

Initial guess (usually superposition of atomic densities for $k=1$)

$$\rho^{(k)}(r) \xleftarrow{k \rightarrow k+1}$$

Evaluate effective potential

$$v_{\text{eff}}(r) = v_{\text{ext}}(r) + v_H(r) [\rho^{(k)}(r)] + v_{xc} [\rho^{(k)}(r)]$$

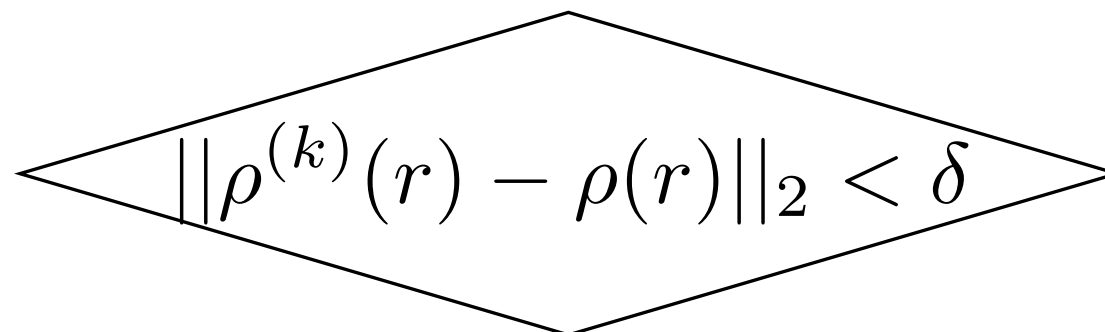
Solve KS equations (for given potential)

$$\left(-\frac{1}{2} \nabla^2 + v_{\text{eff}} [\rho^{(k)}(r)] \right) \psi_i(r) = \epsilon_i \psi_i(r)$$

Evaluate actual density

$$\rho(r) = \sum_i |\psi_i(r)|^2$$

Yes
Compute energy,
forces, stresses....



No