1 (a) $L(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$

$E = \frac{\hbar^2\vec{k}^2}{2m} = \frac{\hbar^2}{2m} \cdot 3 \cdot \frac{\pi^2}{a^2} = \frac{3\hbar^2\pi^2}{2ma^2}$

2. $\Delta x \cdot \Delta k \geq \frac{1}{2}$

$\Delta k < \frac{2\pi}{a} \cdot \frac{1}{1000}$

$\therefore \Delta x \geq \frac{1}{2\Delta k} = \frac{1}{2} \cdot \frac{1000}{2\pi} = \frac{250a}{\pi}$

3. $E = -\frac{13.6ev}{n^2}$

红线: $\Delta E = 13.6ev(\frac{1}{4} - \frac{1}{9}) = \frac{hc}{\lambda_{红}}$

$\therefore \lambda_{红} = 656.39nm$

蓝线: $\Delta E = 13.6ev(\frac{1}{2^2} - \frac{1}{4^2}) = \frac{hc}{\lambda_{蓝}}$

$\therefore \lambda_{蓝} = 486.21nm$

紫线: $\Delta E = 13.6ev(\frac{1}{2^2} - \frac{1}{5^2}) = \frac{hc}{\lambda_{紫}}$

$\therefore \lambda_{紫} = 434.12nm$

4. 1s: $E_1 = \frac{-13.6ev}{1^2} \cdot 2$

2s, 2p: $E_2 = \frac{-13.6ev}{2^2} \cdot 2$

H_N晶体: N个H 1S轨道 = N个能级

对于 H, Li, Na, $E = E_{1S} - 2T\cos ka$

$k = \frac{2m\pi}{Na}$ 晶格常数 Na > Li > H

则能带展宽 Na > Li > H

而 m^* 反比于能带宽度

则有效质量 H > Li > Na

则 Na_N 的能带展宽大, H_N 的能带有效质量较大

6. $Eq = ma$

$\therefore Ee = m^* \frac{dv}{dt}$

$v = \frac{\hbar k}{m^*}$

$\therefore Ee = \hbar \frac{dk}{dt}$

$\therefore dk = \frac{Ee}{\hbar} dt$

$\therefore \Delta t = \frac{\hbar}{Ee} \cdot \frac{\pi}{a}$

$\therefore \Delta t = \frac{\pi\hbar}{aeE}$

$\therefore$ 周期 $\Delta t = \frac{\pi\hbar}{aeE}$

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7. 晶格：

$E(\vec{k}) = \int \psi(x,t)^* \hat{E} \psi(x,t) dV$

$= \sum_R e^{i\vec{k}\cdot\vec{R}} \int \psi_{1s}(\vec{x})^* \hat{H} \psi_{1s}(x-\vec{R}) dV$

$= E_{1s} - 2T(\cos k_x a + \cos k_y a)$

能带底 $= E_{1s} - 2T(2 - \frac{1}{2}(k_x a)^2 - \frac{1}{2}(k_y a)^2)$

$= E_{1s} - 4T + T(k_x a)^2 + T(k_y a)^2 + O(k^4)$

~~$g(E) = \frac{dz}{dE} = \frac{(Na)^2}{(2\pi)^2} \cdot$~~

~~$dz =$~~

近似认为 $\Delta k = \frac{2\pi}{Na}$ $\therefore \frac{dz}{d\vec{k}^2} = \left(\frac{1}{\Delta k}\right)^2 = \left(\frac{Na}{2\pi}\right)^2$

~~$dz = \frac{2\pi k dk}{(\frac{2\pi}{Na})^2}$~~ 考虑电子自旋：

$dz = \left(\frac{Na}{2\pi}\right)^2 \cdot 4\pi d\vec{k}^2$

$\therefore dz = 2\left(\frac{Na}{2\pi}\right)^2 \cdot 2\pi k dk = \frac{(Na)^2}{\pi} k \frac{dk}{dE} \cdot dE$

$E = \frac{\hbar^2 k^2}{2m^*} + C$ $\therefore \frac{dk}{dE} = \frac{2m^*}{\hbar^2 \cdot 2k} dE$

$\therefore dz = \frac{(Na)^2}{\pi} k \cdot \frac{m^*}{\hbar^2 \cdot k} \cdot dE = \frac{m^*(Na)^2}{\pi\hbar^2}$

$\therefore g(E) = \frac{dz}{dz} = \frac{(Na)^2 m^*}{\pi\hbar^2}$

8. ① ~~$\frac{2\pi}{a}$~~ $K = \frac{2\pi}{a}$

$\therefore K^3 = \left(\frac{2\pi}{a}\right)^3 = 1.98 \times 10^{30}\ m^3$

② 能带表达式：

$E = \int \psi^* \hat{E} \psi dV = E_{1s} - 2T(\cos k_x a + \cos k_y a + \cos k_z a)$

$\therefore E = E_{1s} - 2T(\cos k_x a + \cos k_y a + \cos k_z a)$

$a = 0.5nm$, $T = 1eV$

③ 等能面：$\cos k_x a = 1 - \frac{1}{2} a^2 k_x^2$

$\therefore E = E_{1s} - 6T + T[(k_x a)^2 + (k_y a)^2 + (k_z a)^2]$

$Ta^2 = \frac{\hbar^2}{2m^*}$

$\therefore m^* = \frac{\hbar^2}{2Ta^2} = 1.39 \times 10^{-31}\ kg$

能带顶：~~$\cos k_x a = 1 +$~~

$E = E_{1s} + 6T - Ta^2[(k_x - \frac{\pi}{a})^2 + (k_y - \frac{\pi}{a})^2 + (k_z - \frac{\pi}{a})^2]$

$\therefore m_p^* = \frac{\hbar^2}{2Ta^2} = -m^*$

④ $\Delta x \Delta k \geq \frac{1}{2}$

$\Delta k < \frac{2\pi}{a} \cdot \frac{1}{1000}$

$\therefore \Delta x \geq \frac{1000a}{4\pi} = 3.98 \times 10^{-8}\ m$

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