First Principles Workshop

An introduction and hands-on tutorial with the Quantum ESPRESSO

Quantum Espresso & Wannier90

by N. T. Hung, A. R. T. Nugraha and R. Saito group

http://flex.phys.tohoku.ac.jp

Ultra-dense electron structure

NANO LETTERS

Letter

pubs.acs.org/NanoLett

Electron–Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene

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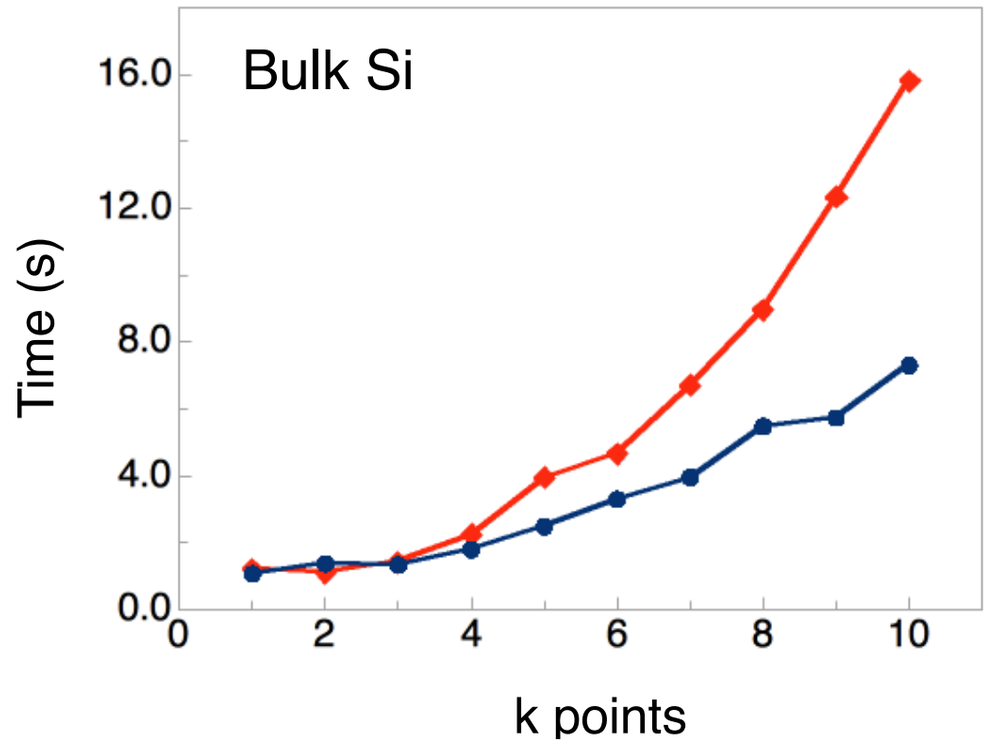
The transport Eliashberg function

$$\alpha^2_{\mathrm{tr}}F(\omega) = \frac{1}{N_\uparrow}\sum_{m'm\nu}\int\int \frac{d\mathbf{p}}{A_{\mathrm{BZ}}}\frac{d\mathbf{q}}{A_{\mathrm{BZ}}}|g^{\nu}_{m',m}(\mathbf{p},\mathbf{q})|^2 \times \delta(\varepsilon_{m',\mathbf{p}+\mathbf{q}} - E_{\mathrm{F}})\delta(\varepsilon_{m,\mathbf{p}} - E_{\mathrm{F}})\delta(\hbar\omega^{\nu}_{\mathbf{q}} - \hbar\omega) \times \left(1 - \frac{\mathbf{v}_{\mathbf{p}+\mathbf{q},m'}\cdot\mathbf{v}_{\mathbf{p},m}}{|\mathbf{v}_{\mathbf{p},m}|^2}\right)$$



