# 2023 Virtual School on Many-Body Calculations using EPW and BerkeleyGW

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Tutorial intro Wed.4

# The Special Displacement Method

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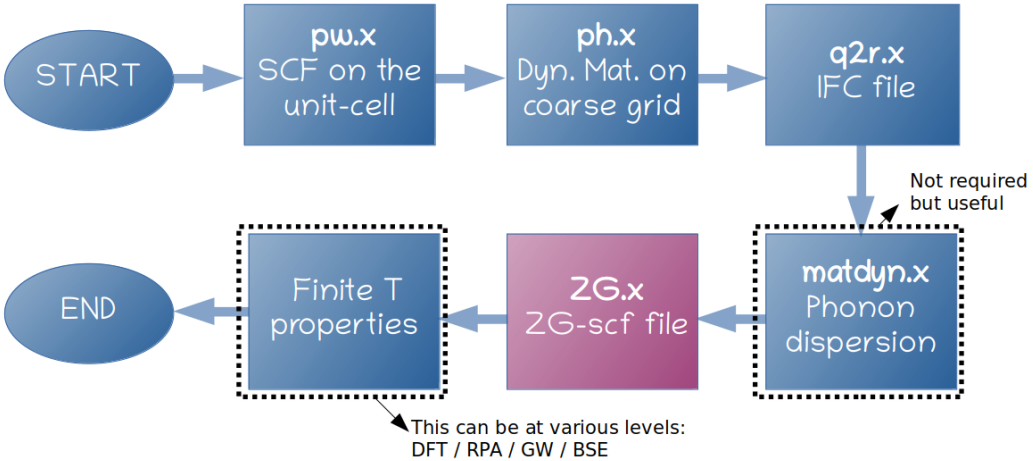
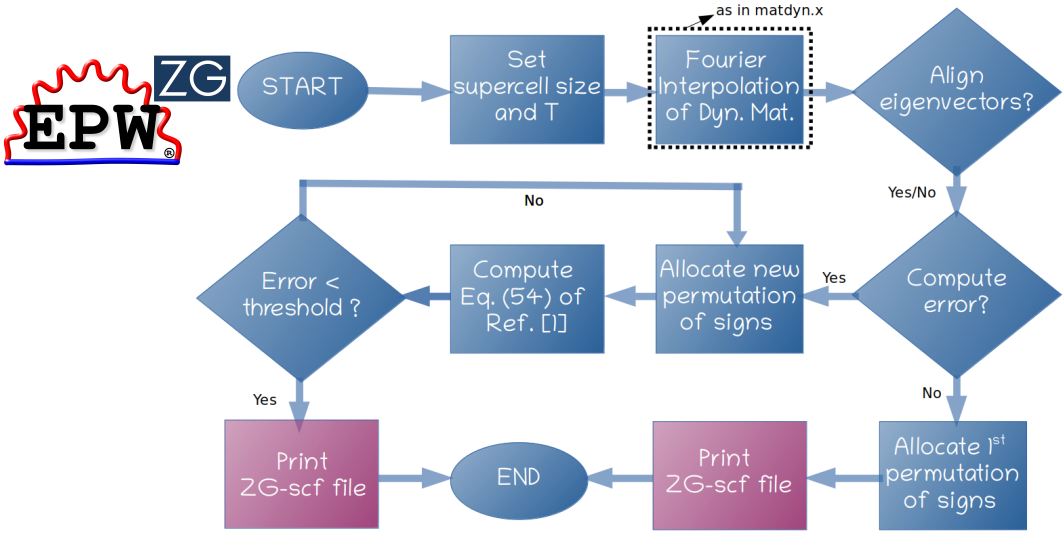
# Instructions

- All exercises except `exercise3` (anharmonicity, A-SDM) can run with QE v7.2.
- To run exercise3 we compiled a modified version of `ZG.x`:
  `/work2/06868/giustino/SCHOOL/q-e-qe-7.2_ZG_anh/bin/`
- Running the tutorial locally (not in FRONTERA) and want to run `exercise3` download the `files` from https://epw2023.dryfta.com/74-schedule
  Then type: `cp ZG.f90 pathqe/EPW/ZG/src/ZG.f90; cd pathqe/EPW/ZG/src/; make; cd -`
- Running the tutorial locally you might get different ZG coordinates; this is reasonable since the phases of eigenvectors might vary for different machines.
- The tutorial is long so you are expected to run the first three exercises.
- For help please go to breakout rooms or post questions in the chat.

