1. LCAO untuk molekul/ion hidrogen H2+

$$|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$$

$$H|\psi\rangle = E|\psi\rangle$$

- Dikalikan dengan $\langle\psi_1|$ dari kiri

$$\langle\psi_1|H|\psi\rangle = \langle\psi_1|E|\psi\rangle$$
$$\langle\psi_1|H\ \{c_1|\psi_1\rangle + c_2|\psi_2\rangle\} = \langle\psi_1|E\ \{c_1|\psi_1\rangle + c_2|\psi_2\rangle\}$$
$$\langle\psi_1|Hc_1|\psi_1\rangle + \langle\psi_1|Hc_2|\psi_2\rangle = \langle\psi_1|Ec_1|\psi_1\rangle + \langle\psi_1|Ec_2|\psi_2\rangle$$
$$c_1\langle\psi_1|H|\psi_1\rangle + c_2\langle\psi_1|H|\psi_2\rangle = c_1\langle\psi_1|E|\psi_1\rangle + c_2\langle\psi_1|E|\psi_2\rangle$$
$$c_1\langle\psi_1|H|\psi_1\rangle + c_2\langle\psi_1|H|\psi_2\rangle = c_1E\langle\psi_1|\psi_1\rangle + c_2E\langle\psi_1|\psi_2\rangle$$
$$c_1\langle\psi_1|H|\psi_1\rangle + c_2\langle\psi_1|H|\psi_2\rangle = c_1E + c_2E\langle\psi_1|\psi_2\rangle$$

- Dikalikan dengan $\langle\psi_2|$ dari kiri

$$\langle\psi_2|H|\psi\rangle = \langle\psi_2|E|\psi\rangle$$
$$\langle\psi_2|H\ \{c_1|\psi_1\rangle + c_2|\psi_2\rangle\} = \langle\psi_2|E\ \{c_1|\psi_1\rangle + c_2|\psi_2\rangle\}$$
$$\langle\psi_2|Hc_1|\psi_1\rangle + \langle\psi_2|Hc_2|\psi_2\rangle = \langle\psi_2|Ec_1|\psi_1\rangle + \langle\psi_2|Ec_2|\psi_2\rangle$$
$$c_1\langle\psi_2|H|\psi_1\rangle + c_2\langle\psi_2|H|\psi_2\rangle = c_1E\langle\psi_2|\psi_1\rangle + c_2E$$

- $c_1\langle\psi_1|H|\psi_1\rangle + c_2\langle\psi_1|H|\psi_2\rangle = c_1E + c_2E\langle\psi_1|\psi_2\rangle$

$$c_1E_1 + c_2U_{12} = c_1E + c_2EI_{12}$$
$$c_1E_1 + c_2(U_{12} - EI_{12}) = c_1E$$
$$c_1E_1 + c_2(V_{12}) = c_1E$$

- $c_1\langle\psi_2|H|\psi_1\rangle + c_2\langle\psi_2|H|\psi_2\rangle = c_1E\langle\psi_2|\psi_1\rangle + c_2E$

$$c_1U_{12}^* + c_2E_2 = c_1EI_{12}^* + c_2E$$
$$c_1(U_{12}^* - EI_{12}^*) + c_2E_2 = c_2E$$
$$c_1(V_{12}^*) + c_2E_2 = c_2E$$

$$c_1E_1 + c_2(V_{12}) = c_1E$$
$$c_1(V_{12}^*) + c_2E_2 = c_2E$$

$$\begin{pmatrix} E_1 & V_{12} \\ V_{12}^* & E_2 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$
$$\boldsymbol{Hc} = E\boldsymbol{c}$$
$$(\boldsymbol{H} - E\boldsymbol{I})\boldsymbol{c} = 0$$
$$\det\,(\boldsymbol{H} - E\boldsymbol{I}) = 0$$

$$\boldsymbol{H} - E\boldsymbol{I} = \begin{bmatrix} E_1 & V_{12} \\ V_{12}^* & E_2 \end{bmatrix} - \begin{bmatrix} E & 0 \\ 0 & E \end{bmatrix}$$

