The Special Displacement Method

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Flowchart for ab-initio calculations with ZG configurations

START

pw.x SCF on the unit-cell

ph.x Dyn. Mat. on coarse grid

q2r.x IFC file

Finite T properties

ZG.x ZG-scf file

matdyn.x Phonon dispersion

This can be at various levels: DFT / RPA / GW / BSE

Not required but useful
Flowchart for ZG.x


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

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:

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

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

All quantities in \( E(\{S_{q\nu}\}) \) can be computed from DFPT; **no extra DFT calculations** 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.
Exercise 1: Generate the ZG displacements in silicon and calculate the total energy.

Exercise 2: Calculate 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:
  
  

- \( q \)-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.

- Achieve 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.`).