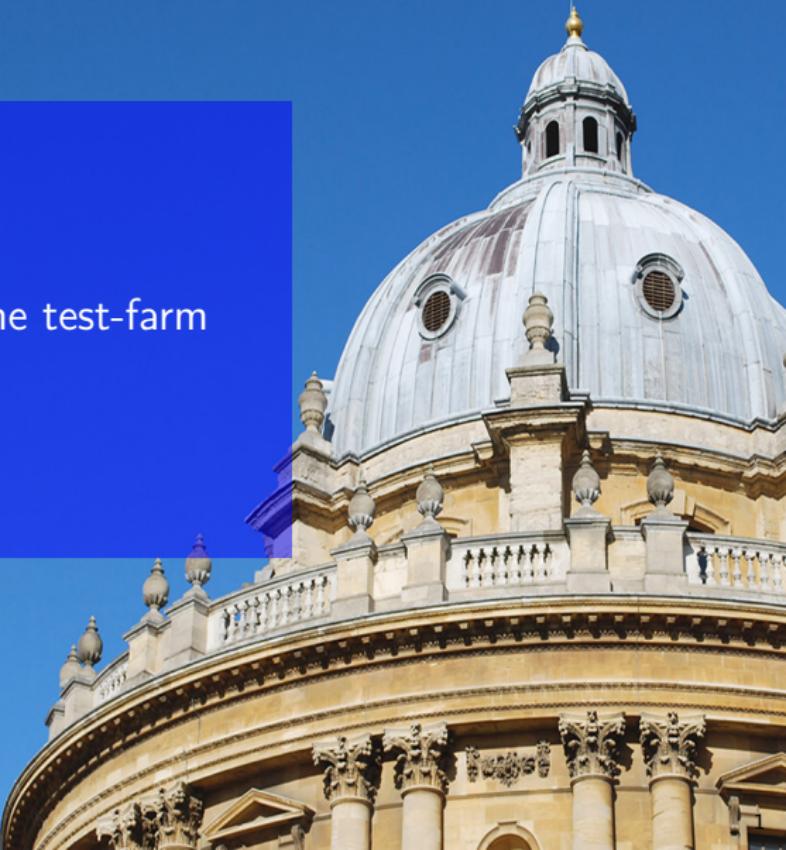




Progress in EPW and the test-farm

Samuel Poncé

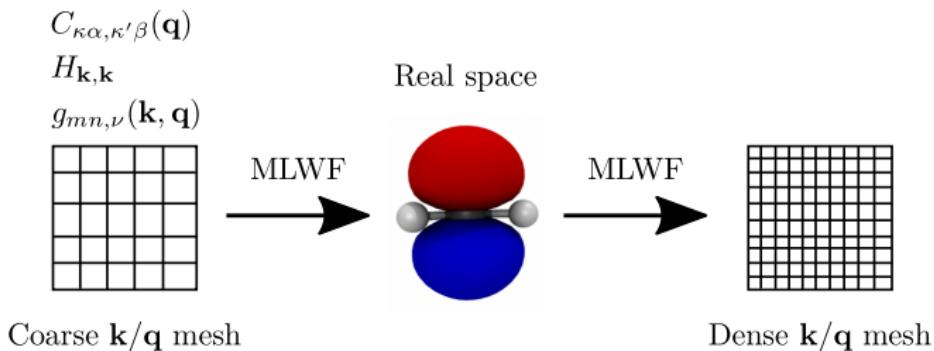
QE Devel meeting 01-02-2018





Electron-phonon Wannier (EPW)

EPW relies on MLWF to interpolate electron-phonon matrix elements.





