EPW®

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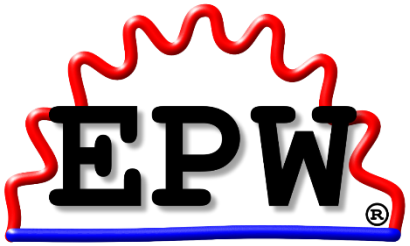
Overview of the code



- Electron-Phonon using Wannier interpolation (EPW)
- Rely on el-ph matrix elements produced by QE
- Interpolate them on a dense k/q grid

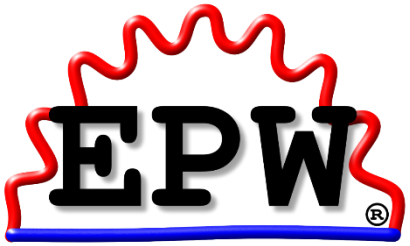
- The code can be used to compute
  - Electron and phonon linewidths & lifetimes
  - ZPR and temperature dependence
  - Eliashberg α^2F, α^2F_T and electronic $A_{n\boldsymbol{k}}(\omega, T)$ spectral function α^2F
  - Anisotropic superconducting gap $\Delta_{n\boldsymbol{k}}$
  - Transport properties

Overview of the code

- EPW rely on some QE routines but need not to modify them

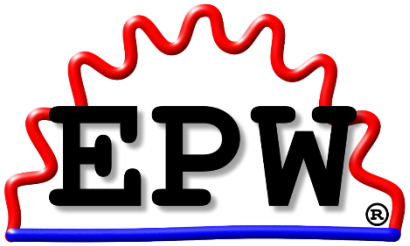
Espresso/EPW/bin
/examples
/src
/tests
/Modules
/Phonon
/PW
/test-suite
/wannier90-2.0.1

Recent developments



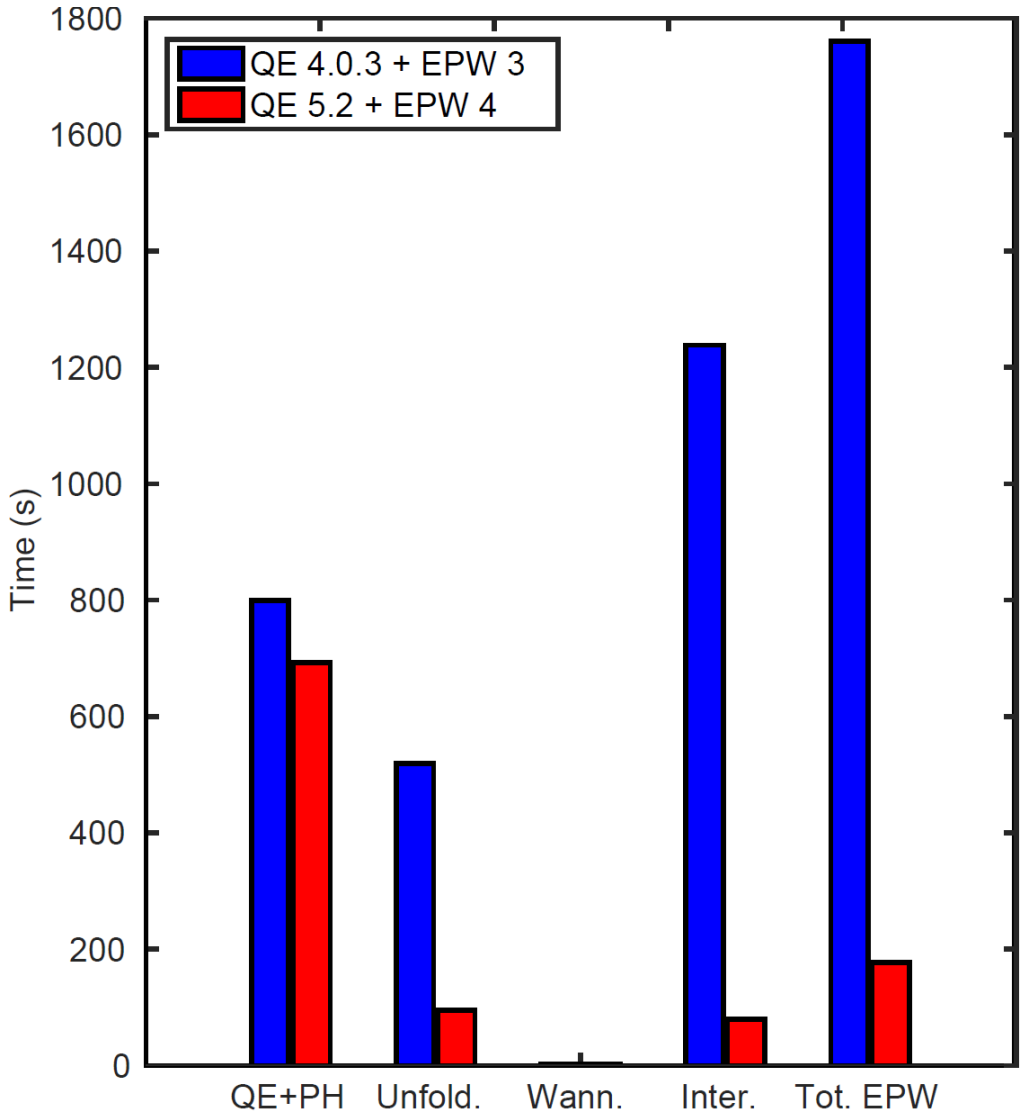
- EPW is now fully compatible with the latest QE trunk and the new Wannier90 2.0.1 lib
- Optimization & cleaning of the code
- Time-reversal symmetry is included
- Polar divergence correctly interpolated
- Spin-orbit coupling included (non-magnetic)
- We plan on releasing EPW in QE in the next 6 weeks

