



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

Electron–Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene

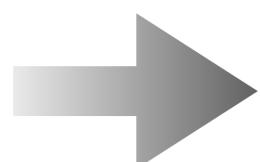
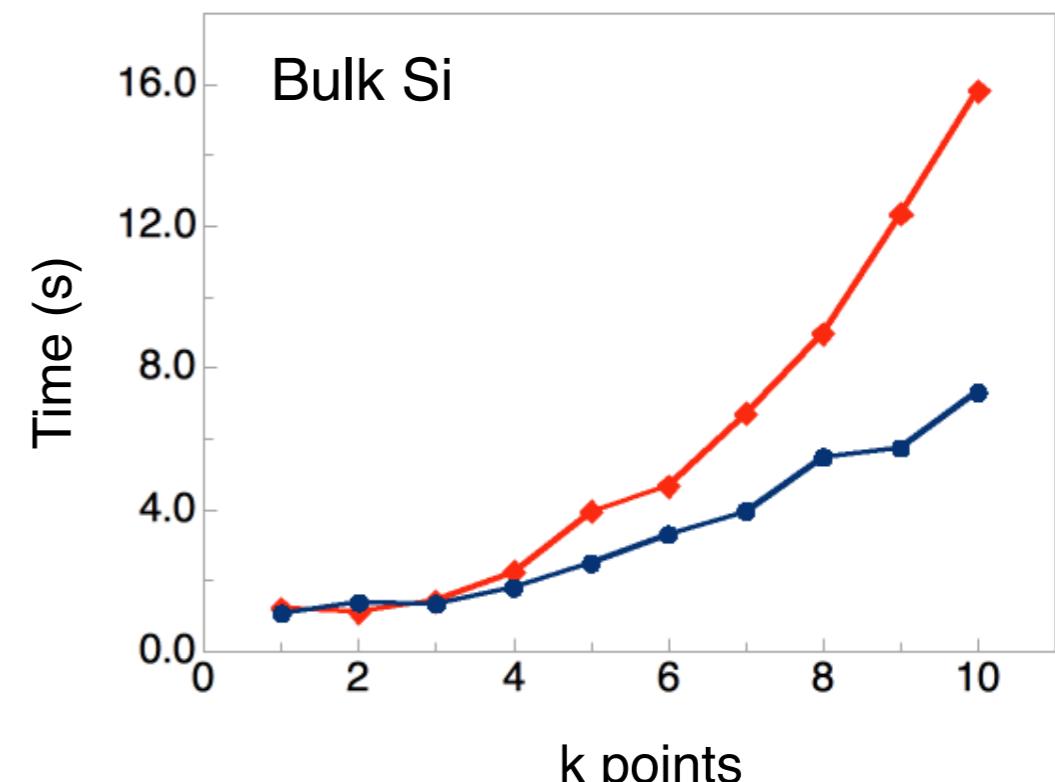
Cheol-Hwan Park,^{*,†,‡,§,¶} Nicola Bonini,^{*,||,¶} Thibault Sohier,[⊥] Georgy Samsonidze,[‡] Boris Kozinsky,[‡] Matteo Calandra,[⊥] Francesco Mauri,[⊥] and Nicola Marzari[†]

The transport Eliashberg function

$$\alpha_{tr}^2 F(\omega) = \frac{1}{N_\uparrow} \sum_{m'm\nu} \iint \frac{d\mathbf{p}}{A_{BZ}} \frac{d\mathbf{q}}{A_{BZ}} |g_{m',m}^\nu(\mathbf{p}, \mathbf{q})|^2 \\ \times \delta(\epsilon_{m',\mathbf{p}+\mathbf{q}} - E_F) \delta(\epsilon_{m,\mathbf{p}} - E_F) \delta(\hbar\omega_q^\nu - \hbar\omega) \\ \times \left(1 - \frac{\mathbf{v}_{\mathbf{p}+\mathbf{q},m'} \cdot \mathbf{v}_{\mathbf{p},m}}{|\mathbf{v}_{\mathbf{p},m}|^2} \right)$$

