

Kohn-Sham DFT

$$\left[-\frac{\nabla^2}{2} + v_{\text{ext}} + V^{\text{Hxc}} \right] \phi_p^{\text{KS}} = \varepsilon_p^{\text{KS}} \phi_p^{\text{KS}}$$

Fundamental gap

GW approximation

$$\varepsilon_p^{\text{GW}} = \varepsilon_p^{\text{KS}} + \langle \phi_p^{\text{KS}} | \Sigma^{\text{GW}}(\varepsilon_p^{\text{GW}}) - V^{\text{x}} | \phi_p^{\text{KS}} \rangle$$

Excitonic effect

Bethe-Salpeter equation

$$\begin{pmatrix} R & C \\ -C^* & R^* \end{pmatrix} \begin{pmatrix} X_m \\ Y_m \end{pmatrix} = \Omega_m \begin{pmatrix} X_m \\ Y_m \end{pmatrix}$$

Molecules

Materials

Clusters