Limitation of the code

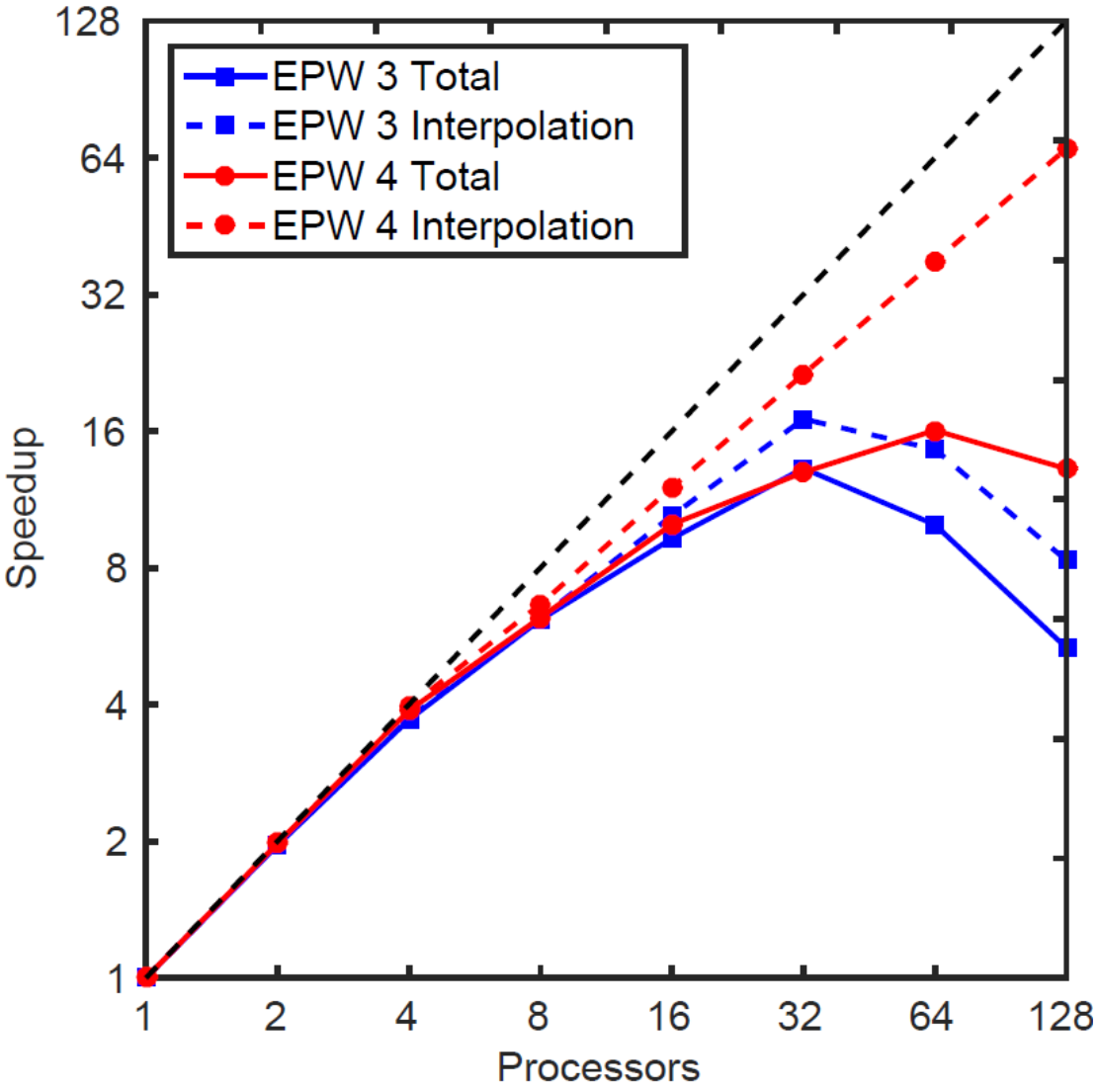


- NC psp only
- No magnetization
- No G-vector parallelization
- Nothing beyond LDA/GGA [not in ph.x]
- No +U [not in ph.x]

Parallelization & Speedup (SiC)



Parallelization & Speedup



Buildbot test farm

- EPW is tested for continuous integration using nightly Buildbot test suites.
- We have 4 hardware slaves: 2 Intel Xeon X5345@2.33Ghz, Opteron P265@1.8Ghz and Intel Core 2 Duo@2.8Ghz
- We plan on adding a Mac

Buildbot test farm

Slaves	OS	Compiler	Flags	Parallel	Library
farmer1	Ubuntu 14.04.3	gcc 4.8.5	-O3 -g -x f95-cpp-input	-	internal
farmer1	Ubuntu 14.04.3	gcc 4.8.5	-O3 -g -x f95-cpp-input	openmpi 1.8.8	internal
farmer1	Ubuntu 14.04.3	intel 12.1.2	-O2 -assume byterecl -g -fpp	openmpi 1.8.8	MKL
farmer1	Ubuntu 14.04.3	intel 13.1.3	-O3 -xHost -assume byterecl -assume buffered_io -fpp	openmpi 1.8.8	MKL + fftw 3.3.4
farmer1	Ubuntu 14.04.3	intel 15.0.3	-O2 -assume byterecl -g -fpp	openmpi 1.8.8	MKL + fftw 3.3.4
farmer2	CentOS 7.1.1503	gcc 5.2.0	-O3 -g -x f95-cpp-input	openmpi 1.8.8	internal
farmer2	CentOS 7.1.1503	pgf90 15.7	-fast	mpich 3.1.3	fftw 3.3.4
farmer2	CentOS 7.1.1503	intel 13.0.1	-O3 -xHost -assume byterecl -assume buffered_io -fpp	mpich 3.1.4	MKL + fftw 3.3.4
farmer2	CentOS 7.1.1503	intel 15.0.3	-O3 -g -x f95-cpp-input	Intel mpi 5.1	MKL + fftw 3.3.4
farmer2	CentOS 7.1.1503	Nag 6.0	-O0 -kind=byte -dcfuns -mismatch	-	internal
farmer3	openSUSE 13.2	gcc 4.9.3	-O3 -g -x f95-cpp-input	mpich 3.1.3	fftw 3.3.4
farmer3	openSUSE 13.2	intel 15.0.3	-O3 -xHost -assume byterecl -assume buffered_io -fpp	mvapich2 2.2a	MKL + FFT MKL