Band velocities and delta function need ultra-dense electron structure

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

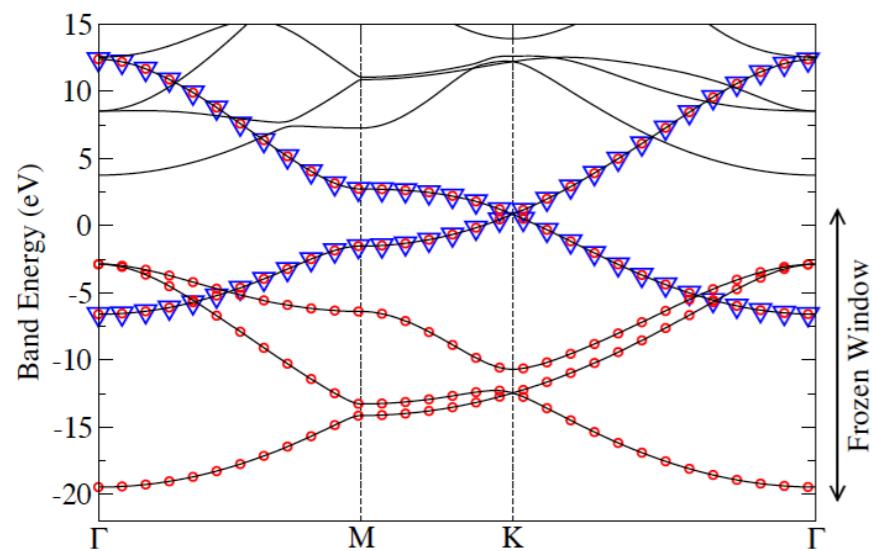


How we can do that with density function theory ???

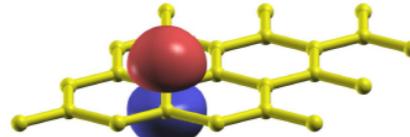
Tight-binding

Compact mapping of **Bloch states** into **local orbitals**

Graphene



sp^2 orbitals



p_z orbitals

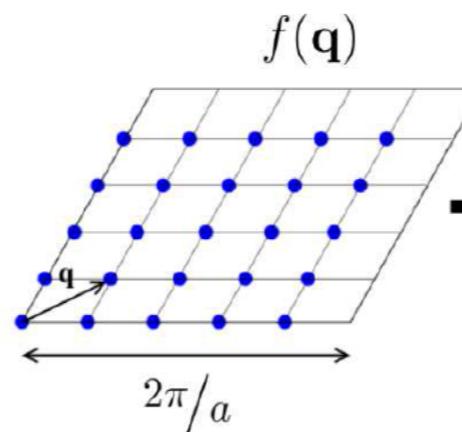
N. Marzari et al, Rev. Mod. Phys. 84, 1419 (2012)

Wannier
functions

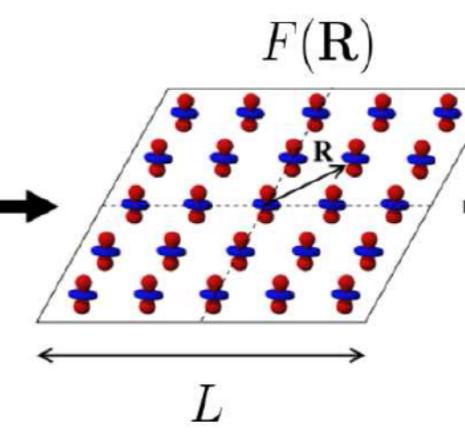
$$w_n(\mathbf{r} - \mathbf{R}) = \frac{V}{8\pi^3} \int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r}) d\mathbf{k}$$

Wave functions from
DFT calc.

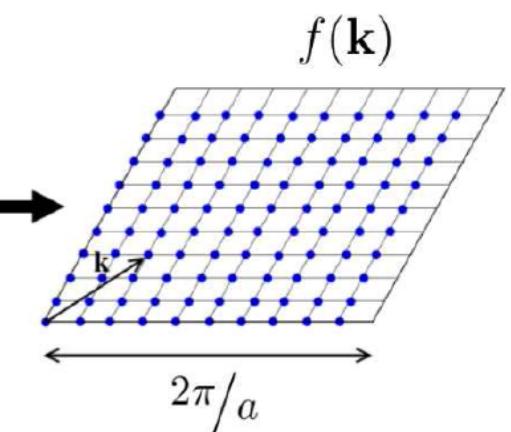
$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_R}} \int_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} w_n(\mathbf{r} - \mathbf{R}) d\mathbf{k}$$



DFT calc. on
coarse grid



Wannier
interpolation



Cheap calc. on
fine grid

How to run a Wannier90 calculation

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

The screenshot shows the Wannier90 website. At the top, there is a blue header bar with the text "WANNIER90". Below it is a white navigation bar with links: Home, History, Download, User Guide, Forum, Papers, Features, and People. The "Download" link is highlighted with a red oval and a red arrow pointing down to it from the title above. The main content area has a "Welcome!" section with a brief description of the software. Below that is a "Latest News" section dated "2 APRIL 2015" announcing the availability of version 2.0.1 for download. There is also a link to the news archive. Further down, there is a "Please cite" section with a reference to a paper in "Comput. Phys. Commun." and a request to cite it in publications. At the bottom, there are logos for various institutions: University of Oxford, Imperial College London, Universidad del País Vasco, Euskal Herriko Unibertsitatea, Rutgers, and EPFL.