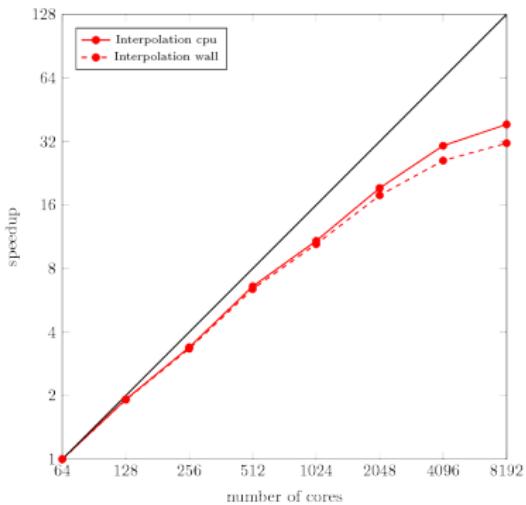
EPW developments in 2017

- ▶ Testing scaling on the KNL architecture.
- ▶ Migration of the test-farm using Buildbot from Oxford to CINECA on a virtual machine (C. Cavazzoni).
- ▶ Calculation of carrier mobility (will be release March 2018).
- ▶ Electron-plasmon (partially analytical) coupling using `plselfen` variable (F. Caruso).
- ▶ Electron spectral function with the cumulant expansion method (F. Caruso)
- ▶ Screening of the el-ph matrix element by the RPA or TF dielectric function using `lscreen` variable (C. Verdi).



Scaling on the KNL architecture

Scalability of the interpolation part of EPW v4.2 on CSD3 for polar SiC on a 64x64x64 k-point grid and 8x8x8 q-grid.



Done with Intel 17.0.4+intel mpi+mkl and with -xAVX -mavx -axCOMMON-AVX512 vectorization flags on Intel(R) Xeon Phi(TM) CPU 7210 @ 1.30GHz. Intel Omni-Path HPC interconnect.

Buildbot test-farm

The test-farm using Buildbot moved from Oxford to CINECA and can be accessed at <http://130.186.13.198:8010>.

- ▶ Automatically send an email when a slave failed to a list of developer
 - ▶ Send me an email at samuel.pon@gmail.com if you want to be on the list



Test-suite

We need to test more parts of the code.

Existing tests:

- ▶ 180 tests for PW
- ▶ 14 tests for PH (we need more)
- ▶ 17 tests for CP
- ▶ 42 tests for EPW
- ▶ 0 test for TDDFPT
- ▶ 0 test for GWW
- ▶ 0 test for QHA
- ▶ 0 test for NEB





Test-suite and Buildbot test-farm

I added some doc in Doc/developer_man.tex to add new tests to the QE test-suite

13.1 How to add tests for a new executable

Let us take the example of adding a new test for the TDDFPT module.

extract-PROG_NAME.x This script extracts the physical quantities from the output and parse it in a format for the testcode.py script. The script need to contain all the different output you want to parse (for chain calculations). For example, in this case we want to parse the output of `pw.x`, `turbo_lanczos.x` and `turbo_spectrum.x`. It is crucial to add as many parameter to be tested as possible to increase the code coverability.

run-PROG_NAME.sh This bash script contains the paths of the different programs and source the `ENVIRONMENT` file

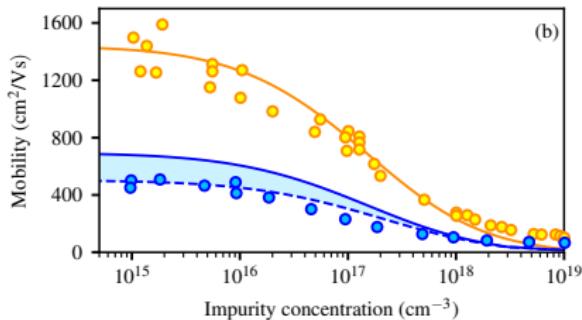
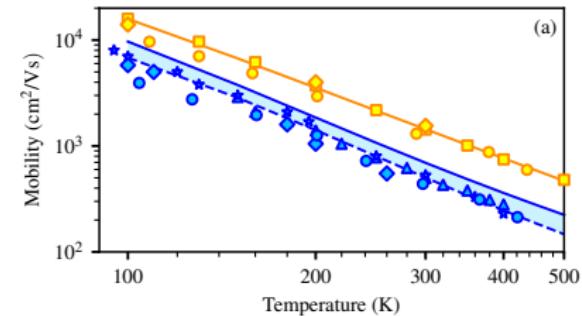
jobconfig You need to edit this file to add all the new tests as well as the new program. You can chain different programs with different output in one test. In this case we added

```
[tddfpt_*]  
program = TDDFPT
```



