

Teori Fungsional Kerapatan

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1 Interaksi Coulomb

Energi interaksi antara dua elektron:

$$E_{ee} = \frac{e^2}{4\pi\epsilon_0 d_{ee}} \quad (1)$$

Energi interaksi antara dua inti atom dengan nomor atom Z :

$$E_{nn} = \frac{Z^2 e^2}{4\pi\epsilon_0 d_{nn}} \quad (2)$$

Energi interaksi antara elektron dan inti atom:

$$E_{en} = -\frac{Z e^2}{4\pi\epsilon_0 d_{en}} \quad (3)$$

Persamaan Schroedinger:

$$\left[\frac{\mathbf{p}^2}{2m_e} + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (4)$$

Fungsi gelombang banyak-partikel:

$$\Psi = \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N; \mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{N_{at}}) \quad (5)$$

References