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Tutorial intro Fri.4

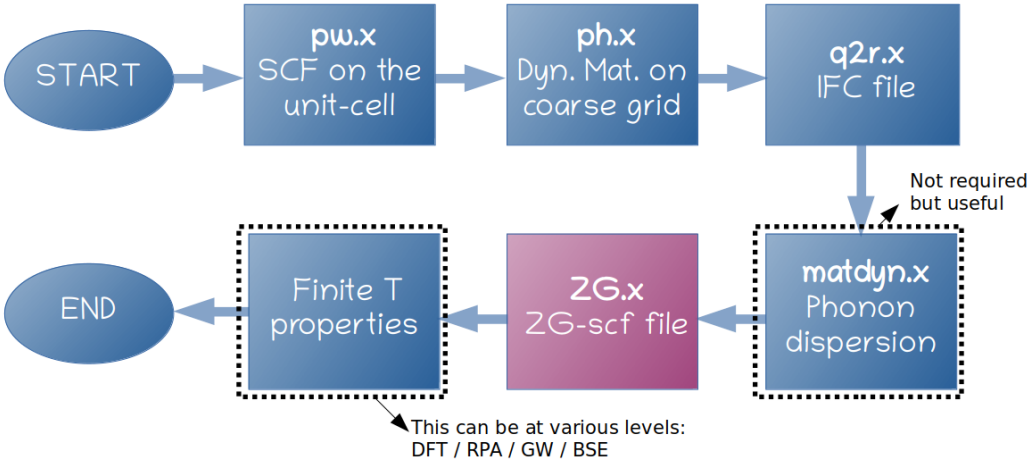
The Special Displacement Method

Marios Zacharias

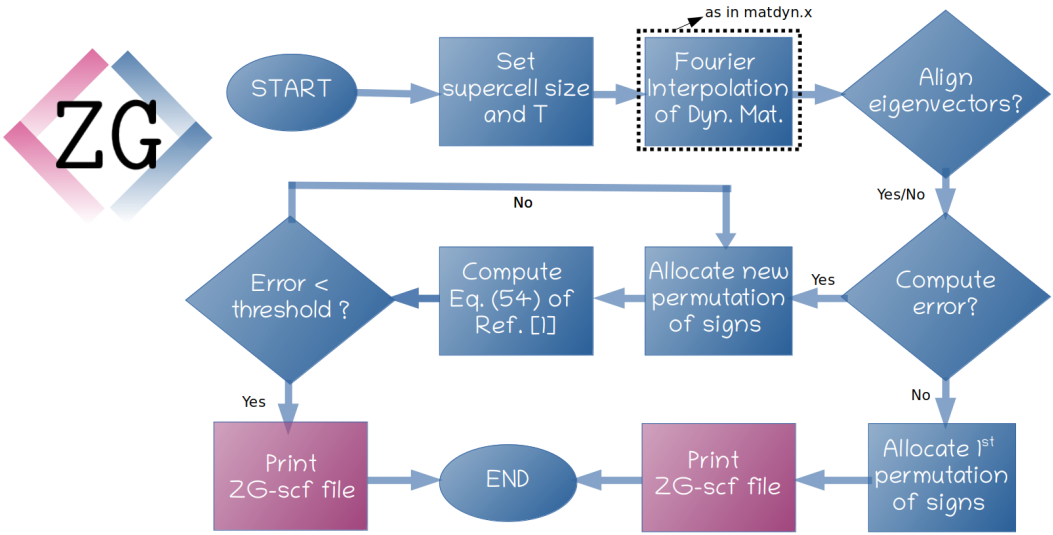
INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

Univ. Rennes

Flowchart for ab-initio calculations with ZG configurations



Flowchart for ZG.x



Ref. [1]: M. Zacharias, F. Giustino, Phys. Rev. Research 2, 013357 (2020)

Compute and minimize the function $E(\{S_{\mathbf{q}\nu}\}, T)$

Find the best ZG displacements for a given *supercell size* and *temperature* by setting
`compute_error = .true.`, `error_thresh = 0.05`
so that the function:

$$E(\{S_{\mathbf{q}\nu}\}, T) = \sum_{\substack{\kappa\alpha \\ \kappa'\alpha'}} \frac{\left| \sum_{\substack{\mathbf{q}\in\mathcal{B} \\ \nu<\nu'}} \Re[e^*_{\kappa\alpha,\nu}(\mathbf{q}) e_{\kappa'\alpha',\nu'}(\mathbf{q})] \sigma_{\mathbf{q}\nu,T} \sigma_{\mathbf{q}\nu',T} S_{\mathbf{q}\nu} S_{\mathbf{q}\nu'} \right|}{\left| \sum_{\substack{\mathbf{q}\in\mathcal{B} \\ \nu}} \Re[e^*_{\kappa\alpha,\nu}(\mathbf{q}) e_{\kappa'\alpha',\nu}(\mathbf{q})] \sigma^2_{\mathbf{q}\nu,T} \right|}$$

is lower than `error_thresh` based on the choice of $\{S_{\mathbf{q}\nu}\}$.

All quantities in $E(\{S_{\mathbf{q}\nu}\})$ can be computed from DFPT;
no extra DFT caclualtions are required to find the optimum ZG configuration.

Example input file for ZG.x (similar structure to matdyn.x)

```
--
&input
  flfrc='si.444.fc',
  asr='simple', amass(1)=28.0855, atm_zg(1) = 'Si',
  flscf = 'si.scf.in'
  T = 0.00,
  dim1 = 5, dim2 = 5, dim3 = 5
  compute_error = .true., synch = .true., error_thresh = 0.05
  incl_qA = .false.
/
```

Tutorials and description of the input flags are available online in https://epwdoc.gitlab.io.

Tutorial Summary

- **Exersice 1**: Generate the ZG displacements in silicon and calculate the total energy.
- **Exersice 2**: Caclualte the zero-point band gap renormalization of silicon and temperature dependent band structure via band structure unfolding.
- **Exercise 3**: Calculate phonon-assisted spectra of silicon.
- **Exercise 4**: Calculate phonon-induced diffuse scattering patterns of graphene.
- **Exercise 5**: Calculate phonon dispersions of P-doped silicon using phonon unfolding.

Things to have in mind when applying SDM via `ZG.x`:

- Make sure that the phonon dispersion is correct. For *anharmonicity* one can upgrade the IFC file using the methods:

  O. Hellman *et al.*, Phys. Rev. B 84, 180301(R) (2011)

  I. Errea *et al.*, Phys. Rev. B 89, 064302 (2014)

- **q**-grid for phonons should not be necessarily the same with the supercell size. Use a coarse **q**-grid and generate any size of ZG configurations.
- Achive convergence of the T-dependent observable with the supercell size.
- Make sure `error_thresh` is small (< 0.1).
- Check the anisotropic displacement tensor data at the end of the output `ZG_XXX.out` (as in `exercise1`).
- Pointless to minimize the error function for systems with many atoms (> 15) in the unit-cell (set `compute_error = .false.`).