User friendly: tests & tutorials

- EPW has a fully dedicated website: http://epw.org.uk
- Tutorials, tests, documentations and theory are available
- Video tutorials are planned (screen recording + sound)

User friendly: tests & tutorials

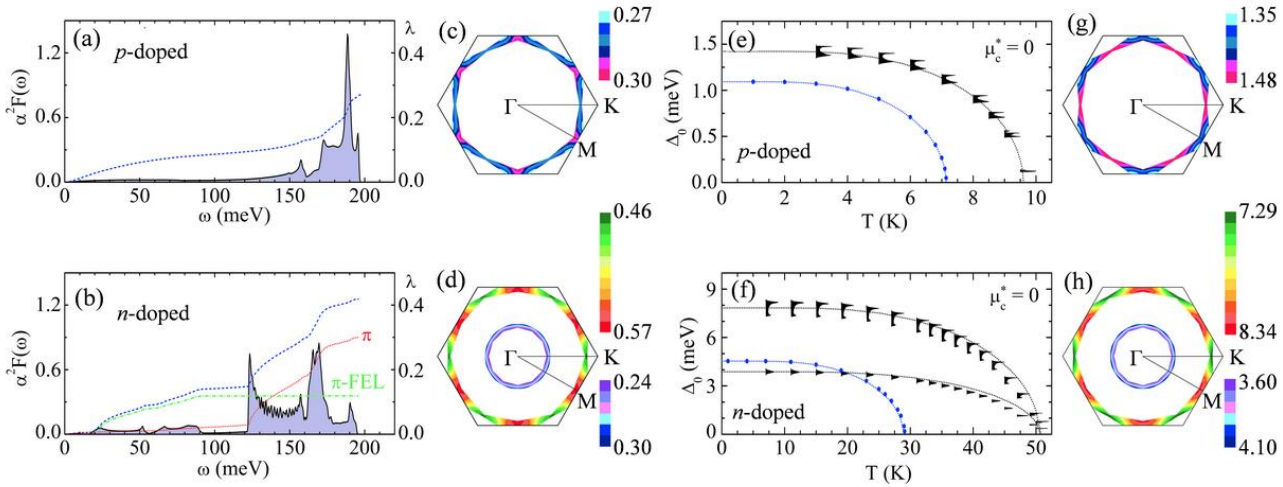
EPW Documentation/Documentation - Mozilla Firefox

epw.org.uk/Documentation/Documentation

EPW

DOCUMENTATION

Here you can find the documentation on the Inputs variables of EPW, the theory behind it and some tutorials (navigate using the right-hand side menu).



PROJECT
About
Documentation
Inputs
Theory
Tutorial
Acknowledge
FAQ
Papers using EPW
Contact

SOURCE CODE
Download and Install
Subversion
Test Farm
Troubleshoot

Edit

EPW dependences on QE

- To not re-invent the wheel, we import modules from QE:
- Modules/
  - mp*, **wavefunctions**, ions_base, cell_base, noncol, io_files, io_global, fft_base, recvec, control_flags
- S3DE/iotk/src/iotk_module
- PW/src/
  - pwcom, start_k, **symm_base**
- PHonon/PH/
  - **phcom, smallgq, set_small_group_of_q**
- PP/src/sym_band, cryst_to_car
- Wannier90-2.0.1/src
  - parameters, wannier_libs, wannierise

