Quantum ESPRESSO Lattice Optimization Workflow

1

Start Program

Program Initialization
QE begins, loads pseudopotential, and sets limits

2

Crystal Definition
Defines crystal structure, parameters, and symmetry

System Setup

3

K-Points & G-Vectors

Grid Generation
Generates k-point grid and G-vectors for calculations

4

Electronic Setup
Builds initial potential and wavefunctions for SCF

Initial Potential: From free atomic potentials

5

Initial SCF

Ground-State Calculation
Computes ground-state energy and electronic structure

Geometry Relaxation
-Update atomic positions to minimize enthalpy.
-For each BFGS step, a SCF calculation is perform.

BFGS Optimization

7

Final SCF

Convergence Check
Performs final SCF to confirm relaxed structure

8

Data Output
Saves final cell parameters, atomic positions, and timing

Save Results

9

Job End

Process Completion
QE job finishes and reports final results