Band velocities and delta function need ultra-dense electron structure

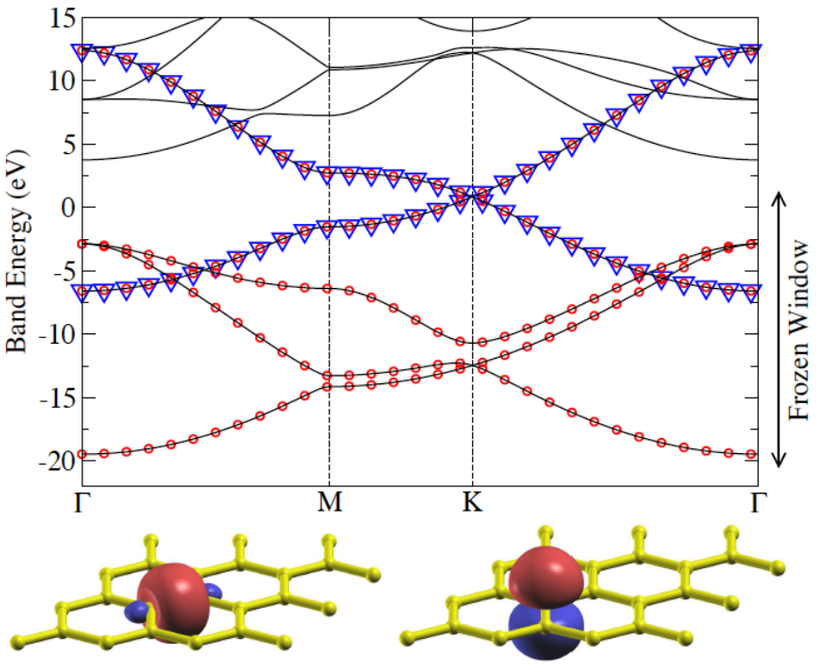
For example: 1000 × 1000 k-points or q-points

How we can do that with density function theory ???

Tight-binding

Compact mapping of Bloch states into local orbitals

Graphene



sp^2 orbitals

p_z orbitals

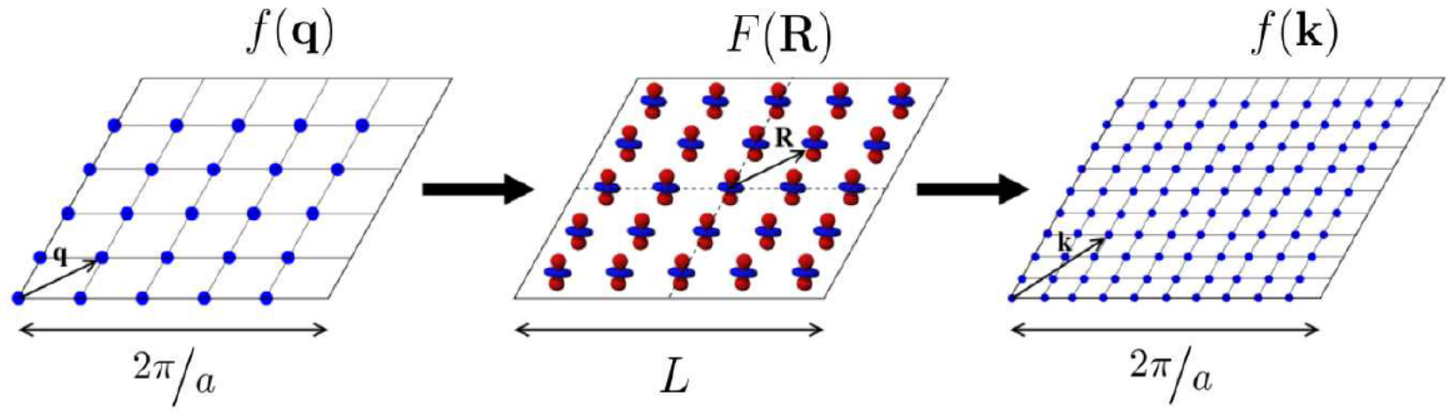
N. Marzari et al, Rev. Mod. Phys. 84, 1419 (2012)

Wannier funcitions

Wave functions from DFT calc.

$$w_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{\mathbf{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})\,d\mathbf{k}$$

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_R}}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} w_n(\mathbf{r}-\mathbf{R})\,d\mathbf{k}$$



DFT calc. on coarse grid

Wannier interpolation

Cheap calc. on fine grid

How to run a Wannier90 calculation

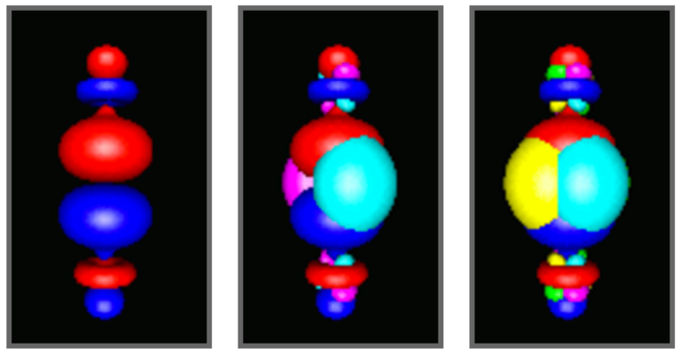
http://www.wannier.org/download.html

WANNIER90

Home History Download User Guide Forum Papers Features People

Welcome!

