Lab2

First-principles calculations of electronic properties of materials: the case study of bulk CaO

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Outline

1. Introduction to the Quantum ESPRESSO project

2. Description of the input file for the pw.x code

3. Performing the calculation

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The Quantum ESPRESSO project

www.quantum-espresso.org

QUANTUM ESPRESSO

Is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

READ MORE

The Quantum ESPRESSO project

IOP Publishing

Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **29** (2017) 465901 (30pp)

https://doi.org/10.1088/1361-648X/aa8f79

Advanced capabilities for materials modelling with QUANTUM ESPRESSO

P Giannozzi[1], O Andreussi[2,9], T Brumme[3], O Bunau[4], M Buongiorno Nardelli[5], M Calandra[4], R Car[6], C Cavazzoni[7], D Ceresoli[8], M Cococcioni[9], N Colonna[9], I Carnimeo[1], A Dal Corso[10,32], S de Gironcoli[10,32], P Delugas[10], R A DiStasio Jr [11], A Ferretti[12], A Floris[13], G Fratesi[14], G Fugallo[15], R Gebauer[16], U Gerstmann[17], F Giustino[18], T Gorni[4,10], J Jia[11], M Kawamura[19], H-Y Ko[6], A Kokalj[20], E Küçükbenli[10], M Lazzeri[4], M Marsili[21], N Marzari[9], F Mauri[22], N L Nguyen[9], H-V Nguyen[23], A Otero-de-la-Roza[24], L Paulatto[4], S Poncé[18], D Rocca[25,26], R Sabatini[27], B Santra[6], M Schlipf[18], A P Seitsonen[28,29], A Smogunov[30], I Timrov[9], T Thonhauser[31], P Umari[21,32], N Vast[33], X Wu[34] and S Baroni[10]

The Quantum ESPRESSO project

ESPRESSO: opEn Source Package for Research in Electronic Structure, Simulation and Optimization

Density Functional Theory (DFT):
ground state properties (total energy, forces, stress tensor…)

Density Functional Perturbation Theory (DFPT):
lattice vibrations

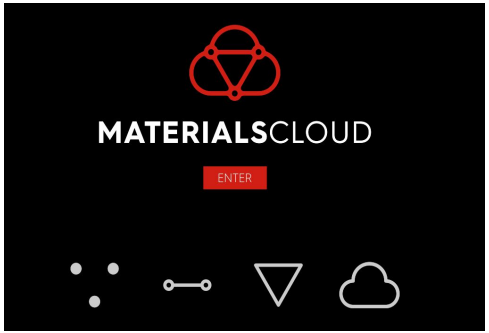
Car-Parrinello molecular dynamics

Time-dependent DFPT
spectroscopy

… and there are many other components of this project.

The Quantum ESPRESSO project

Tutorials and lectures:



https://www.materialscloud.org/learn/sections

https://www.quantum-espresso.org/resources/tutorials

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Input file for the pw.x code

In this lab we will study electronic properties of the bulk CaO – calcium oxide
The input file for this system looks like this (CaO_primitive.scf.in):

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    prefix = 'CaO'
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    nat = 2
    ntyp = 2
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/
&electrons
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K_POINTS automatic
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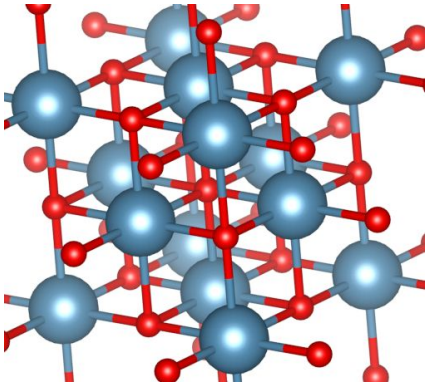

https://www.quantum-espresso.org/Doc/INPUT_PW.html

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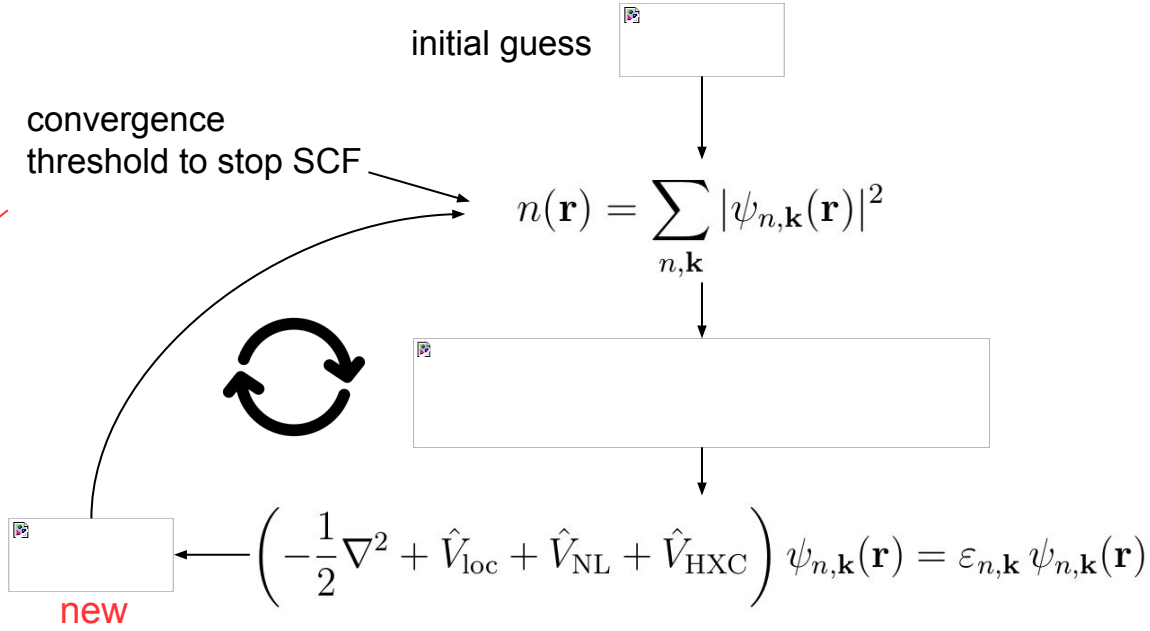
Self-consistent field (SCF): iterative solution of the Kohn-Sham (KS) equations:



