

nonrel. 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 with various components and their physical interpretations. The equation is enclosed in large parentheses and consists of four terms added together: $-\frac{\hbar^2}{2m} \vec{\nabla}_{\vec{r}}^2$ (orange box), $v_{\text{ext}}(\vec{r})$ (pink box), $v_H(\vec{r})$ (pink box), and v_{xc} (pink box). Annotations with arrows point to these terms: 'nonrel. Schrödinger equation or relativistic Dirac equation' points to the kinetic energy term; 'crystal ions or pseudopotential' points to $v_{\text{ext}}(\vec{r})$; 'LDA or GGA or hybrids' points to v_{xc} ; and 'Poisson equation or equation ??' points to $v_H(\vec{r})$. To the right of the parentheses is an equals sign, followed by $\phi_i(\vec{r})$ (grey box) and E_i (blue box), with another $\phi_i(\vec{r})$ (grey box) to the right. Annotations with arrows point to these results: 'physical orbitals or not mesh density and basis set' points to the first $\phi_i(\vec{r})$; 'band structure or not' points to E_i ; and the same text 'physical orbitals or not mesh density and basis set' also points to the second $\phi_i(\vec{r})$.

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

crystal ions or
pseudopotential

Poisson equation
or equation ??

band structure
or not