New features in EPW

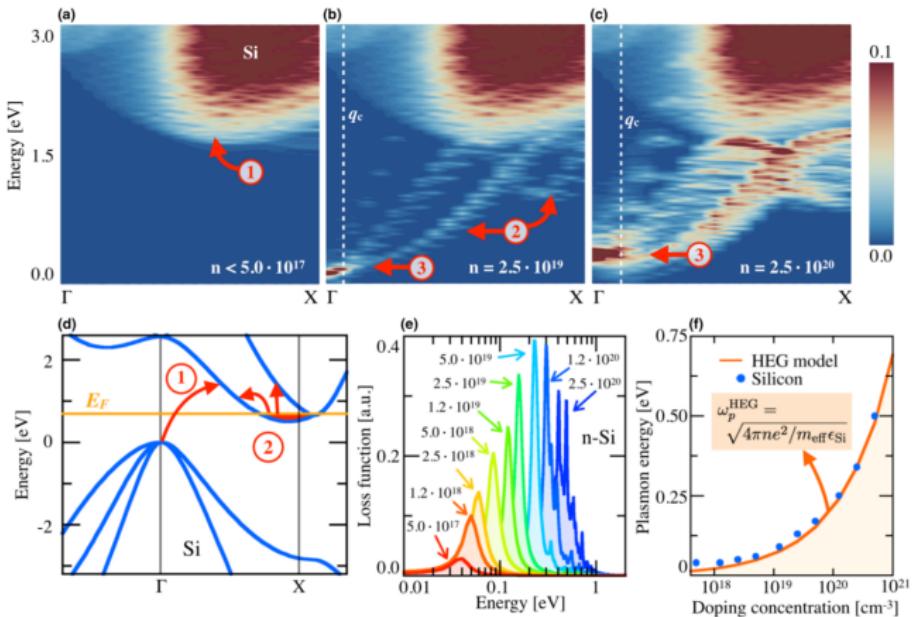
Carrier mobility in semiconductors: will be released before the ICTP ep-ph school in March 2018.





Electron-plasmon coupling (model) in Silicon

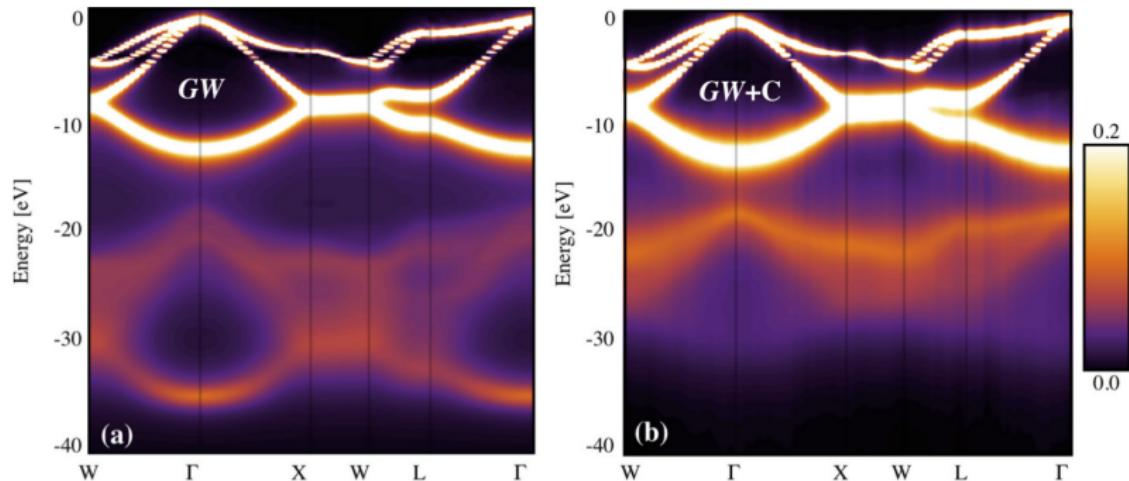
See new input variables: `plselfen`, `epsiHEG`, `meff`, `nel`





