## Lecture Schedule

## Soft Material

## by Takehiko Mori

Electronic structure of solids. Band structure of solids, and the practical applications. I am ready to lecture the following items, from which some will be selected.

(1) Fundamentals of quantum mechanics
 (2) Atomic orbitals to molecular orbitals
 (3) Extension of molecular orbitals to solids
 (4) Free electron model
 (5) Fermi Dirac statistics
 (6) Tight-binding model
 (7) Energy band
 (8) Symmetry of crystals
 (9) Transport properties of solids
 (10) Physics of semiconductor devices
 (11) Magnetism
 (12) Electron correlation
 (13) Organic electronics

Quantum mechanics is derived from the following two theorems, which represent duality of wave and particle.

(1) A wave with frequency  $\nu$  acts as a particle with energy  $E = h \nu (= \hbar \omega)$ .

(1) Planck's photon  $\rightarrow$  Black body (2) Photoelectron

(2) A particle with momentum *p* acts as a wave with wavelength  $\lambda = h/p$  (de Broglie wave).

(1) Electron diffraction

(2) Line spectra of hydrogen atoms

This leads to the correspondence:

Particle (Energy, Momentum) Wave (Frequency, Wavelength)













General wave 
$$\phi(x,t) = \phi_0 e^{\frac{2\pi i \left(\frac{1}{h} - t^{n}\right)}}$$
 is differentiated by x,  
to give  

$$\frac{\lambda}{dx} = \frac{2\pi}{2\pi} \phi \frac{1}{b} \frac{1}{p} \rho \qquad \therefore \quad p \phi = \left(\frac{h}{t} \frac{\partial \phi}{\partial x}\right) (1)$$
Similarly differentiated by t, to give  

$$\frac{k = h^{k}}{d} = -2\pi i \phi \frac{1}{b} - \frac{1}{h} p \phi \qquad \therefore \quad E \phi = \left(h \frac{\partial \phi}{\partial x}\right) (2)$$
We can obtain p and E by differentiating  $\phi$  by x and t, and  
multiplying  $h(t)$  (or  $h)$ .  
We can replace p, E to differential operators:  

$$p \rightarrow \frac{h}{t} \frac{\partial}{\partial x} = E \phi$$
 has an eigenfunction  $\phi(x) = e^{hx}$ .  
The corresponding eigenvalue is  $E = \frac{h^{2} k^{2}}{2m} \frac{1}{dx} = p \phi$  at the same time.  
The corresponding eigenvalue is  $\left(\frac{h}{h} \frac{\lambda}{2m}\right)$  and is an eigenfunction  $\phi(x) = e^{hx}$ .  
The place wave  $\phi(x) = e^{hx}$  has nomentum  $p = \left(-hk^{-1}\right)$  and energy  $E = \left(\frac{h^{2} k^{2}}{2m}\right)$  and is an eigenfunction.  
 $\phi(x) = e^{-hx}$  has nomentum  $p(-hk^{-1})$  and energy  $E = \left(\frac{h^{2} k^{2}}{2m}\right)$  and is an eigenfunction.  
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 $\psi(x) = e^{-hx}$  has nomentum  $\phi(x) =$ 





Problem				
When <i>l</i> =	D, show $R(r)$	$=e^{-\tilde{G}}$ is a s	olution of	
$\frac{d^2R}{dr^2} +$	$\frac{2}{r}\frac{dR}{dr} + \left[\frac{2m}{\hbar^2}\right](E)$	$+\frac{Ze^2}{4\pi\varepsilon_0 r})-\frac{l(a)}{4\pi\varepsilon_0 r}$	$\frac{l+1)}{r^2}]R=0$	
and obta	in $\zeta$ and $E$ .			
Solution $\mathbf{F}$	Put $R(r) = e^{-\zeta r}$ $\frac{2\zeta}{r} + [\frac{2m}{\hbar^2}(E +$	into the above $\frac{Ze^2}{4\pi\varepsilon_0 r}$ ] = 0	ove equation	, to give,
The te	rm of 1/ <i>r</i> is 0.1	leading to 7	$=$ $Zme^2$	<u>Z</u>
		,	$4\pi\hbar^2\varepsilon_0$	$a_0$ Bohr radius
SO	$E = -\frac{\hbar^2}{2}\zeta^2 =$	$=-\frac{Z^2me^4}{22 + 2} =$	$=-Z^2Rhc$	0.529 Å
	2m	$32\pi^2 \varepsilon_0^2 h^2$	Rydber	g constant
	1 6			13.6 eV

Laguerre polynomials guarantees orthogonality of 1s, 2s, 3s orbitals, but complicates molecular orbital calculations.

They are not important in the usual distances of chemical bonds, so that we neglect them to

 $\phi \propto e^{-\varphi} Y_{lm}(\theta, \phi)$  Slater orbital

 $\zeta = \frac{Z}{a_0}$  increases as Z increases (and the orbital size decreases).

The "outer most electron" is screened by other "Z-1" electrons from the Z+ nuclear charge.

If the screening is complete, it feels Z = 1 charge, but the screening is incomplete, because the focused electron is not always out of other electrons, so that the effective  $Z^*$  is  $1 < Z^* < Z$ .

Accordingly  $\zeta$  changes as shown in the next page.

C < N < 0













(large )ionization energy, and (deep) atomic orbital. Going right leads to electronically negative.











1	$\alpha - E$	β	0	0	0	$\beta$	
6 2	β	$\dot{\alpha} - E$	β	0	0	0	
5 3	0	β	$\alpha - E$	β	0	0	
4	0	0	β	$\alpha - E$	β	0 = 0	
	0	0	0	β	$\alpha - E$	β	
	β	0	0	0	β	$\alpha - E$	
$\alpha - 2\beta - \beta$	2( a	2+2β)	)+4(a	( +β)	—6α	$= \left[ 8 \beta \right]$	
αρ	Compared with three doublebonds						
$\alpha + \beta$	$3 \times 2\beta = 6\beta$ , there is $2\beta$ energy gain						
$\chi + 2\beta$	4n+2	memb	on ene	ergy). ng de	elocali	zation aromatic	