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.

UNIVERSITY OF OXFORD

Imperial College London

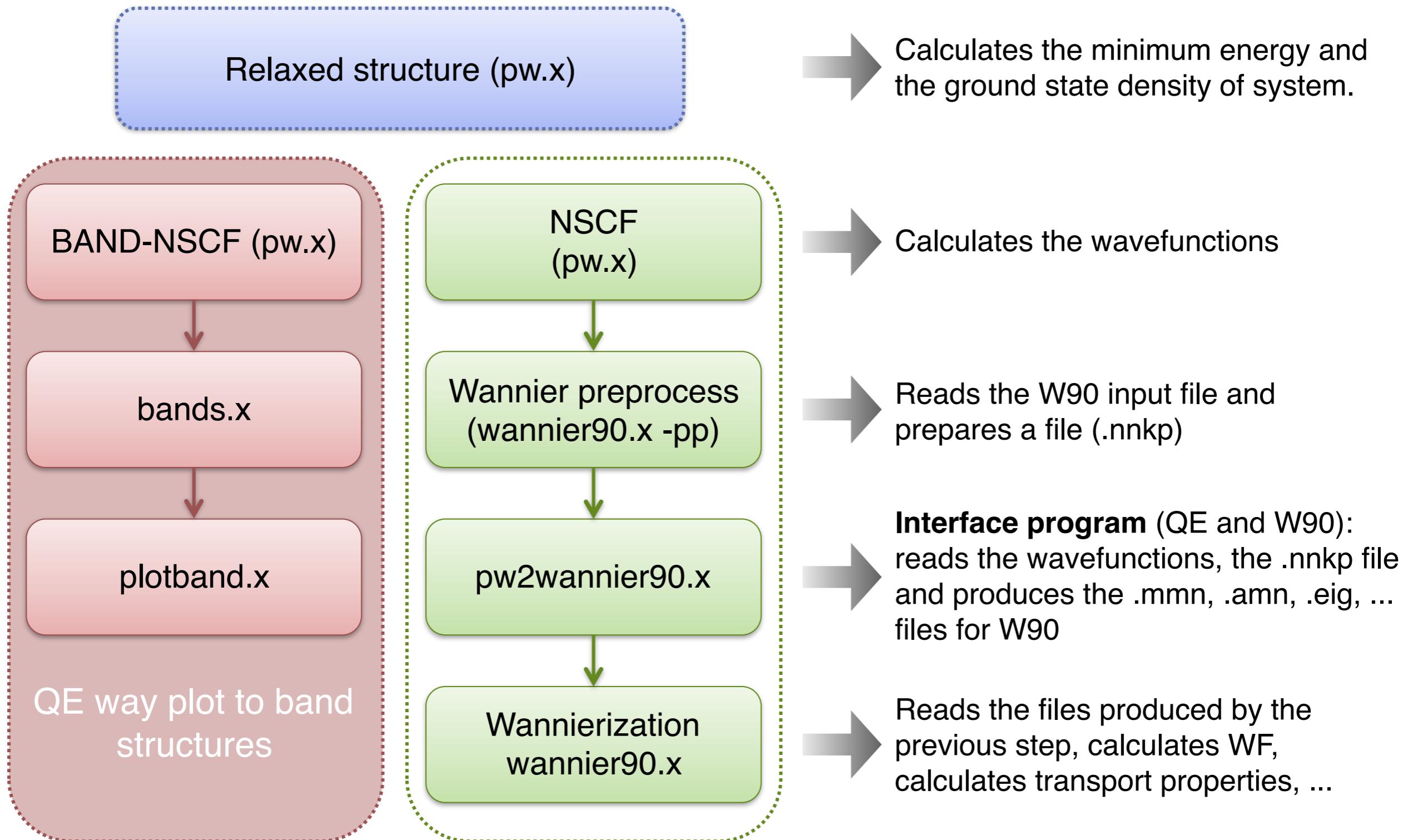
Universidad del País Vasco

