SOLID STATE PHYSICS - TEST N°2 25/05/20

Part I: Just a little theory

① Effective mass of the charge carriers proportional to the effective potential ⇒ the highest the interaction with nuclei (positive ions), the highest is the mass, so the lowest will be the mobility.

② Dispersion relation: $E_k = \frac{\hbar^2}{2m_{eff}} k^2$

with $m_{eff} = \frac{m^2 a^2 |V|}{\hbar^2}$

③ $\frac{d^2E_k}{dk^2} = \frac{\hbar^2}{m_{eff}} \Leftrightarrow$ $\boxed{m_{eff} = \frac{\hbar^2}{d^2E_k/dk^2}}$

④ The highest is the local curvature $\left(\frac{d^2E}{dk^2}\right)$ the lowest the effective mass. In point C, the curvature is lower and effective mass higher.

⑤ Lowest mass ⇒ higher mobility.
(point A) (point A)

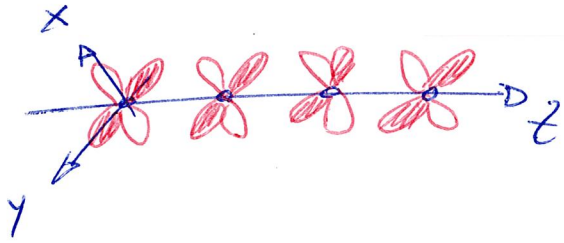
⑥ Band gap between A and B: $\boxed{\Delta E = 0{,}7\ eV}$

(7) The highest the curvature, the lowest the DOS. DOS is high at point C. [2]

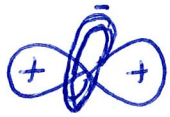
Part II: A chemist view ---

(1) d_{z^2} large overlap (σ) ⇒ broad band (high dispersion)

$d_{x^2-y^2}$, d_{xy} small overlap (δ) ⇒ narrow band (small dispersion)



(2) d_{z^2} Bonding state for $k = 0$
Anti-bonding $k = \frac{\pi}{a}$



p_z Anti-bonding state for $k = 0$
Bonding state for $k = \frac{\pi}{a}$

(3) N states with N the number of atoms (groups)

$$k = n\frac{2\pi}{L} = n\frac{2\pi}{Na}$$

- full length of 1st Brillouin zone = $\frac{2\pi}{a}$
- number of states $\frac{2\pi}{a} / \frac{2\pi}{Na} = N$ or $2N$ spins

④ The lowest the distance, the broadest the band. [3]

Part III. Few more questions

① Cours - Bands and conductivity.

② The highest is the dispersion, the highest is the overlap between orbitals = the highest the coupling and mobility of electrons = the highest the conductivity. [CHEMIST]

Current density $\vec{j} = -e \int \frac{d\vec{k}}{4\pi^3} \cdot \frac{dE(\vec{k})}{d\vec{k}}$

The highest the dispersion, the highest the integral (sum) over $d\vec{k}$ of $\frac{dE(\vec{k})}{d\vec{k}}$ = the highest the conductivity. [PHYSICIST]

③ METAL.