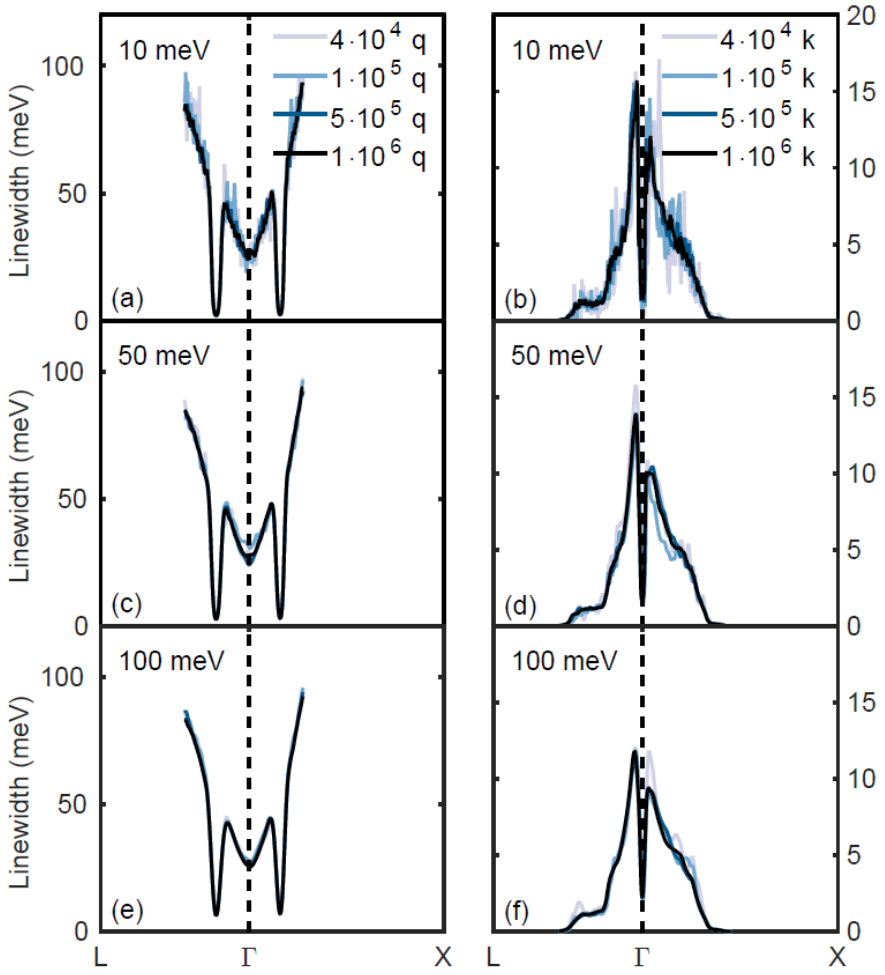
Test case: B-doped diamond

- Electron linewidth $= \Im\Sigma_{n\boldsymbol{k}}$

$$\Sigma_{n\mathbf{k}}(\omega, T) = \sum_{m\nu} \int_{BZ} \frac{d\mathbf{q}}{\Omega_{BZ}} |g_{mn,\nu}(\mathbf{k}, \mathbf{q})|^2 \left[\frac{n_{\mathbf{q}\nu}(T) + f_{m\mathbf{k}+\mathbf{q}}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}\nu} + i\delta} + \frac{n_{\mathbf{q}\nu}(T) + 1 - f_{m\mathbf{k}+\mathbf{q}}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}\nu} + i\delta} \right]$$

- Phonon linewidth $= \Im\Pi_{n\boldsymbol{k}}$

$$\Pi_{\mathbf{q}\nu}(\omega, T) = \sum_{mn} \int_{BZ} \frac{d\mathbf{k}}{\Omega_{BZ}} |g_{mn,\nu}(\mathbf{k}, \mathbf{q})|^2 \frac{f_{n\mathbf{k}}(T) - f_{m\mathbf{k}+\mathbf{q}}(T)}{\omega - \varepsilon_{m\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}\nu} + i\delta}$$