Euskal Herriko Unibertsitatea

RUTGERS THE STATE UNIVERSITY OF NEW JERSEY

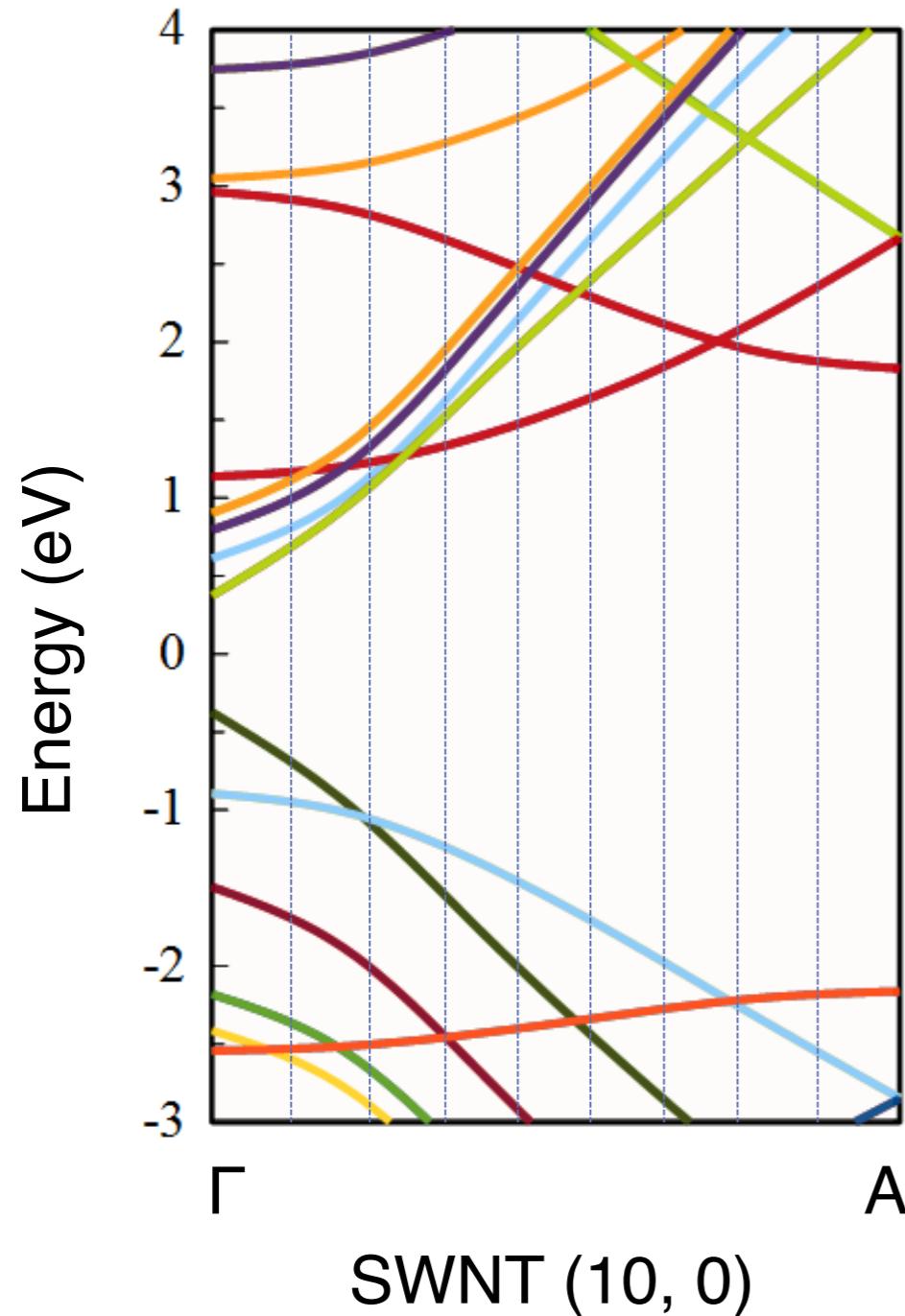
EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

