Updates on high-throughput DFPT


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22/05/2019
1. Introduction

2. High-throughput DFPT

3. Phonons database

4. Abinit for HT

5. Further developments
Outline

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Aim of the project

Diffusion of large databases based on DFT calculations

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High-throughput workflows for Abinit

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DFPT phonon band structures at Materials Project
Where were we?

ABIDEV 2017:

- Infrastructure to run high-throughput calculations with Abinit
  - dependencies on different python frameworks
  - high-throughput framework: Abiflows

- Preliminary results:
  - Convergence study
  - Workflows at NERSC
Where were we?

ABIDEV 2017:
- Infrastructure to run high-throughput calculations with Abinit
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  - high-throughput framework: Abiflows
- Preliminary results:
  - Convergence study
  - Workflows at NERSC

ABIDEV 2019:
- Results
  - Materials project
- Problems encountered
- Next steps
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High-throughput framework

- **Abinit**
  - DFT + DFPT code

- **pymatgen**
  - Generic material analysis framework

- **abipy**
  - Abinit python analysis framework

- **FireWorks**
  - Workflow manager

- **abiflows**
  - Abinit workflows framework

Available on Github: https://github.com/abinit/abiflows
Extended workflow to cover all possible DFPT calculation available
Extended workflow to cover all possible DFPT calculation available
Convergence study

Find optimal k-points and q-points sampling for high-throughput
Petretto, Gonze, Hautier, Rignanese, Comp. Mat. Sci., 144, 331 (2018)

- Set of 48 semiconductors
  - Various sizes, crystal symmetries, gaps
- Several K and Q grids
- Statistic on error with respect to dense grids:
  - relative and absolute error
  - mean and maximum error

| NaLi2Sb  | Ca(CdP)2 | CdS   | SrLiP | InS   | GaN   | RbYO2  | SiO2  | BP   | AlSb | LiZnP | MgCO3 | ScF3   | ZnGeN2 | LiMgAs | P2Ir | Si   | Li3Sb | K2O   | Ga3Os | Be3P2  | ZnSe  | MgO  | AgCl | SiC   | YWN3  | SrO   | PbF2   | MgSiP2 | SiO2  | GaP   | Be2C  | SnHgF6 | MgMoN2 | ZnO    | ZrSiO4 | Ba(MgP)2 | Ba(MgAs)2 | Ca(MgAs)2 | C    | Rbl   | FeS2   |
|----------|----------|-------|-------|-------|-------|--------|-------|------|------|-------|-------|--------|--------|--------|-------|------|------|-------|-------|--------|--------|-------|------|------|-------|--------|--------|--------|-------|-------|-------|--------|--------|--------|--------|--------|-------|-------|

G. Petretto (MODL, UCL)
Convergence study: grids density

- absolute and relative errors on $\omega$, $E_{at}$, $Z^*$ and $\epsilon$
- 1500 points per reciprocal atom $\Rightarrow N_{kpt} \times N_{atoms} \lesssim 1500$
  $\Rightarrow$ All materials converged with 0.5 cm$^{-1}$ MAE and 0.6% MARE
- Better using a Q-grid commensurable with K-grid
  $\Rightarrow$ Smoother close to $\Gamma$

![Graph showing frequency vs error on $\omega$ for AgCl at different qpt grids with 6x6x6 and 12x12x12 k-points](image)
Convergence study: symmetry of the grid

Convergence rate of phonon frequencies $\omega$ for symmetric versus non-symmetric grids

Grids should preserve the symmetries of the system
Results validation

Validation versus experimental data

Vibrational entropy at 300K

Γ phonon frequencies
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Open access database: 1521 semiconductor materials (and growing...)
1508 of those materials with less than 13 atomic sites
~ 5M CPU-hours
Open access database: **1521 semiconductor materials** (and growing...) 1508 of those materials with less than 13 atomic sites

$\sim$ 5M CPU-hours

- Interatomic force constants (DDB files)
- Phonon dispersion
- Born effective charges
- Dielectric tensor
- Thermodynamic prop.: $\Delta F, \Delta E_{ph}, C_v, S$

Materials Project phonons database

All the data available on the website and through REST service.