$$= \begin{bmatrix} E_1 - E & V_{12} \\ V_{12}^* & E_2 - E \end{bmatrix}$$

$$\det(\boldsymbol{H} - E\boldsymbol{I}) = \begin{vmatrix} E_1 - E & V_{12} \\ V_{12}^* & E_2 - E \end{vmatrix} = 0$$

$$(E_1 - E)(E_2 - E) - (V_{12}^*)(V_{12}) = 0$$
$$(E_1E_2 - E_1E - EE_2 + E^2) - |V_{12}|^2 = 0$$
$$E^2 - (E_1 + E_2)E + (E_1E_2 - |V_{12}|^2) = 0$$

$$x\pm = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$E\pm = \frac{(E_1 + E_2) \pm \sqrt{(E_1 + E_2)^2 - 4(E_1E_2 - |V_{12}|^2)}}{2(1)}$$
$$E\pm = \frac{E_1 + E_2}{2} \pm \frac{1}{2}\sqrt{E_1^2 + E_2^2 + 2E_1E_2 - 4E_1E_2 + 4|V_{12}|^2}$$
$$E\pm = \frac{E_1 + E_2}{2} \pm \frac{1}{2}\sqrt{E_1^2 + E_2^2 - 2E_1E_2 + 4|V_{12}|^2}$$
$$E\pm = \frac{E_1 + E_2}{2} \pm \sqrt{\frac{(E_1 - E_2)^2}{2} + |V_{12}|^2}$$

2. Uraikan lagi tentang solusi LCAO untuk Li_3. Jelaskan mana konfigurasi yang lebih stabil antara bentuk segitiga dan garis lurus.

$\mathrm{Li} = 1\mathrm{s}^2\ 2\mathrm{s}^1$

- Bentuk segitiga

$$\boldsymbol{H} = \begin{bmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{bmatrix}$$
$$\boldsymbol{H} = \begin{bmatrix} 0 & t & t \\ t & 0 & t \\ t & t & 0 \end{bmatrix}$$
$$\boldsymbol{H} = \begin{vmatrix} -E & t & t \\ t & -E & t \\ t & t & -E \end{vmatrix} \begin{matrix} -E & t \\ t & -E \\ t & t \end{matrix}$$

$$|\boldsymbol{H} - E\boldsymbol{I}| = 0$$

$$0 = -E^3 + t^3 + t^3 + Et^2 + Et^2 + Et^2$$
$$0 = -E^3 + 2t^3 + 3Et^2$$

$$0 = E^3 - 3Et^2 - 2t^3$$
$$0 = E(E^2 - 3t^2) - 2t^3$$
$$0 = (E + t)(E + t)(E - 2t)$$

$$\mathrm{E} = -\mathrm{t} \;\; \mathrm{V} \;\; \mathrm{E} = -\mathrm{t} \;\; \mathrm{V} \;\; \mathrm{E} = 2\mathrm{t}$$
$$E_{tot} = 2\ 2t + (-t)$$
$$= 3t$$

- Garis lurus

$$\boldsymbol{H} = \begin{bmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{bmatrix}$$
$$\boldsymbol{H} = \begin{bmatrix} 0 & t & 0 \\ t & 0 & t \\ 0 & t & 0 \end{bmatrix}$$
$$\boldsymbol{H} = \begin{vmatrix} -E & t & 0 \\ t & -E & t \\ 0 & t & -E \end{vmatrix} \begin{matrix} -E & t \\ t & -E \\ 0 & t \end{matrix}$$

$$|\boldsymbol{H} - E\boldsymbol{I}| = 0$$

$$0 = -E^3 + 0 + 0 - 0 + Et^2 + Et^2$$
$$0 = -E^3 + 2Et^2$$
$$0 = E^3 - 2Et^2$$
$$0 = E(E^2 - 2t^2)$$

$$\mathrm{E} = 0 \;\; \mathrm{V} \;\; \mathrm{E} = \mathrm{t}\sqrt{2} \;\; \mathrm{V} \;\; \mathrm{E} = -\mathrm{t}\sqrt{2}$$
$$E_{tot} = 2\ t\sqrt{2} + 0$$
$$\approx 2.8t$$

$$\therefore \mathrm{E_{tot}}\ (\text{segitiga}) < \mathrm{E_{tot}}\ (\text{garis lurus})$$