

2016 / 9 / 23

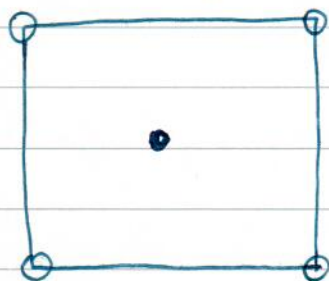
(2)

(1)

$$H_{\text{bilayer}} = 2t_0 (\cos k_x + \cos k_y) 6_0 \tau_0 \nu_0$$

$$+ 4t' \cos \frac{k_x}{2} \cos \frac{k_y}{2} 6_0 \tau_x \nu_0$$

$$+ 4t_{\text{id}} \cos \frac{k_x}{2} \cos \frac{k_y}{2} 6_z \tau_y \nu_0$$

 d_{xy} d_{yz} d_{zx}

$$|J_z = \frac{1}{2}\rangle = \frac{1}{\sqrt{3}} \left(|d_{yz} \downarrow\rangle + i |d_{zx} \downarrow\rangle + |d_{xy} \uparrow\rangle \right)$$

$$|J_z = -\frac{1}{2}\rangle = \frac{1}{\sqrt{3}} \left(|d_{yz} \uparrow\rangle - i |d_{zx} \uparrow\rangle - |d_{xy} \downarrow\rangle \right)$$

2016/9/23 (2) (3). (2)

Rotation & Slater-Koster parameters.

$$\text{p-orbital at } \theta = \text{p-orbital at } 0 \cos \theta + \text{p-orbital at } 90^\circ \sin \theta$$

$$\langle a | H | b \rangle = 0 \sin \theta + V_{pp\sigma} \cos \theta.$$

$$\text{d-orbital at } \theta = \text{d-orbital at } 0 \cos \theta + \text{d-orbital at } 90^\circ \sin \theta$$

$$= V_{sp\sigma} \cos \theta + 0 \sin \theta$$

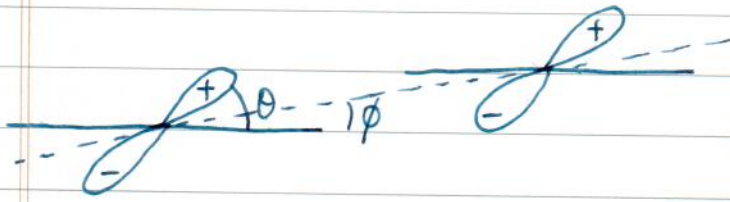
$$\text{p-orbital}^2 \text{ at } \theta = \text{p-orbital}^2 \text{ at } 0 \cos^2 \theta + \text{p-orbital}^2 \text{ at } 90^\circ \sin^2 \theta$$

$$= V_{pp\sigma} \cos^2 \theta + V_{pp\pi} \sin^2 \theta.$$

$$\text{p-orbital}^2 \text{ at } \theta = \text{p-orbital}^2 \text{ at } 0 \cos^2 \theta - \text{p-orbital}^2 \text{ at } 90^\circ \sin^2 \theta$$

$$= V_{pp\sigma} \cos^2 \theta - V_{pp\pi} \sin^2 \theta$$

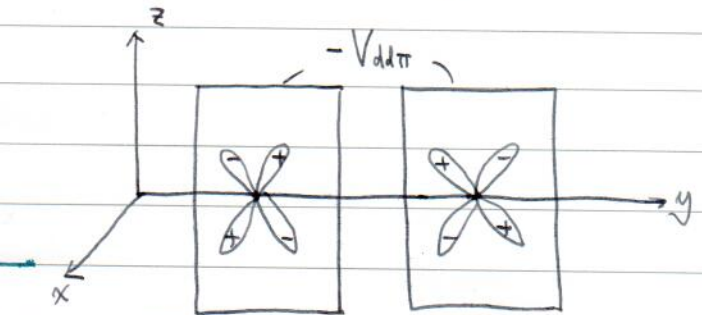
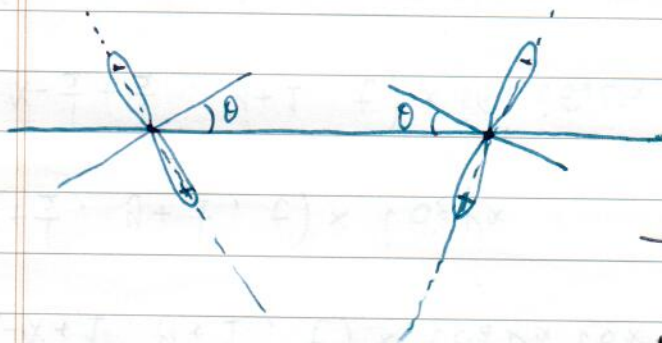
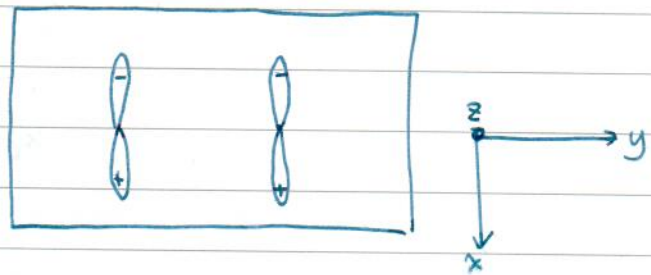
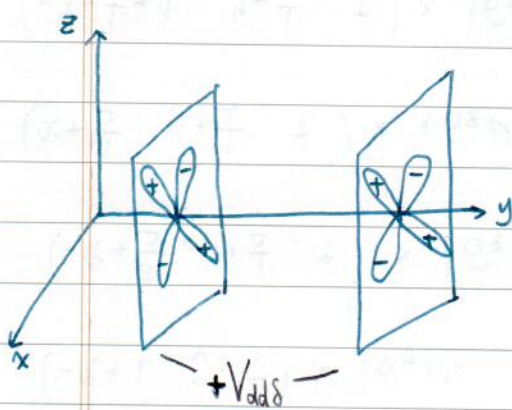
2016 / 9 / 23 (2) (3)



$$= V_{pp6} \cos(\theta - \phi) \cos(\theta + \phi) - V_{pp\pi} \sin(\theta - \phi) \sin(\theta + \phi)$$

check! $\theta = 0$, $\phi = \frac{\pi}{2}$ should be $V_{pp\pi}$

$$: V_{pp6} \cos\left(-\frac{\pi}{2}\right) \cos\frac{\pi}{2} - V_{pp\pi} \sin\left(-\frac{\pi}{2}\right) \sin\frac{\pi}{2} = V_{pp\pi}$$



$$-V_{dd\pi} \cos^2\theta - V_{dd6} \sin^2\theta$$

$$+V_{dd6} \cos^2\theta - V_{dd\pi} \sin^2\theta$$