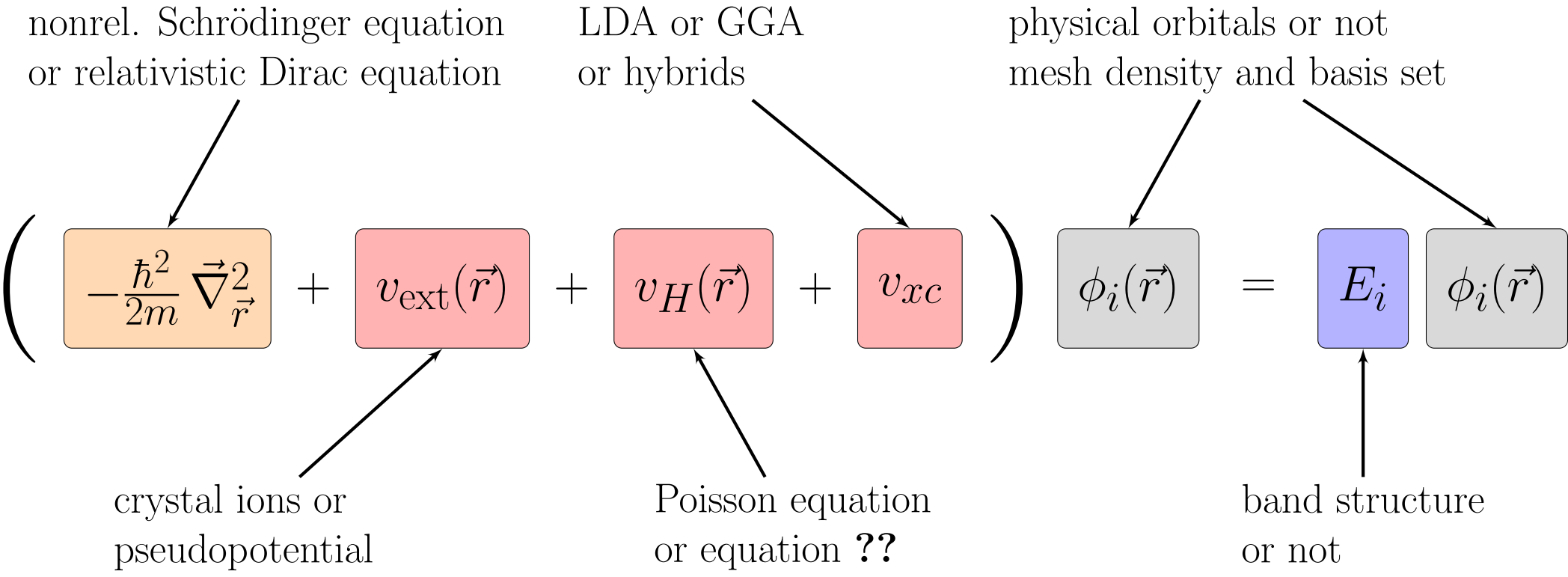
nonrel. Schrödinger equation
or relativistic Dirac equation
LDA or GGA
or hybrids
physical orbitals or not
mesh density and basis set
$-\frac{\hbar^2}{2m}\vec{\nabla}^2_{\vec{r}}$
+
$v_{\text{ext}}(\vec{r})$
+
$v_H(\vec{r})$
+
v_{xc}
$\phi_i(\vec{r})$
=
E_i
$\phi_i(\vec{r})$
crystal ions or
pseudopotential
Poisson equation
or equation **??**
band structure
or not