

- Teori kuantum
 - { elektron : potensial sederhana
 - atom : hidrogen, Born-Oppenheimer
 - molekul : LCAO
 - kristal : TB model, DFT, dll..

- Sifat material : interaksi / gangguan



$$\langle \hat{O} \rangle = \langle \Psi | \hat{H} | \Psi \rangle$$

Diagram illustrating a transition between two energy levels:

- The initial state is $|i\rangle$ and the final state is $|f\rangle$.
- The energy difference between the states is $\hbar\omega$.
- The transition is labeled "intensitas" (intensity).

$$O_{i \rightarrow f} = \langle \Psi_f | H_{int} | \Psi_i \rangle$$

$$I \propto |O|^2$$

$$\begin{aligned} S &: [V/K] \\ \sigma &: [1/m\Omega] \\ \kappa &: [W/mK] \end{aligned} \quad \left\{ \begin{aligned} PF &= S^2 \sigma \\ (PF) &= \frac{V^2}{K^2} \cdot \frac{1}{\Omega m} \end{aligned} \right.$$

$$= \frac{W}{mK^2}$$

$$\begin{aligned} (ZT) &= \frac{[S^2 \sigma]}{[\kappa]} \cdot [T] \\ &= \frac{W/mK^2}{W/mK} \cdot \text{K} \end{aligned}$$

$$= 1 \text{ (dimensionless)}$$

efficiency:

$$\eta = \frac{P_{\text{output}}}{P_{\text{input}}} \times 100\%$$

• Sifat termoelektrik ingredients ⁴ per hitungan

$$\boxed{\mathcal{E}(k)}$$

: energy dispersion



$$\text{DOS } (g(\mathcal{E}))$$

density of states

$$\mathcal{E} = \hbar \omega$$



v : group velocity.

$$\boxed{v = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{d\mathcal{E}}{dk}}$$