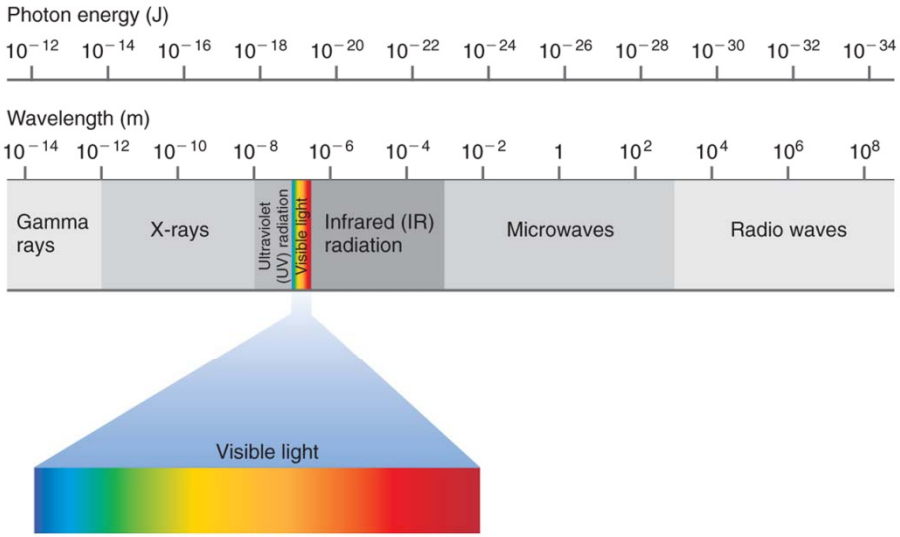


Figure: 18-01

Copyright © 2008 Pearson Prentice Hall, Inc.

TABLE 18.1 Important Spectroscopies and Their Spectral Range

Spectral Range	λ (nm)	$\nu/10^{14}$ (Hz)	$\tilde{\nu}$ $(cm)^{-1}$	Energy (kJ/mol)	Spectroscopy
Radio	$\sim 1 \times 10^{9}$	$\sim 10^{-6}$	~0.01	$\sim 10^{-8}$	NMR
Microwave	~100,000	$\sim 10^{-2}$	~100	$\sim 10^{-2}$	Rotational
Infrared	~1000	~3.0	~10,000	$\sim 10^{3}$	Vibrational
Visible (red)	~700	~4	~14,000	$\sim 10^{5}$	Electronic
Visible (blue)	~450	~6	~22,000	$\sim 3 \times 10^{5}$	Electronic
Ultraviolet	<300	>10	>30,000	$>5 \times 10^{5}$	Electronic

Table: 18_01

Copyright © 2008 Pearson Prentice Hall, Inc.