# Flowchart for ab-initio calculations with ZG configurations



# Flowchart for `ZG.x` to generate ZG-configuration




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 $\{S_{\mathbf{q}\nu}\}$.

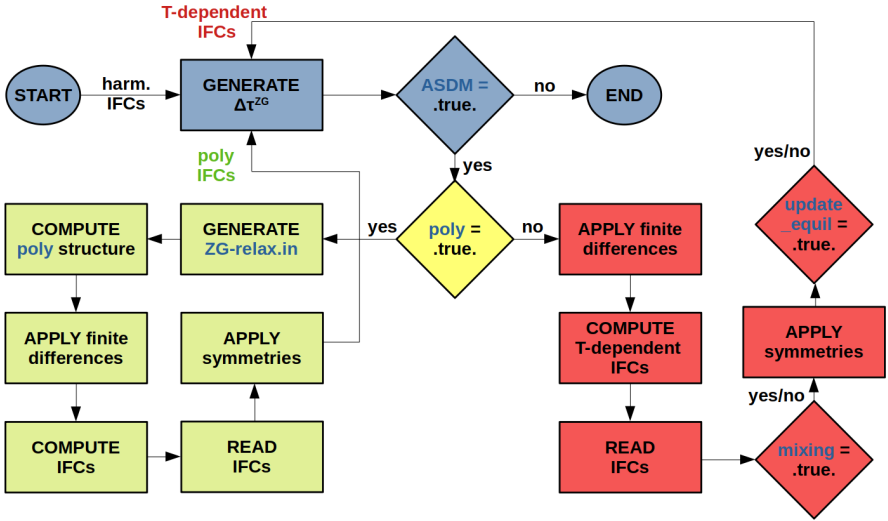
All quantities in $E(\{S_{\mathbf{q}\nu}\})$ can be computed from DFPT;
**no extra DFT** calculations are required to find the optimum ZG configuration.

# 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.

# Appendix: Flowchart for ASDM in ZG.x




M. Zacharias, G. Volonakis, F. Giustino, J. Even arXiv:2212.10633

# Inputs for ZG.x (A-SDM)

```
&input                                                                ZG_4
    flfrc='poly_iter_00.fc', flscf = 'scf.in', asr='crystal',
    amass(1)=132.90545, amass(2)=207.2, amass(3)= 79.904,
    atm_zg(1) = 'Cs', atm_zg(2) = 'Pb', atm_zg(3) = 'Br'
    T = 380.00,
    dim1 = 2, dim2 = 2, dim3 = 2
    compute_error = .true., synch = .true., error_thresh = 0.5
    ASDM = .true., na_ifc = .true.
/
&A_ZG
   iter_idx = 1
   apply_fd = .true.
   incl_epsil = .true.
/
```

Note: `T = 380 K`, `flfrc = 'poly_iter_00.fc'` (computed from iter 0), and `na_ifc = .true.` for nonanal contrib

# Tutorial Summary

- **Exercise 1**: ZG displacements in silicon and total energy via SDM
- **Exercise 2**: Zero-point band gap renormalization of silicon and temperature dependent band structure via band structure unfolding
- **Exercise 3**: Anharmonic lattice dynamics of Zr via A-SDM
- **Exercise 4**: Phonon-assisted spectra of silicon with ZG displacements
- **Exercise 5**: Phonon-induced diffuse scattering in graphene
- **Exercise 6**: Phonon dispersions of P-doped silicon using phonon unfolding

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

- Always make sure that the phonon dispersion has no instabilities. For *anharmonic* systems one can upgrade the IFC file using the A-SDM.
- **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 fairly small ($< 0.2$).
- 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.`).
- If you work in a 2×2×2 supercell set `incl_qA = .true.`. Useful for anharmonic phonons with A-SDM. In this case `error_thresh` can be ($< 0.5$).