This is the home of maximally-localised Wannier functions (MLWFs) and Wannier90, the computer program that calculates them. Wannier90 is released under the GNU General Public License.



Latest News

2 APRIL 2015

Wannier90 (v2.0.1) is now available for download here.

See here for our news archive.

Please cite

Wannier90: A Tool for Obtaining Maximally-Localised Wannier Functions
A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari
Comput. Phys. Commun. **178**, 685 (2008) [ONLINE JOURNAL]

in all publications resulting from your use of Wannier90.

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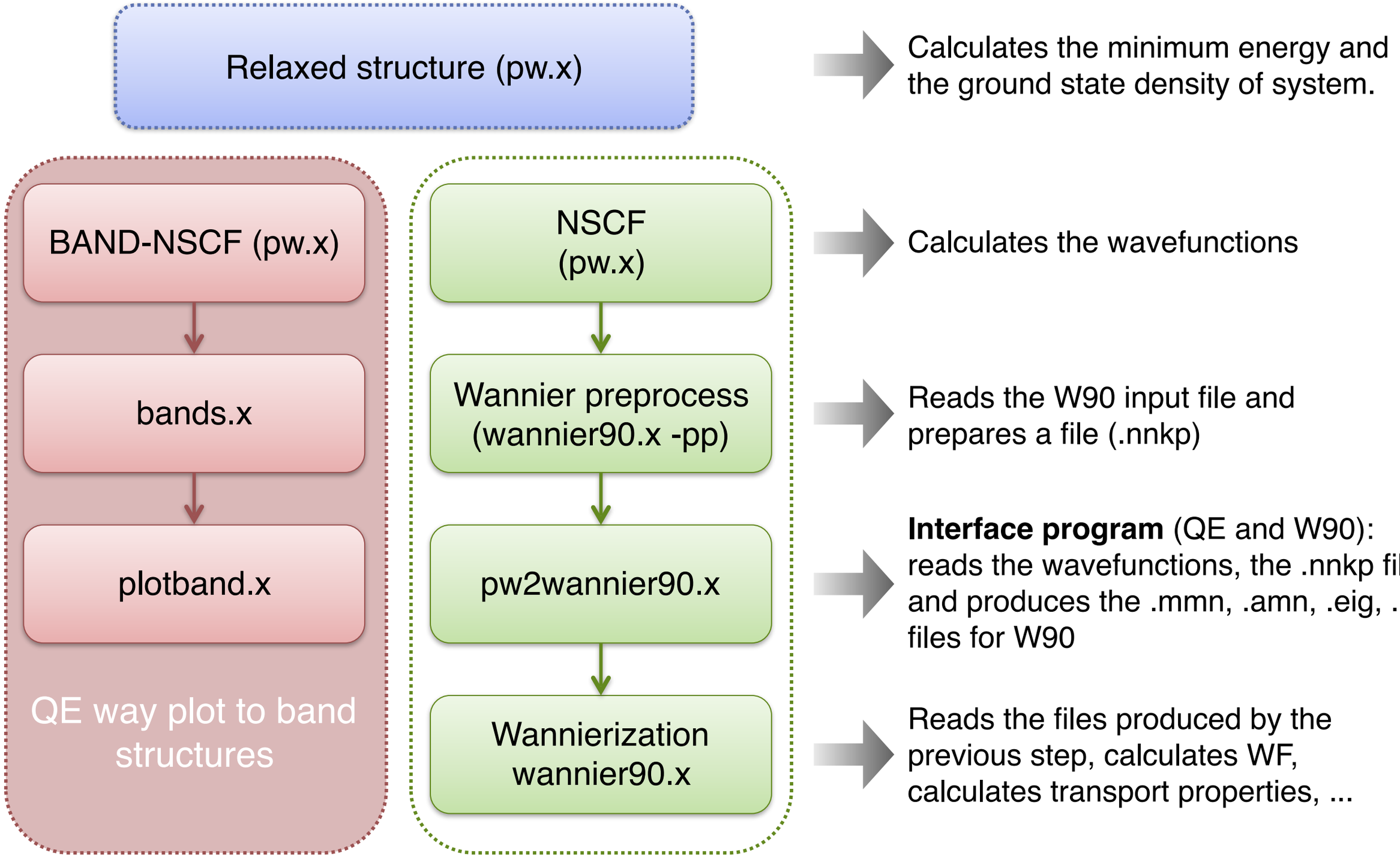
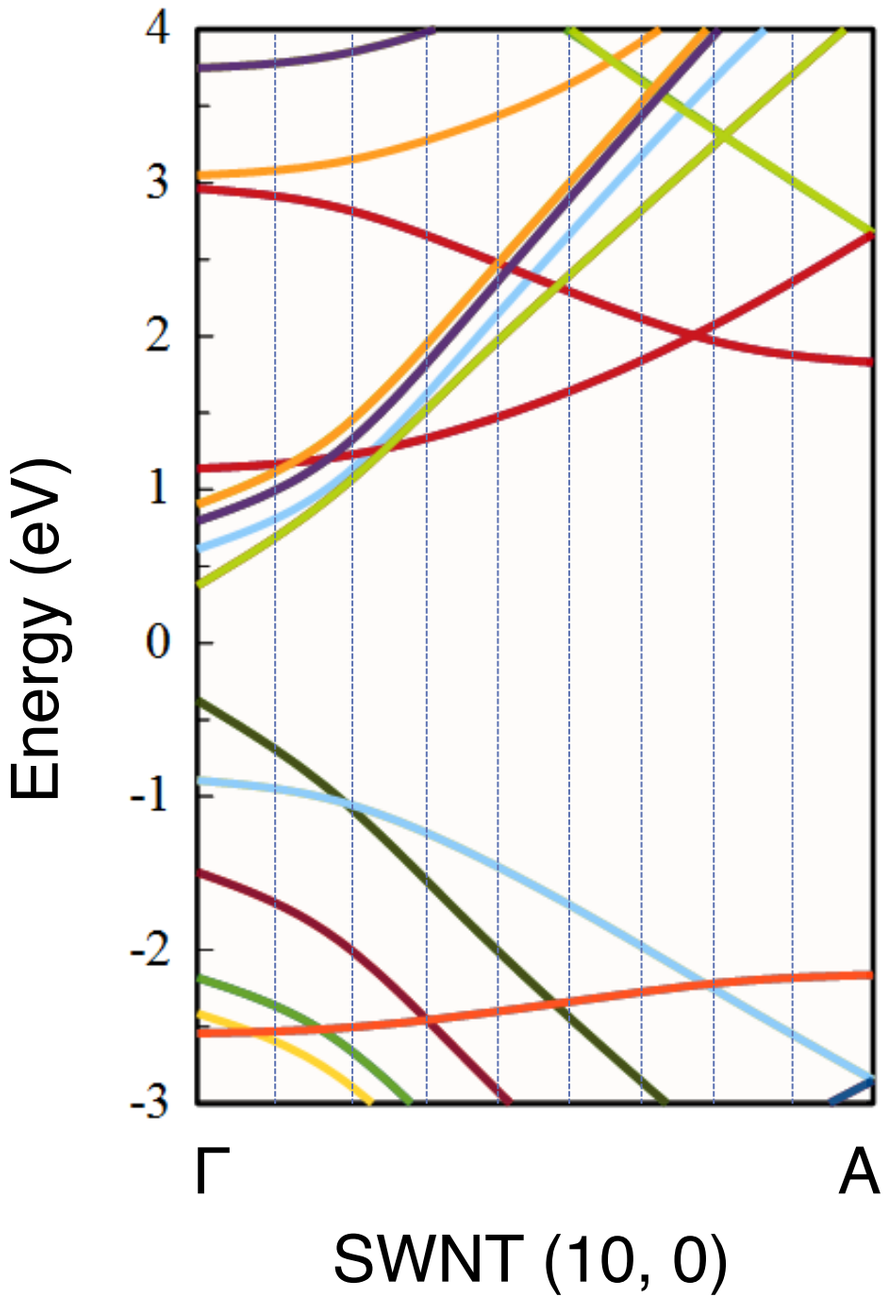
How to run a Wannier90 calculation



