

non-rel. Schrödinger equation
or relativistic Dirac equation

LDA or GGA
or hybrids

physical orbitals or not
mesh density and basis set

The diagram illustrates the Kohn-Sham equation and its components. On the left, a large left parenthesis $($ is followed by four terms in boxes: an orange box containing $-\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2$, a red box containing $v_{\text{ext}}(\vec{r})$, a red box containing $v_H(\vec{r})$, and a red box containing v_{xc} . These are separated by plus signs. A large right parenthesis $)$ follows. To the right of the parenthesis is a gray box containing $\phi_i(\vec{r})$, followed by an equals sign $=$, a blue box containing E_i , and another gray box containing $\phi_i(\vec{r})$. Arrows point from the descriptive text above and below to the corresponding terms in the equation.

$$\left(-\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 + v_{\text{ext}}(\vec{r}) + v_H(\vec{r}) + v_{xc} \right) \phi_i(\vec{r}) = E_i \phi_i(\vec{r})$$

crystal ions or
pseudopotential

Poisson equation
or Hartree potential

band structure
or not