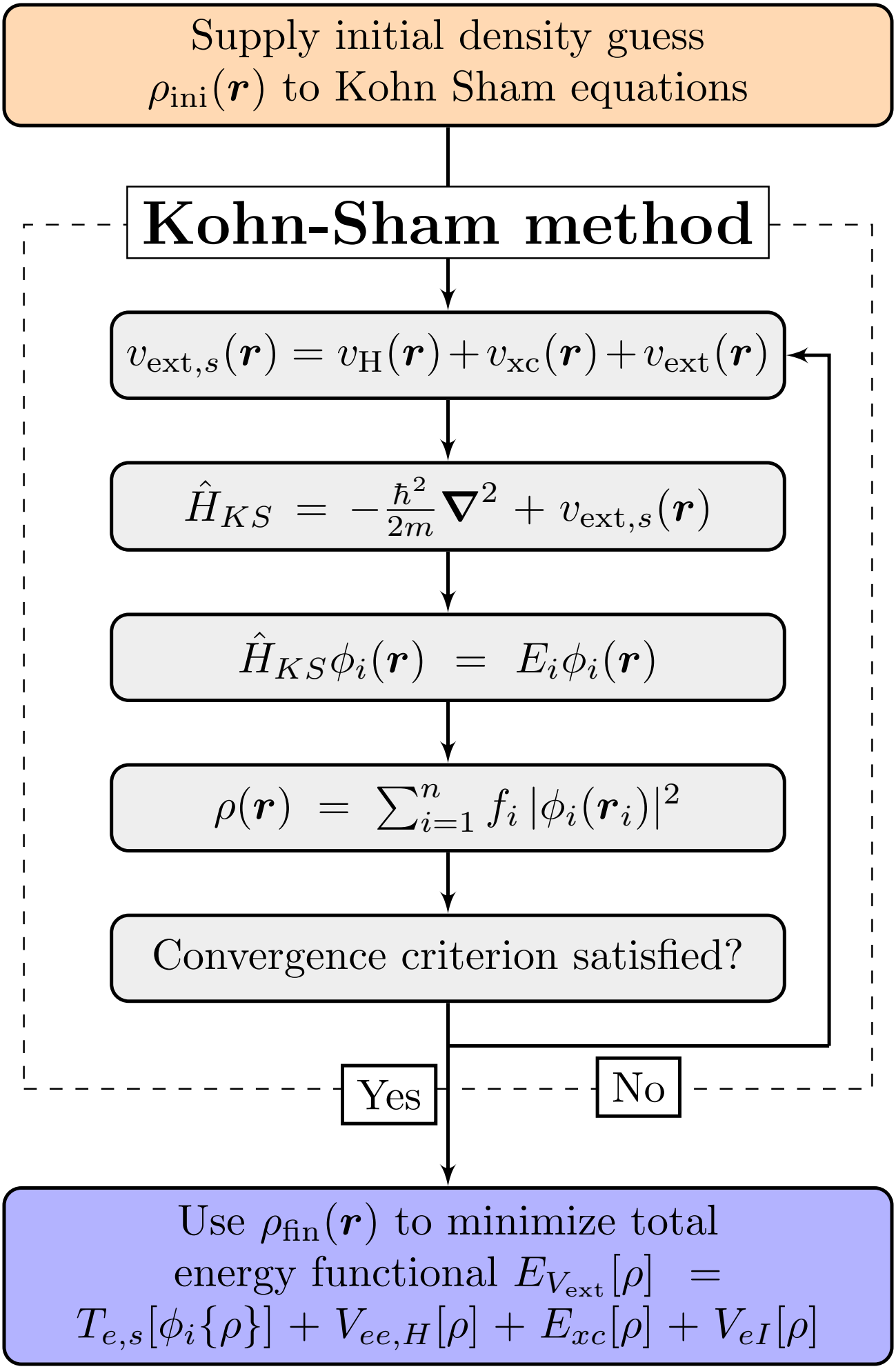
Supply initial density guess
$\rho_{\mathrm{ini}}(\boldsymbol{r})$ to Kohn Sham equations
Kohn-Sham method
$v_{\mathrm{ext},s}(\boldsymbol{r}) = v_{\mathrm{H}}(\boldsymbol{r}) + v_{\mathrm{xc}}(\boldsymbol{r}) + v_{\mathrm{ext}}(\boldsymbol{r})$
$\hat{H}_{KS} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + v_{\mathrm{ext},s}(\boldsymbol{r})$
$\hat{H}_{KS}\phi_i(\boldsymbol{r}) = E_i\phi_i(\boldsymbol{r})$
$\rho(\boldsymbol{r}) = \sum_{i=1}^{n} f_i \left|\phi_i(\boldsymbol{r}_i)\right|^2$
Convergence criterion satisfied?
Yes
No
Use $\rho_{\mathrm{fin}}(\boldsymbol{r})$ to minimize total
energy functional $E_{V_{\mathrm{ext}}}[\rho]$ =
$T_{e,s}[\phi_i\{\rho\}] + V_{ee,H}[\rho] + E_{xc}[\rho] + V_{eI}[\rho]$