How to run a Wannier90 calculation

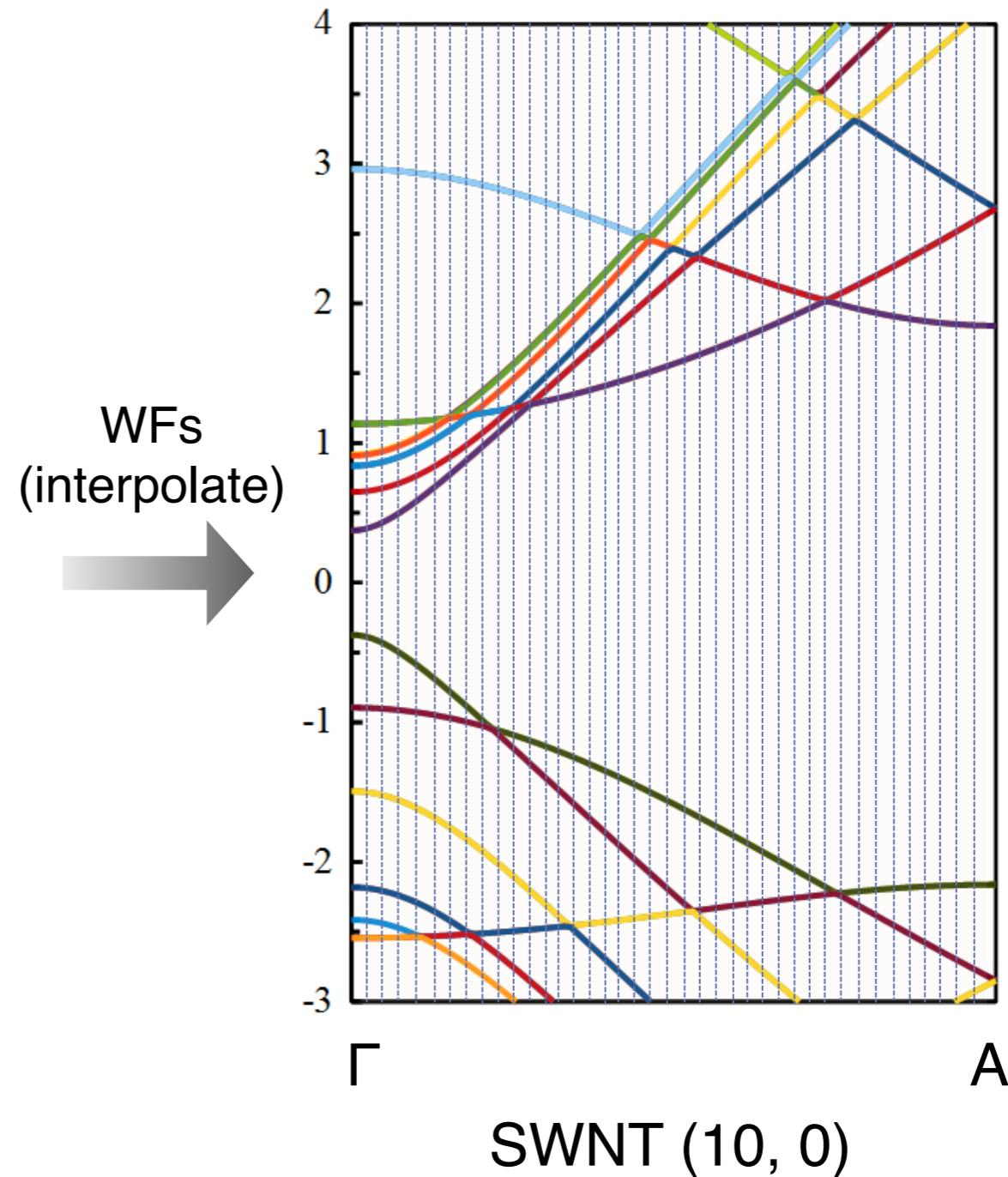


QE & Wannier90

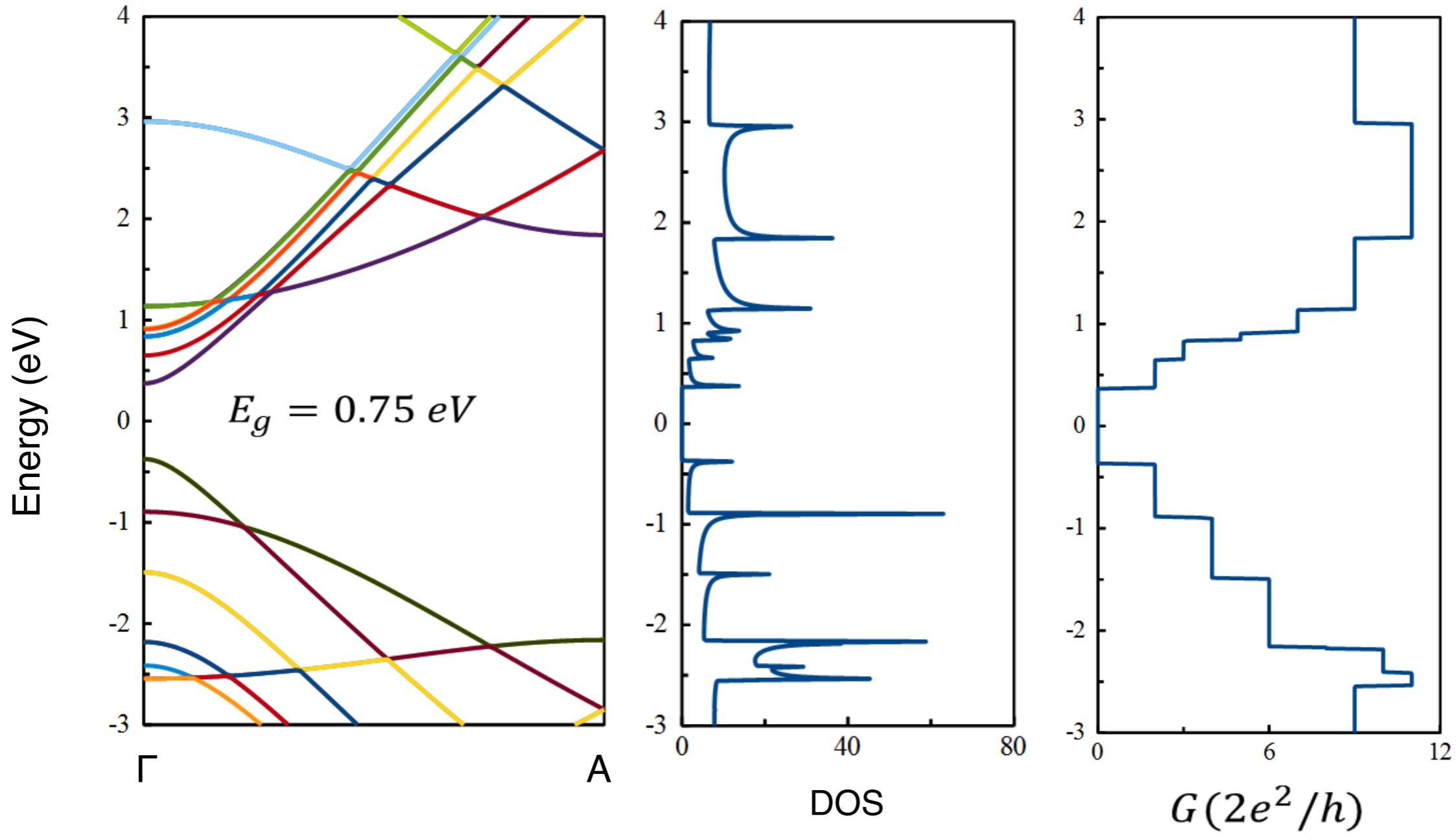
QE with coarse
10-grid



QE & W90 with
fine 100-grid



QE & Wannier90



SWNT (10, 0)

Thermoelectricity

■ Ab initio (DFT)