Cumulant spectral function in Silicon

See new input variables: `cumulant`, `bnd_cum`

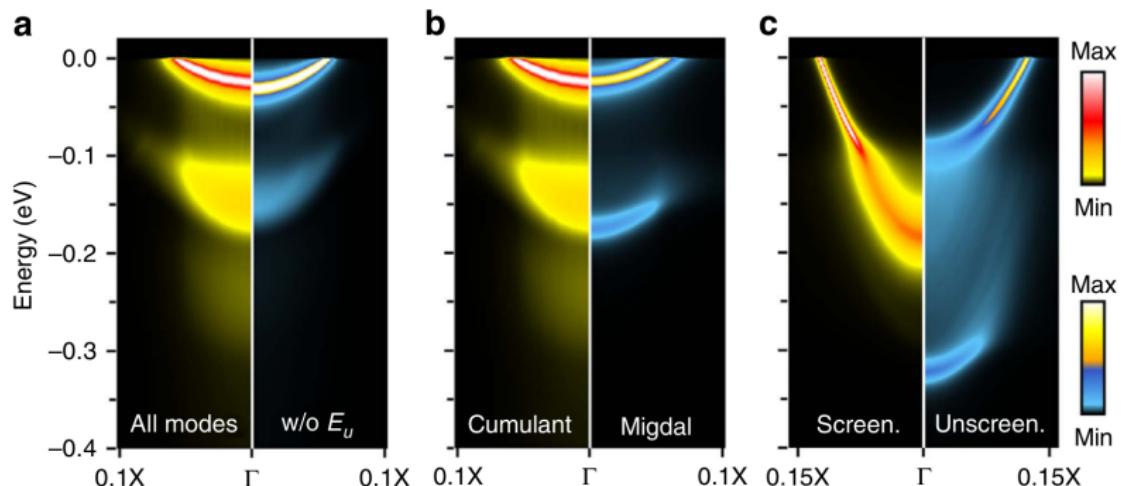


B. Gumhalter, V. Kovač, F. Caruso, H. Lambert and F. Giustino, Phys. Rev. B, **94**, 035103 (2016).



Screening of el-ph in TiO_2

See new input variables: `lscreen`, `scr_typ`, `smear_rpa`



C. Verdi, F. Caruso and F. Giustino, Nat. Commun. **8**, 15769 (2016)



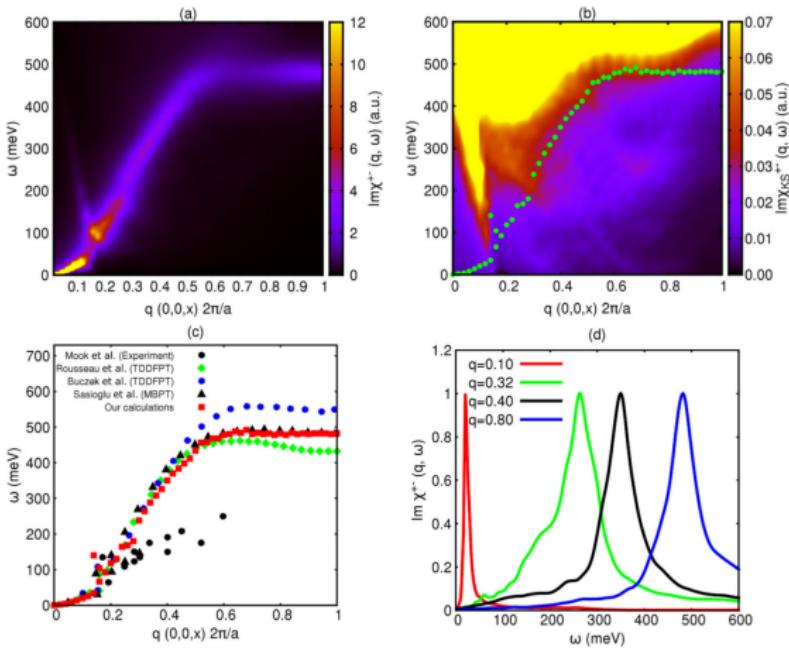
Miscellaneous

- ▶ Possibility to print the electron-phonon vertex using the new `prtgkk` input variable
- ▶ Memory optimization (`etf_mem = 2`). Useful for very big system (20 atoms +)
- ▶ New memory report using the `VmPeak cat` directly from the node.
- ▶ Real and Imaginary part of the phonon self-energy well as the phonon spectral function
- ▶ Restart option (`restart` and `restart_freq`) during the interpolation step



New Magnon implementation [K. Cao]

Comparison between the TDDFPT and KS susceptibility of fcc Ni.





New Magnon implementation [K. Cao]

A lot of work is needed before release of the code

- ▶ Need alignment with QE trunk. Currently compatible with QE 5.0.3
- ▶ Need cleaning, documentations and tests
- ▶ Implementation can be found at
<https://github.com/mmdg-oxford/magnon-dev>
- ▶ The code is open and if people are interested, we are happy to collaborate and join efforts
- ▶ The code is not ready for general use but if anyone is interested we are happy to discuss



Acknowledgments



The Leverhulme Trust





More info



<http://epw.org.uk>



<http://epwforum.uk>



<https://gitlab.com/QEF/q-e>