Self-Consistent Field Calculation Steps in DFT

Initialize the System

Start with a guess for the electron density and set up the system.

Compute the New Electron Density

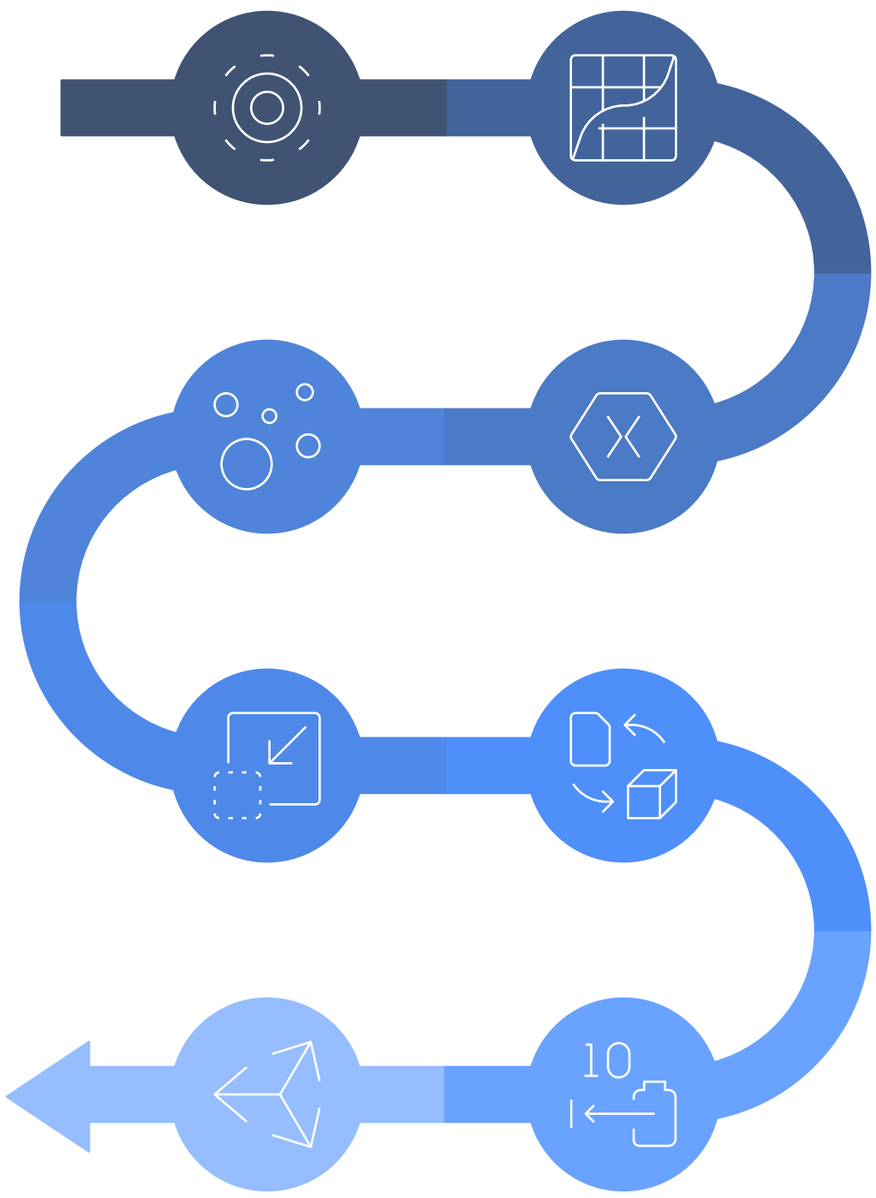
Calculate a new density from the occupied orbitals.

Check for Convergence

Compare the new density with the input density.

Compute Final Quantities

Once converged, calculate key properties for the system.



Compute the Effective Potential

Calculate the effective potential based on the current density.

Solve the Kohn-Sham Equations

Find the Kohn-Sham orbitals and energies by diagonalizing the Hamiltonian.

Mix the Densities

Blend the new and old densities to stabilize the next iteration.

Iterate Until Convergence

Repeat steps 2–6 until the density or energy converges.