Ultra-dense electronic structure

Boltzmann transport equation

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

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

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

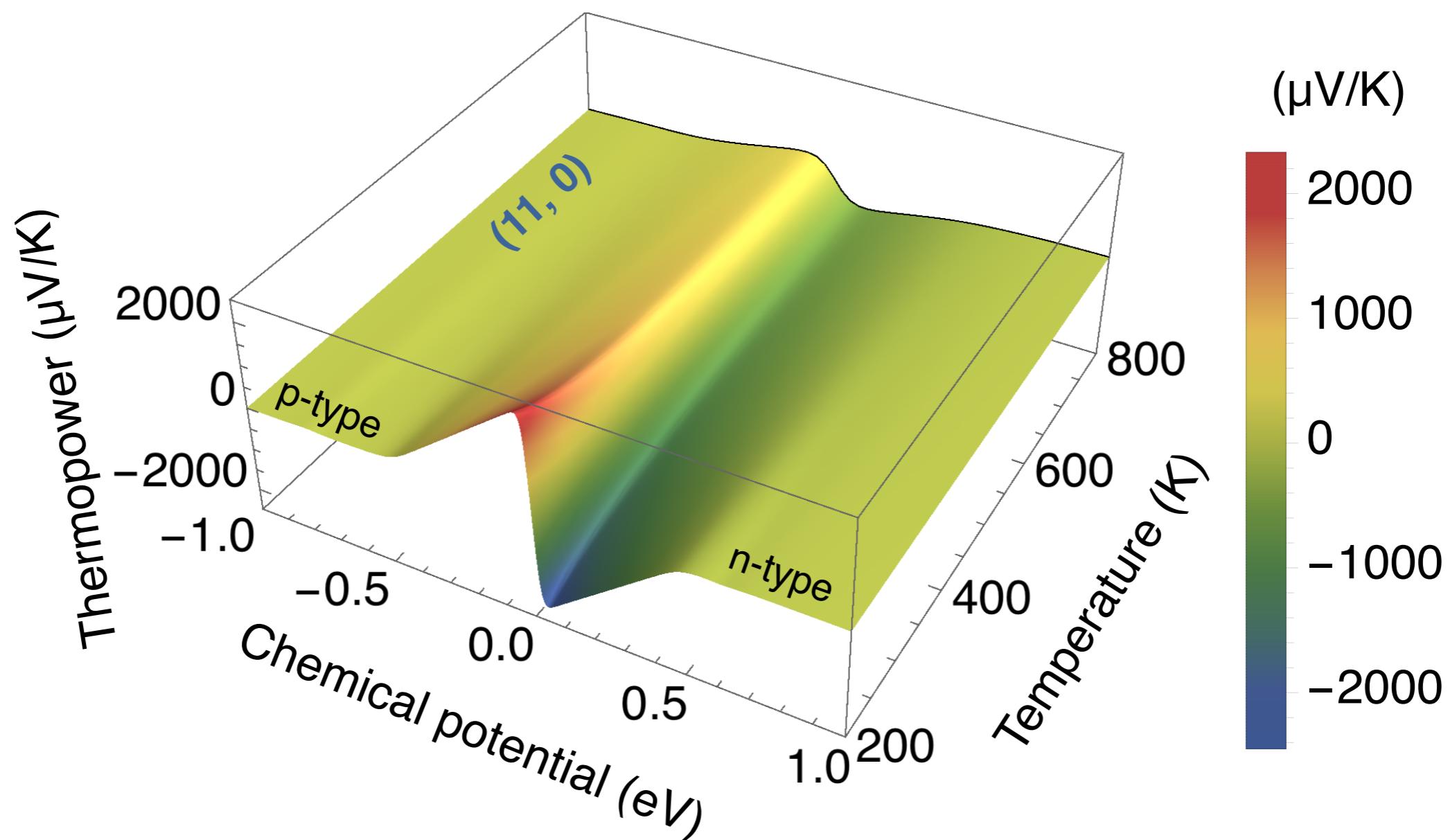
$$\kappa_{\alpha\beta}^0(T, \mu) = \frac{1}{eT\Omega} \int \sigma_{\alpha\beta}(\epsilon) (\epsilon - \mu)^2 \times \left[-\frac{\partial f_0(T, \epsilon, \mu)}{\partial \epsilon} \right] d\epsilon \quad \text{Electronic thermal conductivity}$$