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The prefix for temporary files

The name and the path to the folder, where temporary files will be written

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Calculation of the stress tensor

Calculation of the forces

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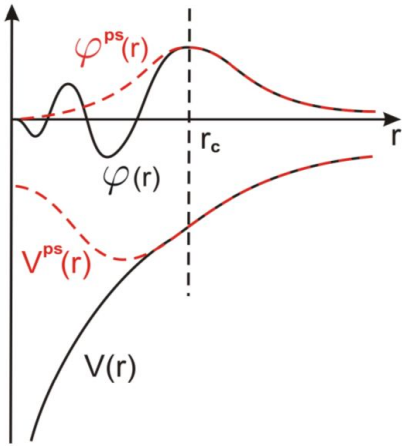
The path to the location of the pseudopotential



Pseudopotential file names

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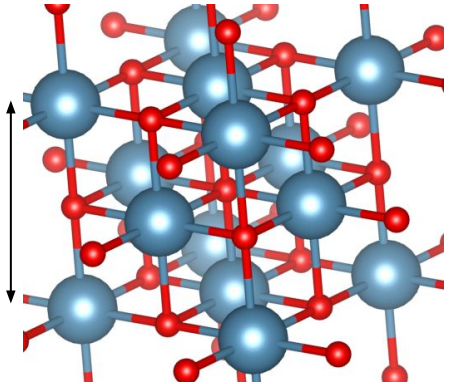
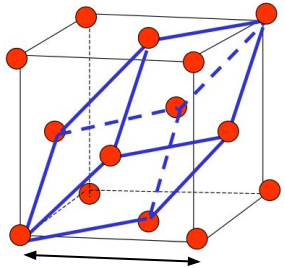
Bravais lattice index (FCC)

lattice parameter, units are bohr





lattice parameter = 9.0 bohr

atomic coordinates (unit cell), in fractional units, i.e. units of alat = celldm(1)

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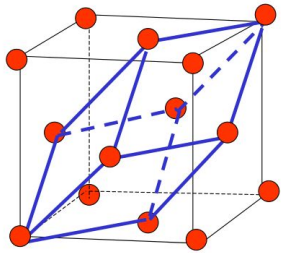
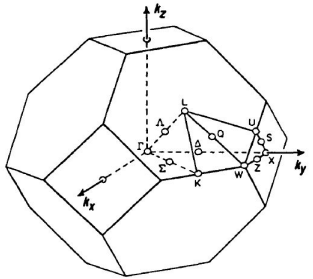
Real space
(unit cell)



Reciprocal space
(first Brillouin Zone)



k points sampling of the Brillouin zone using the Monkhorst-Pack scheme

- 4x4x4 uniform grid
- 0 0 0 means that the grid is not shifted with respect to the center of the BZ

Symmetries ⟺ Irreducible wedge of the BZ

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```

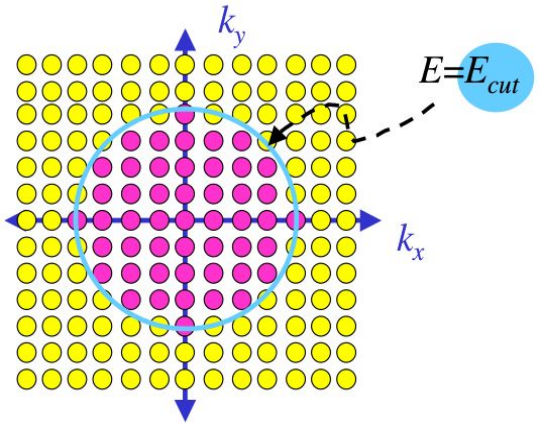
$$\psi_{n,\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{n,\mathbf{k}+\mathbf{G}}\, e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

KS wavefunctions are expanded in a plane-wave basis set up to a cutoff G_{cut}

Kinetic energy cutoff E_{cut} units are Ry

E_{cut} defines G_{cut}:

$$\frac{\hbar^2}{2m}|\mathbf{k}+\mathbf{G}|^2 \le E_{cut}$$



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Performing the calculation

To perform a single pw.x calculation, it is necessary to execute the following command: