

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