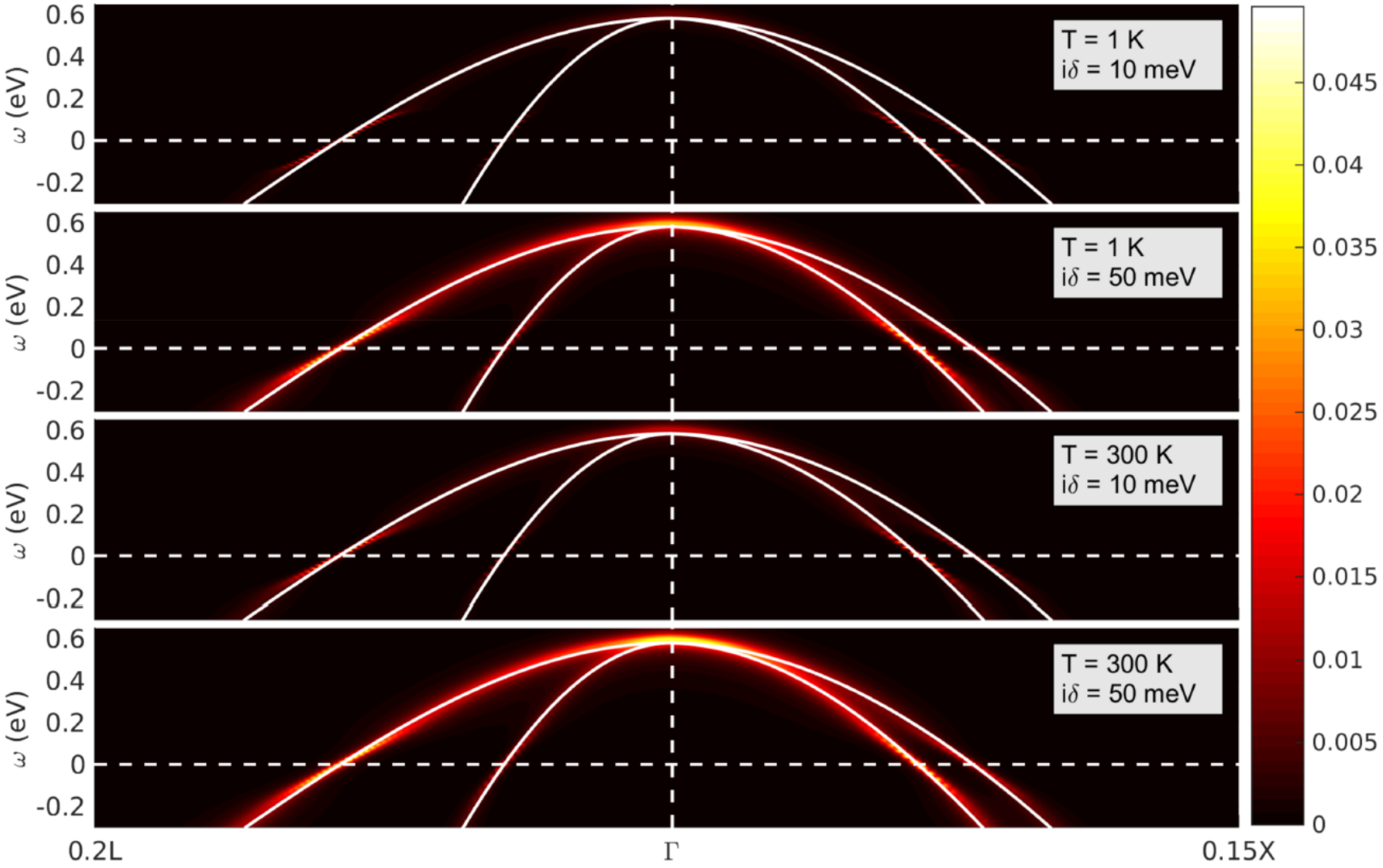


Test case: B-doped diamond

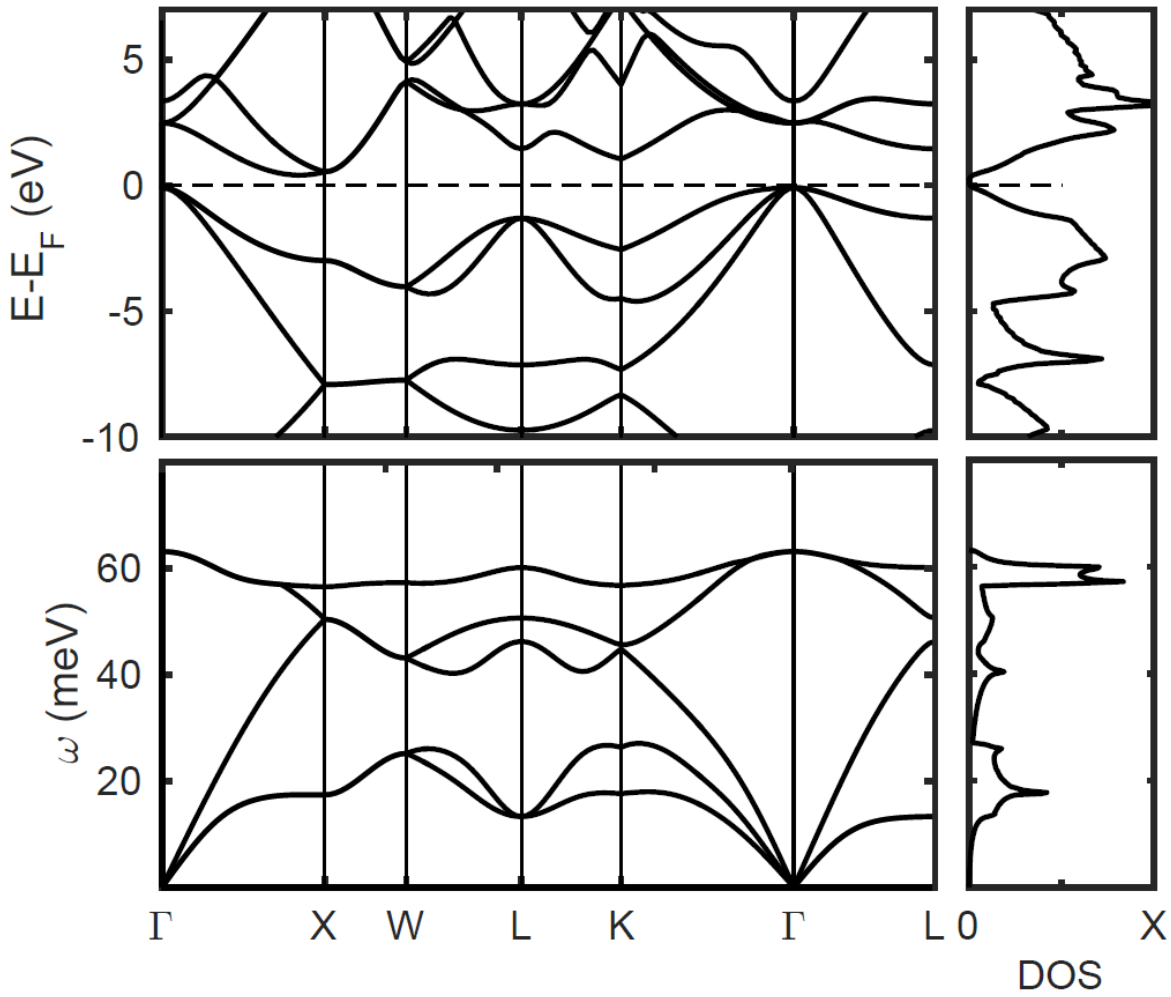
- Spectral function

$$A_{n\mathbf{k}}(\omega, T) = \frac{1}{\pi} \frac{|\Sigma''_{n\mathbf{k}}(\omega, T)|}{|\omega - \varepsilon_{n\mathbf{k}} - \Sigma'_{n\mathbf{k}}(\omega, T)|^2 + |\Sigma''_{n\mathbf{k}}(\omega, T)|}$$