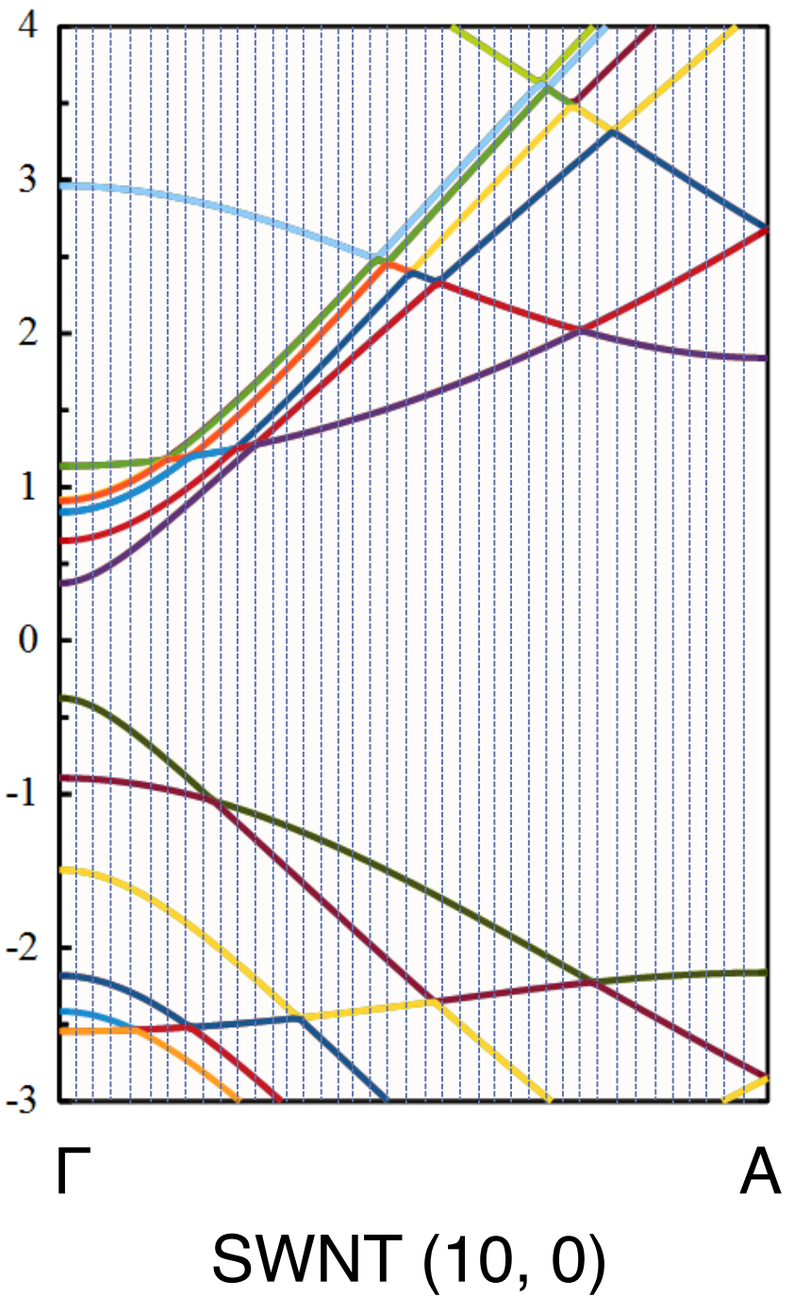
QE & Wannier90

QE with coarse
10-grid

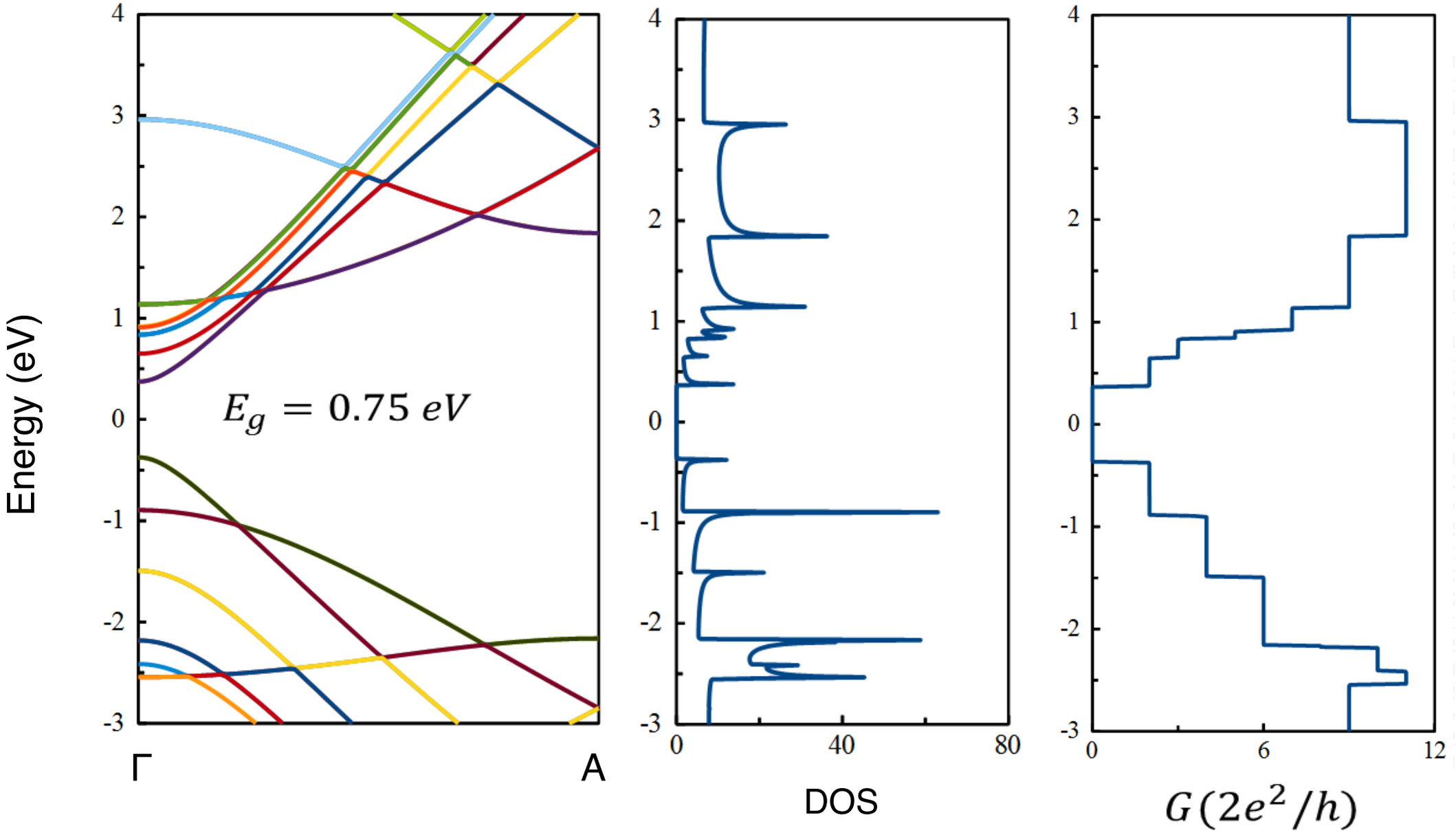


WFs
(interpolate)

QE & W90 with
fine 100-grid



QE & Wannier90



SWNT (10, 0)

Thermoelectricity

Ab initio (DFT)

Ultra-dense electronic structure

Boltzmann transport equation

$$v_\alpha(i,\mathbf{k}) = \frac{1}{\hbar}\frac{\partial\varepsilon(i,\mathbf{k})}{\partial k_\alpha} \quad ; \quad \sigma_{\alpha\beta}(\varepsilon) = \frac{e^2}{N}\sum_{i,\mathbf{k}} \tau(i,\mathbf{k})\, v_\alpha(i,\mathbf{k})\, v_\beta(i,\mathbf{k})\, \delta[\varepsilon - \varepsilon(i,\mathbf{k})]$$

$$\sigma_{\alpha\beta}(T,\mu) = \frac{1}{\Omega}\int \sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right] \mathrm{d}\varepsilon$$ Electrical conductivity

