Supply initial density guess $\rho_{\text{ini}}(\boldsymbol{r})$ to Kohn Sham equations

**Kohn-Sham method**

$$v_{\text{ext},s}(\boldsymbol{r}) = v_{\text{H}}(\boldsymbol{r}) + v_{\text{xc}}(\boldsymbol{r}) + v_{\text{ext}}(\boldsymbol{r})$$

$$\hat{H}_{KS} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + v_{\text{ext},s}(\boldsymbol{r})$$

$$\hat{H}_{KS}\phi_i(\boldsymbol{r}) = E_i\phi_i(\boldsymbol{r})$$

$$\rho(\boldsymbol{r}) = \sum_{i=1}^n f_i \left|\phi_i(\boldsymbol{r}_i)\right|^2$$

Convergence criterion satisfied?

Yes

No

Use $\rho_{\text{fin}}(\boldsymbol{r})$ to minimize total energy functional $E_{V_{\text{ext}}}[\rho] = T_{e,s}[\phi_i\{\rho\}] + V_{ee,H}[\rho] + E_{xc}[\rho] + V_{eI}[\rho]$