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

Thermopower



Thermoelectricity

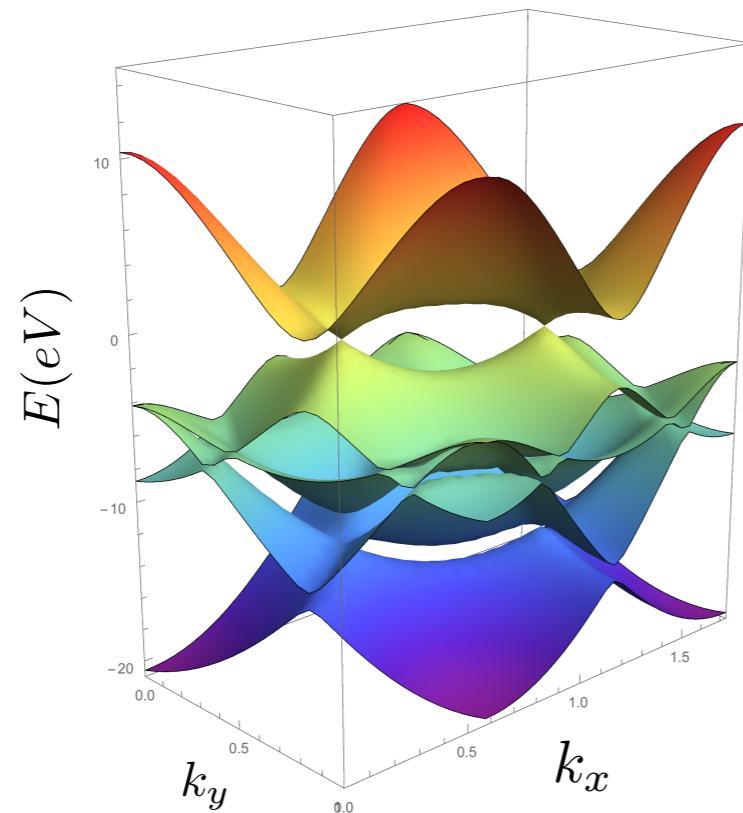
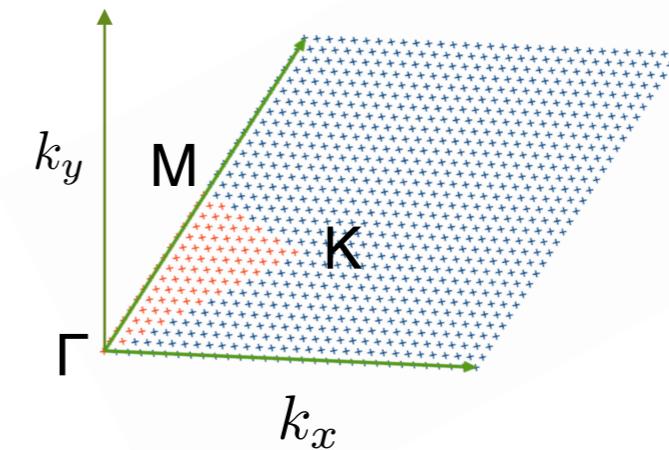
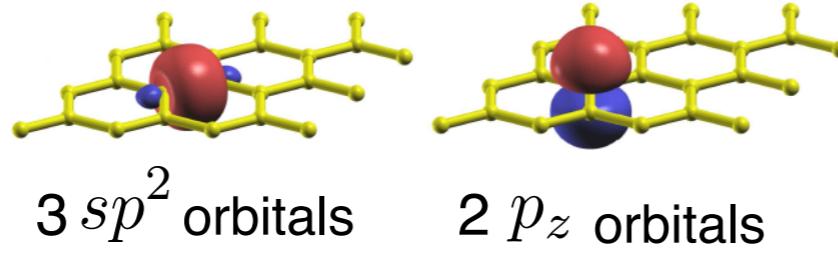


N. T. Hung, et al, PRB 92 (2015) 165426.

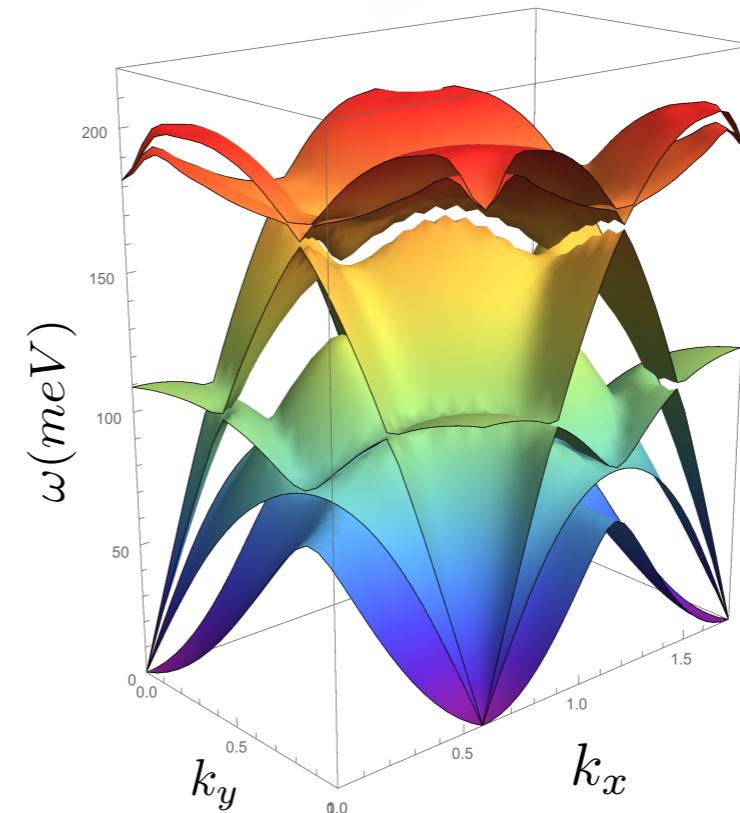
Exercises

Files for Wannier90

/graphene-wannier90/



Band structures
 $10^6 \mathbf{k}$ points



Phonon dispersions
 $10^4 \mathbf{q}$ points

thank you!

