

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, with arrows indicating their physical origins:

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

Arrows point from the following text labels to the corresponding terms in the equation:

- non-rel. Schrödinger equation or relativistic Dirac equation →  $-\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2$
- crystal ions or pseudopotential →  $v_{\text{ext}}(\vec{r})$
- LDA or GGA or hybrids →  $v_{xc}$
- Poisson equation or Hartree potential →  $v_H(\vec{r})$
- physical orbitals or not mesh density and basis set →  $\phi_i(\vec{r})$  (on the left)
- band structure or not →  $E_i$
- physical orbitals or not mesh density and basis set →  $\phi_i(\vec{r})$  (on the right)