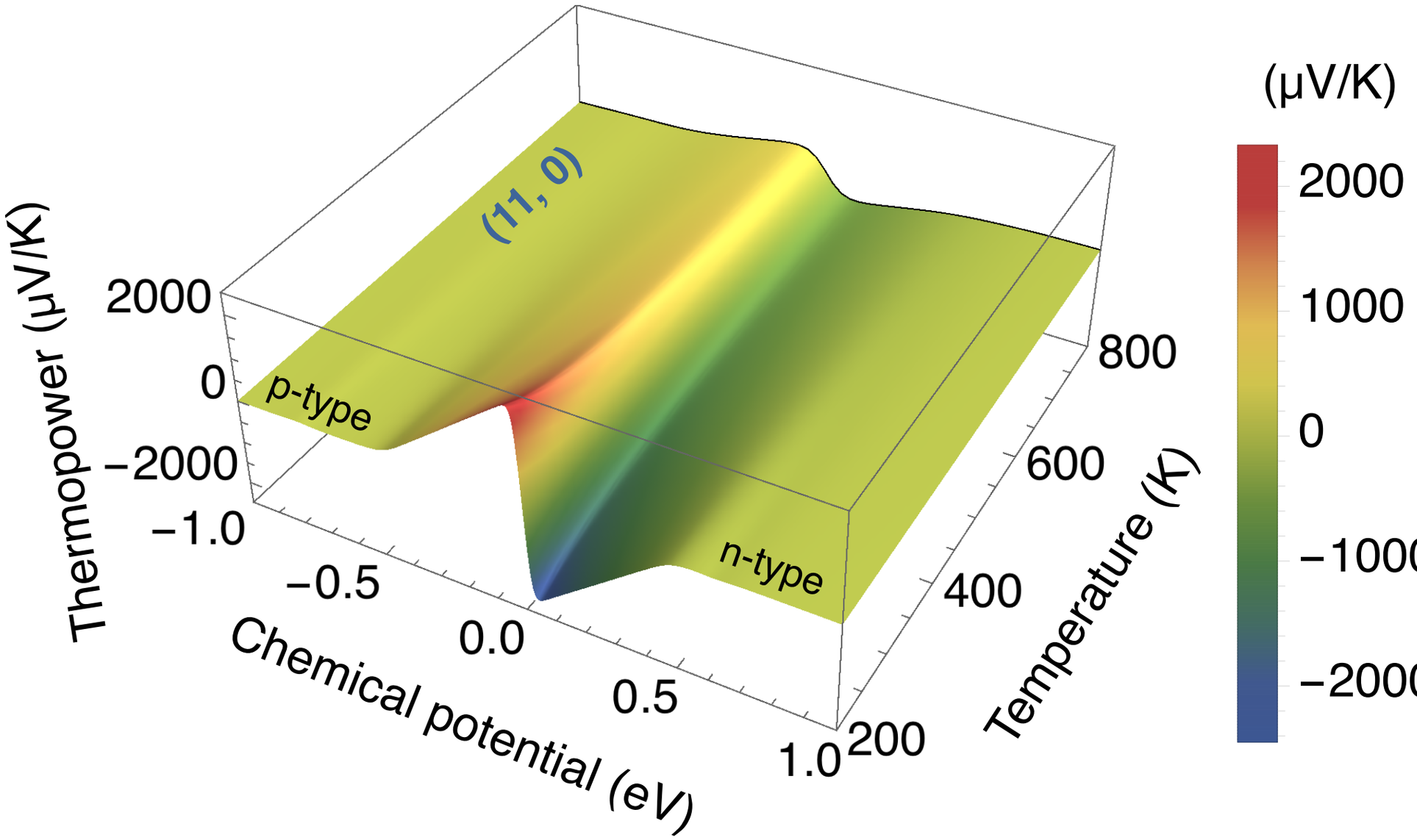
$$S_{\alpha\beta}(T,\mu) = \frac{1}{eT\Omega\sigma_{\alpha\beta}(T,\mu)}\int \sigma_{\alpha\beta}(\varepsilon)(\varepsilon-\mu)\times\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right] \mathrm{d}\varepsilon$$ Seebeck coefficient

$$\kappa^0_{\alpha\beta}(T,\mu) = \frac{1}{eT\Omega}\int \sigma_{\alpha\beta}(\varepsilon)(\varepsilon-\mu)^2\times\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right] \mathrm{d}\varepsilon$$ Electronic thermal conductivity