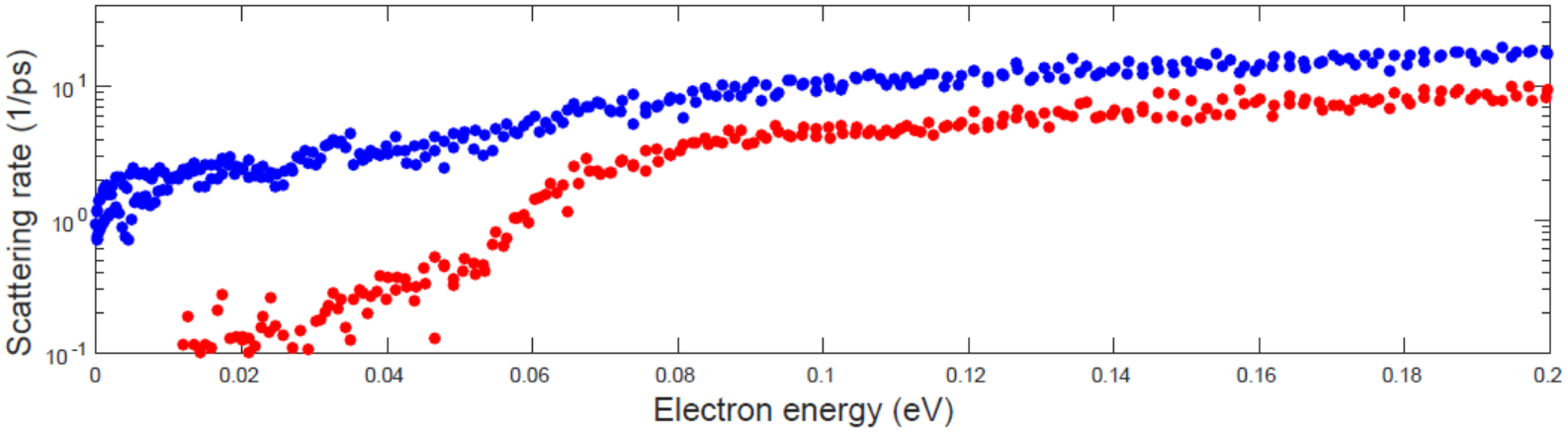
Test case: B-doped diamond

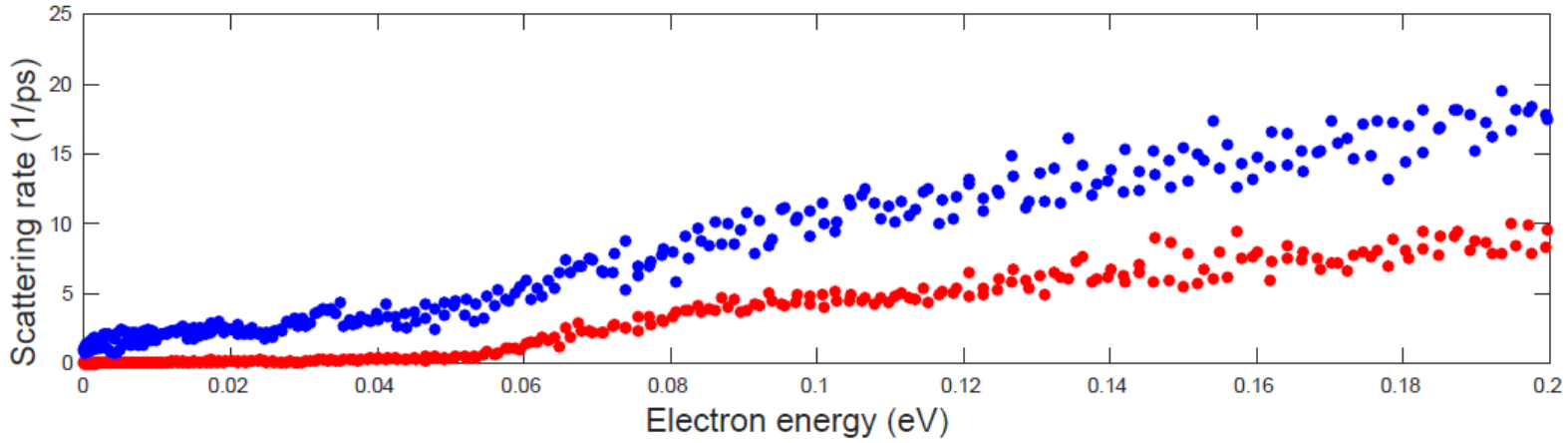


Test case: Si scattering rate



Test case: Si scattering rate from CBM



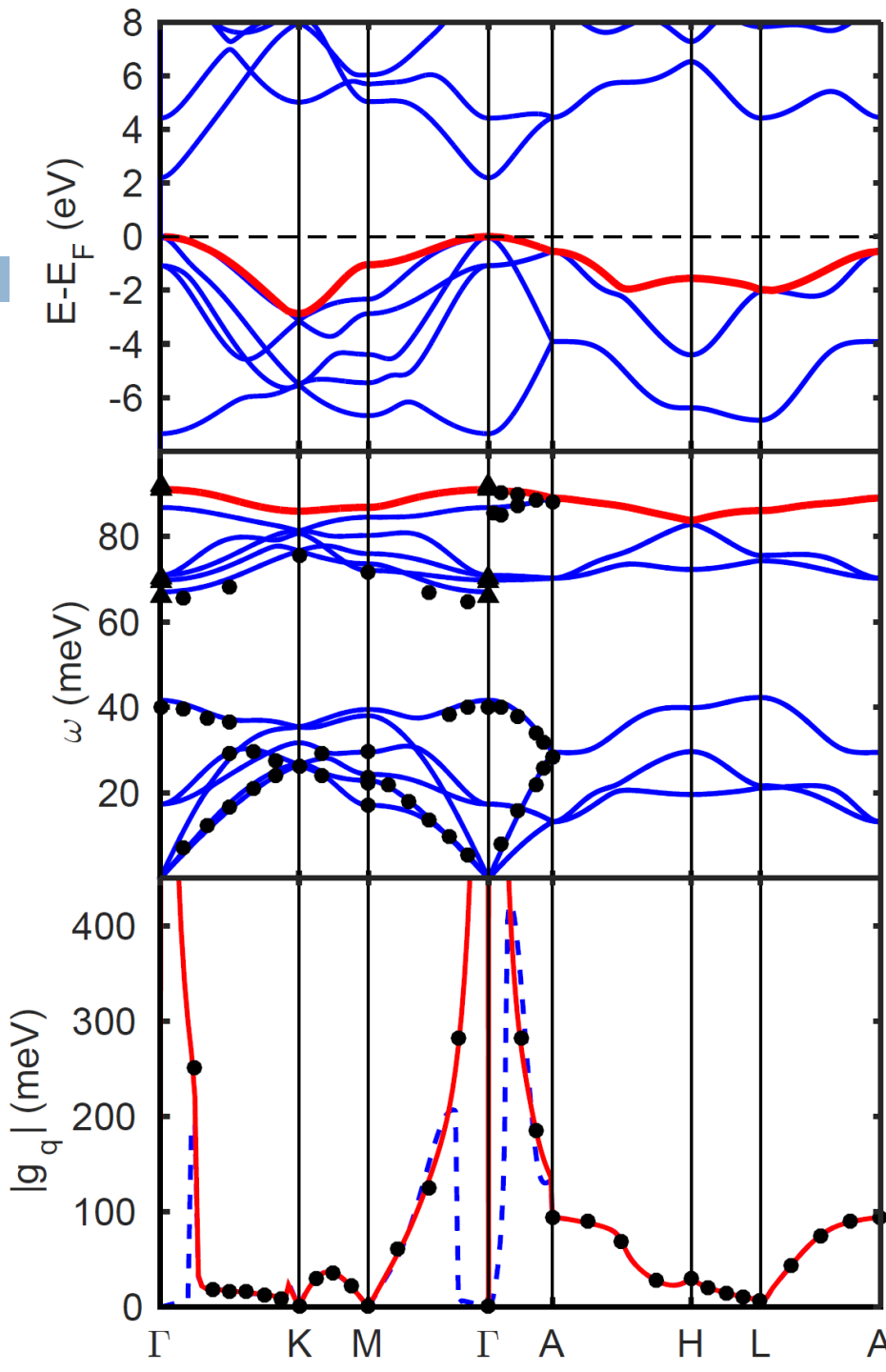


Test case: GaN

- The electron-phonon matrix elements:

$$g_{mn,\nu}(\mathbf{k},\mathbf{q}) = \left(\frac{\hbar}{2m_0\omega_{\mathbf{q}\nu}}\right)^{1/2} \langle \psi_{m\mathbf{k}+\mathbf{q}} | \partial_{\mathbf{q}\nu} V | \psi_{n\mathbf{k}} \rangle$$

- Diverge as $\frac{1}{q}$ for $q \to 0$ in polar materials



Test case: GaN

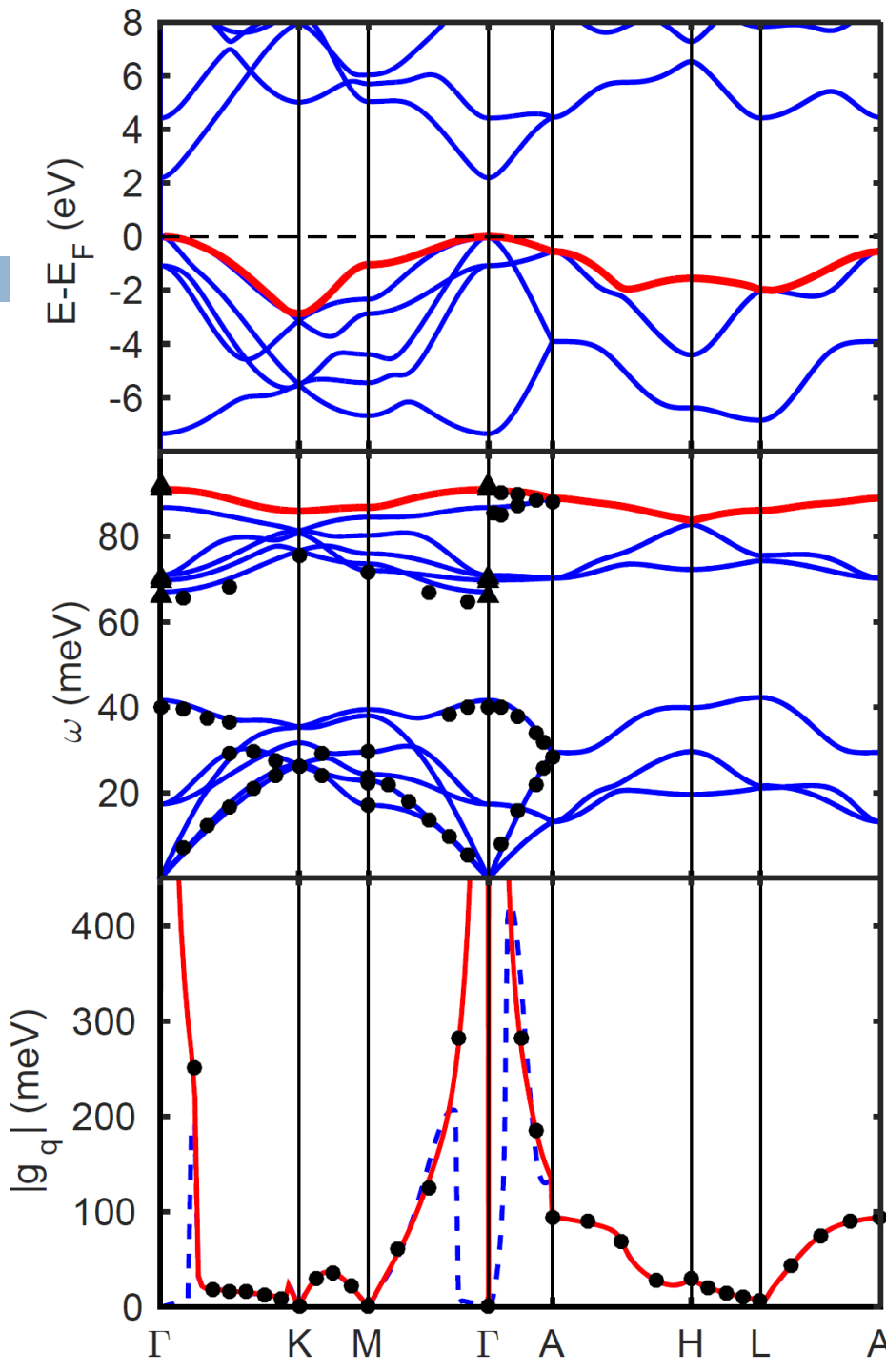
- Correct Wannier interpolation:

$$g_{mn,\nu}(\mathbf{k},\mathbf{q}) = g^{\mathcal{S}}_{mn,\nu}(\mathbf{k},\mathbf{q}) + g^{\mathcal{L}}_{mn,\nu}(\mathbf{k},\mathbf{q})$$

$$g^{\mathcal{L}}_{mn,\nu}(\mathbf{k},\mathbf{q}) = i\sum_{\kappa}\left(\frac{\hbar}{2M_{\kappa}\omega_{\mathbf{q}\nu}}\right)^{1/2}$$

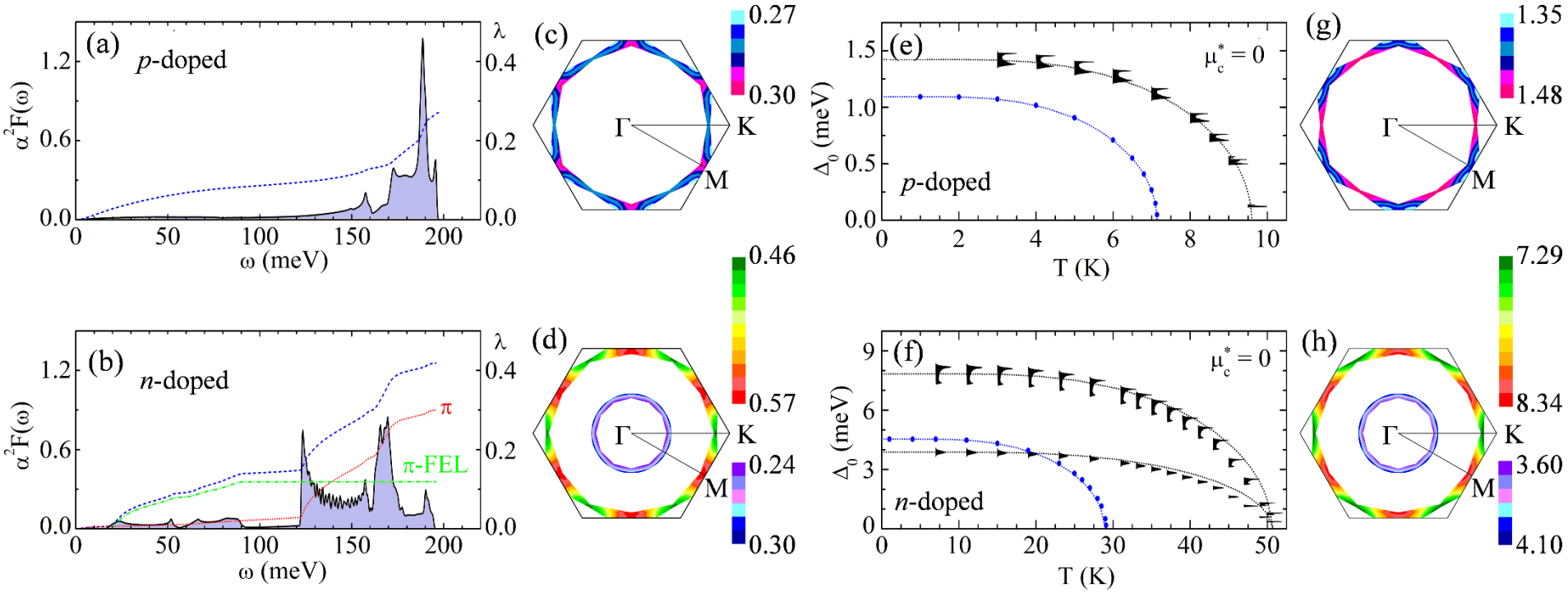
$$\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{(\mathbf{q}+\mathbf{G})\cdot\mathbf{Z}^{*}{}_{\kappa}\cdot\mathbf{e}_{\kappa,\nu}(\mathbf{q})}{(\mathbf{q}+\mathbf{G})\cdot\boldsymbol{\varepsilon}\cdot(\mathbf{q}+\mathbf{G})}\langle\psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle$$

$$\langle\psi_{m\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle = [U_{\mathbf{k}+\mathbf{q}}U_{\mathbf{k}^{\dagger}}]_{mn}$$



Test case: doped-graphene

- Superconducting gap & T_c



Conclusion & future developments

- Current version of EPW4
  - is fully compatible with QE and W90
  - is tested on different hardware & compilers with different libraries
  - has been optimized + new features implemented

- Future
  - G-vector parallelization
  - US (PAW) support
  - Expand the test farm: add mac hardware & power 8 (xlf)
  - Add new features related to transport (conductivity, resistivity etc…)

Acknowledgments

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