Interactive visualization of the phonon dispersion using the phononwebsite

http://henriquemiranda.github.io/phononwebsite/
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Reliability: workflows

For the 1521 phonon band structures:

- Relax workflow
- Phonon workflow (+ anaddb)

Out of all the submitted workflows only \( \sim 30 \) did not complete successfully
Reliability: workflows

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Out of all the submitted workflows only \(\sim 30\) did not complete successfully.

Main reasons:

- Too slow relaxation/relaxation did not converge
- Too small gap (switched to metallic)
- Presence of La
- Poor choice of materials
Warnings available in the database:

- Negative $\omega$ close to $\Gamma$: 24 materials
- ASR break $>30 \text{ cm}^{-1}$: 72 materials
- CNSR break $>0.2e$: 92 materials
Problems encountered

- Current MP cluster: KNL nodes
  - not optimized
  - reserve full node
  - relatively poor performances
  - difficult to fine tune parallelization at high-throughput level

- Relax - `ionmov 22`: seems faster but may fail at small `tolmxf` ($10^{-6}$)
  ⇒ switch `ionmov` at python level.

- Autoparal for DFPT
  - always gives the maximum number of processes allowed
  - often parallelizing over just the k-points is advantageous
  ⇒ could be improved?

- Memory
  - moving to larger materials already caused a few jobs to fail due to memory issues
  ⇒ might be needed to rely on estimation of total memory
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More data on the MP database

Calculations have proceed: almost **500 more materials**

More physical quantities will be extracted from the phonon data:

- Sound velocity as slope of acoustic modes
- Low-frequency dielectric permittivity tensor \( \epsilon_{\alpha\beta}(\omega) \)
- Thermal displacement ellipsoids (Debye-Waller)
Phonons for metals

Extend the calculation to **metals** as well. Materials project:
- 24356 metals
- 8242 with less than 6 atoms

Potential issues:
- Denser k-point grids
- Q-point grids?
- Smearing
- Kohn anomalies
  - Fourier interpolation

New convergence study required

He, Liu, Li, Rignanese, Zhou (2019)
Volume: Grüneisen parameters

Phonons at different volumes (e.g. ±2%) ⇒ Grüneisen

- Tools already available in Abinit (netcdf) and Abipy
- Preferable to have separate workflows

```python
import GrunsNcFile

volumes = ["-2_DDB", "+0_DDB", "+2_DDB"]
g = GrunsNcFile.from_ddb_list(volumes)
g.plot_phbands_with_gruns(with_doses=None)
g.plot_gruns_scatter()
phbst.plot_phbands(units="cm\(^{-1}\)"
```
Volume: Quasi-Harmonic Approximation

Tools for QHA implemented in Abipy:

- **Standard QHA object**
  - generated from GSR and PHDOS netcdf files
  - Fittings
  - Thermal expansion coefficient
  - Interface to Phonopy for further functionalities

  - several electronic energies at different V and 3 phonon calculations
  - extrapolate phonon contribution at other V
  - Satisfactory results

⇒ Interesting for high-throughput
Example QHA-3P for Si

```python
def qha = QHA.from_files(gsr_paths, dos_paths)
qha3p = QHA3P.from_files(gsr_paths, gruns_path, ind_doses=[1,2,3])
fig = qha.plot_thermal_expansion_coeff()
qha3p.plot_thermal_expansion_coeff(ax=fig.axes[0])
```

![Graph showing thermal expansion coefficient for QHA and QHA3P](image-url)
Thank you for your attention
High-throughput framework

What do we need for high-throughput with Abinit?

- Python interface to DFT codes
- Inputs
  - pseudopotentials and cutoffs
  - automatic generation
- Workflow management
- Database interface
- Workflows
- Error handling and data analysis
Materials Project phonons database: rester

Fetching DDB files from MP and analyze results with Abipy

```python
ddb = abilab.DdbFile.from_mpid("mp-1265")  # MgO
phbst, phdos = ddb.anaget_phbst_and_phdos_files(ndivsm=20, nqsmall=20,
                                                  lo_to_splitting=True)
phbst.plot_phbands(units="cm-1")
```

![Graph of phonon bands](image)
q-points convergence

Use subgrids of the q-point grid to check the convergence w.r.t. qpt

- Material dependent
- Suggest good convergence level at 1500 qppa
- reducing by a factor 2 may lead to sizeable errors on average