Quantum Espresso

Guide to running simulations for DLS Spectroscopy

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Introduction

Open Source Software Package

Where to get help?

At Diamond:
Email: joshua.elliott@diamond.ac.uk; Office: 1.12 Z02 (Ring); Ext:
Email: mihai.duta@diamond.ac.uk (installation/compilation problems)

Online:
Web-site: www.quantum-espresso.org

Literature:
Journal of Physics: Condensed Matter 2009, 21 (39), 395502.
Journal of Physics: Condensed Matter 2017, 29 (46), 465901.
Journal of Chemical Physics 2020, 152 (15), 154105.

Source Code:
Doc folder under quantum espresso distribution

Mailing List:
Email: users@lists.quantum-espresso.org
Archive of questions/issues dating back to 2011.
Web-site: https://www.mail-archive.com/users@lists.quantum-espresso.org/

A Software Suite

Important: QE is not a single executable file, rather a collected distribution of several executable programs.

PWscf	Ground state electronic structure, structural optmiziation.
CP	Carr-Parrinello molecular dynamics.
PHonon	Linear-repsonse calculations.
PostProc	Post processing, graphs and visualization.
PWneb	Nudged-Elastic Band driver from reaction paths.
atomic	Generation of pseudopotentials.
PWGui	Graphical User Interface for input.
PWcond	Ballistic conductance calculations.
XSpectra	Core-level excitation spectra based on Fermi-Golden Rule.
GWL	Quasiparticle and Exciton energies based on GW/BSE approximation.
TD-DFPT	Time-dependent Density Functional Perturbation Theory.
EPW	Electron-phonon coupling.
HP	Automation of linear-response DFT+U parameters.

All these packages and others share: (i) installation method, (ii) input file format, (iii) pseudopotential file format, (iv) output format (v) source code.

Density Functional Theory - Theory

Quantum mechanics in terms of the electron density

The total energy of the ground state of a system of electrons may be written as a functional of the electron density.

$$E^{\mathrm{DFT}}[n]; \qquad \int n(\mathbf{r})\ \mathrm{d}\mathbf{r} = N; \qquad n(\mathbf{r}) \geq 0 \tag{1}$$

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We can prove mathmatically that the functional exists, but the form is unknown. Within Kohn-Sham formalism we write the functional:

$$E^{\mathrm{DFT}}[n] = T_s[\{\psi_i\}] + E_{\mathrm{ext}}[n] + E_{\mathrm{Hartree}}[n] + E_{xc}[n] + E_{\mathrm{ions}} \tag{2}$$

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$$n(\mathbf{r}) = \sum_{i}^{M} |\psi_i(\mathbf{r})|^2 \tag{3}$$

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These are used to approximate the kinetic energy

$$T_s[\{\psi_i\}] = -\frac{1}{2}\sum_i^N \int \mathrm{d}\mathbf{r}\ \psi_i^*(\mathbf{r})\nabla^2\psi_i(\mathbf{r}) \tag{4}$$

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The other terms are functionals of the density:

$$E_{\text{ext}}[n] = \int \mathrm{d}\mathbf{r}\ n(\mathbf{r}) V_{\text{ext}}(\mathbf{r}), \tag{5}$$

$$E_{\text{Hartree}}[n] = \frac{1}{2} \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'\ \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \tag{6}$$

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$$E_{\text{ions}} = \sum_{I,J\neq I} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} \tag{7}$$

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Minimization of the functional derivitive of E^{DFT} with respect to the density n gives

$$H^{\text{KS}}\psi_i(\mathbf{r}) = \left[-\frac{1}{2}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{xc}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r}) \tag{8}$$

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$$V_{\mathrm{Hartree}} = \int \mathrm{d}\mathbf{r}' \ \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \tag{10}$$

$$V_{xc} = \frac{\delta E_{xc}}{\delta n} \tag{11}$$