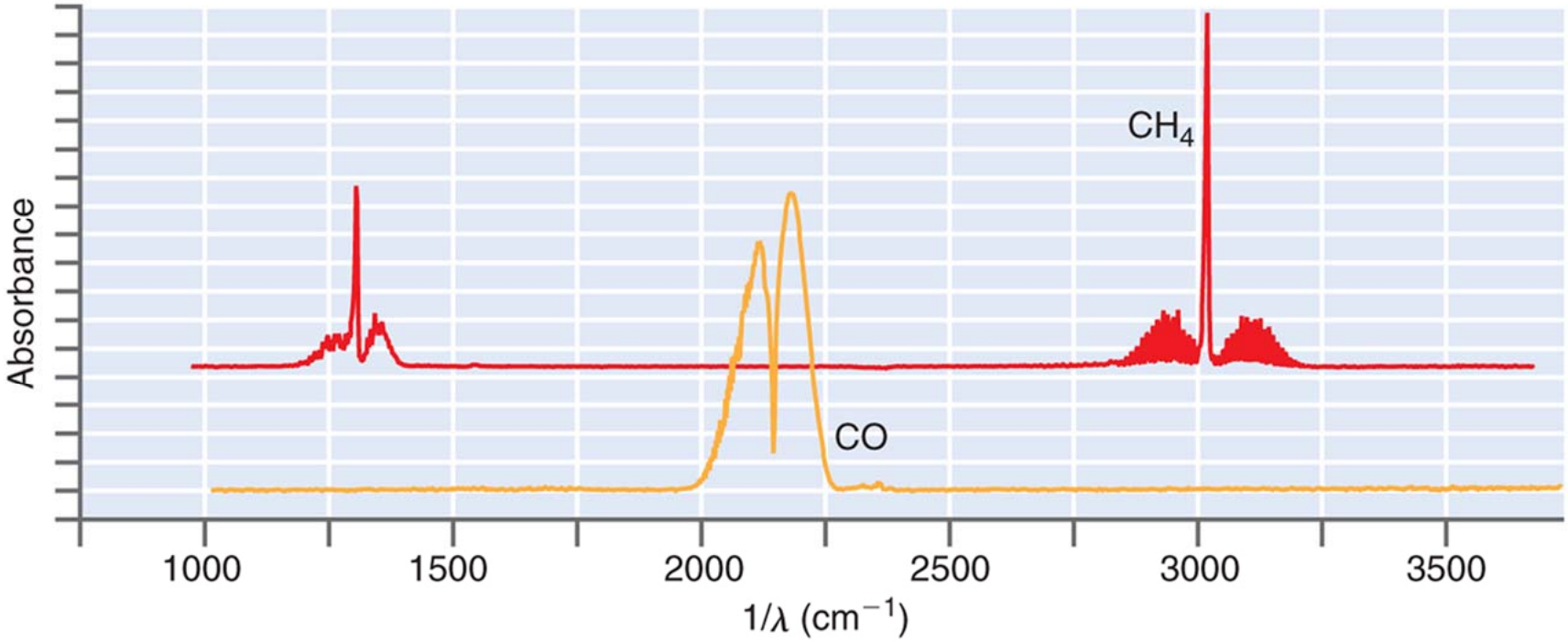
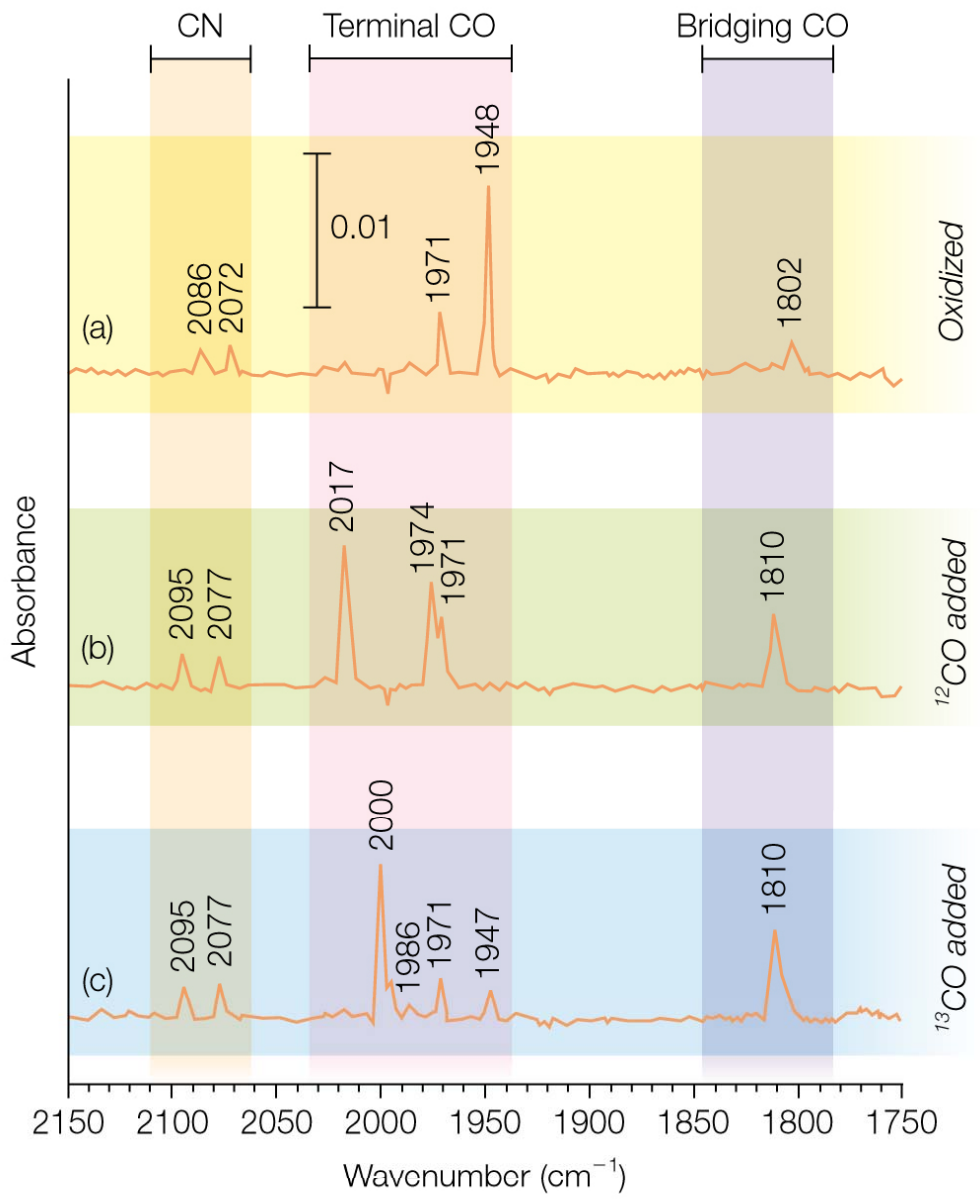


Figure: 18-10

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation



Y.T Lin's Presentation

TABLE 18.2 Vibrational State Populations for Selected Diatomic Molecules

Molecule	$\tilde{\nu}$ (cm^{-1})	ν (s^{-1})	N_1/N_0 for 300 K	N_1/N_0 for 1000 K
H—H	4400	1.32×10^{14}	6.88×10^{-10}	1.78×10^{-3}
H—F	4138	1.24×10^{14}	2.42×10^{-9}	2.60×10^{-3}
H—Br	2649	7.94×10^{13}	3.05×10^{-6}	2.21×10^{-2}
N≡N	2358	7.07×10^{13}	1.23×10^{-5}	3.36×10^{-2}
C≡O	2170	6.51×10^{13}	3.03×10^{-5}	4.41×10^{-2}
Br—Br	323	9.68×10^{12}	0.213	0.628

Table: 18_02

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

TABLE 18.4 Selected Group Frequencies

Group	Frequency (cm^{-1})	Group	Frequency (cm^{-1})
O—H stretch	3600	C═O stretch	1700
N—H stretch	3350	C═C stretch	1650
C—H stretch	2900	C—C stretch	1200
C—H bend	1400	C—Cl stretch	700

Table: 18_04

Copyright © 2008 Pearson Prentice Hall, Inc.

Y.T Lin's Presentation

End of Lecture

版權聲明:

本講義所使用之圖片皆由教科書出版商提供或是由網路上下載使用，同時內容安排及呈現順序為林盈廷老師上課解說，與其學生課後複習之用。禁止任何其他講述者及商業行為之未經授權的複製與使用。

Y.T Lin's Presentation

Slide Downloading

http://ytlab.kmu.edu.tw

Y.T Lin's Presentation