$$\kappa_e = \kappa^0 - S^2\sigma T$$

Thermopower

Thermoelectricity

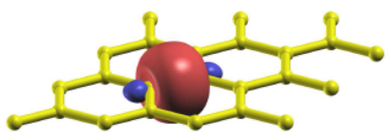


N. T. Hung, et al, PRB 92 (2015) 165426.

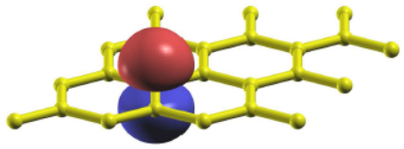
Exercises

Files for Wannier90

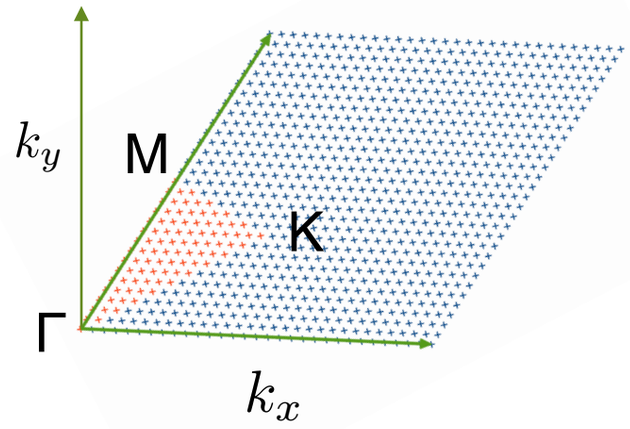
/graphene-wannier90/

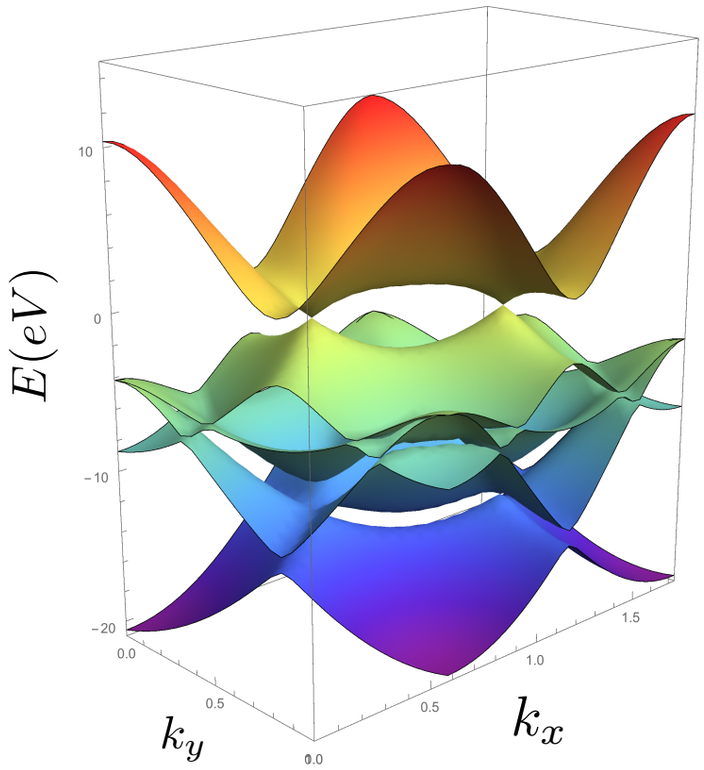


3 sp^2 orbitals



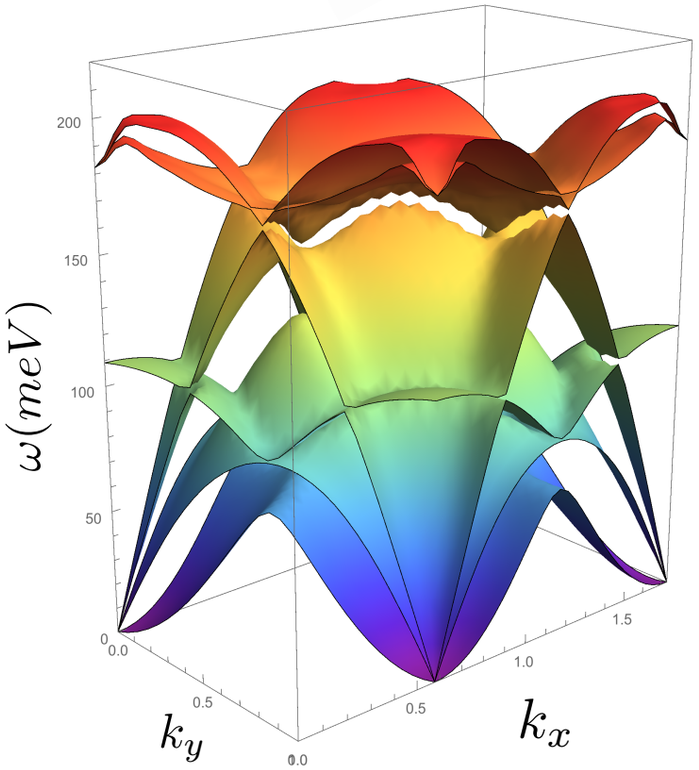
2 p_z orbitals





Band structures

10^6 **k** points



Phonon dispersions

10^4 q points

thank you!