GW calculations in nanowires

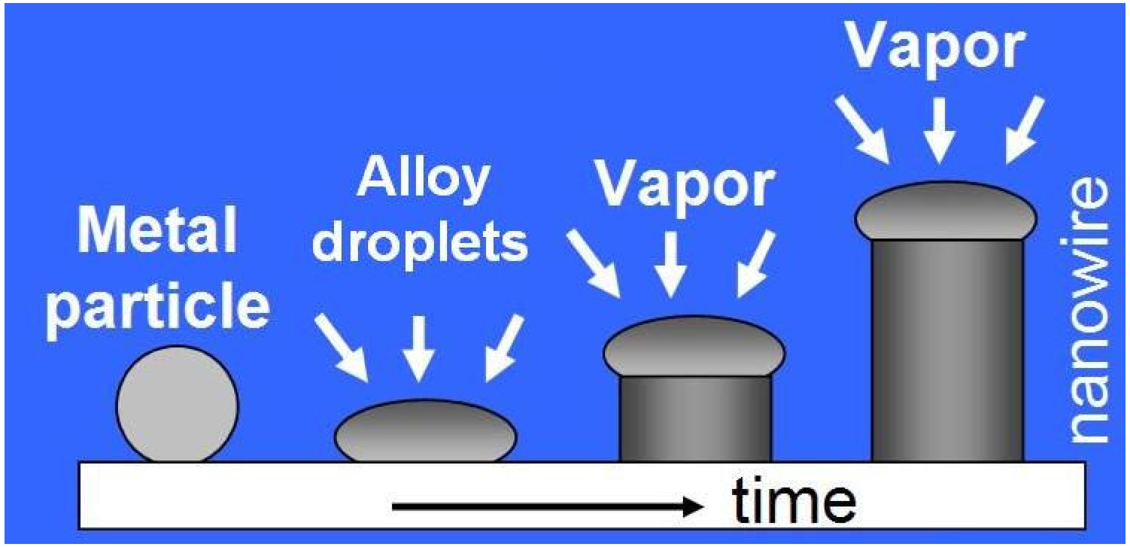
H. Peelaers, B. Partoens, M. Giantomassi, T. Rangel, E. Goossens, G.-M. Rignanese, X. Gonze, and F. M. Peeters

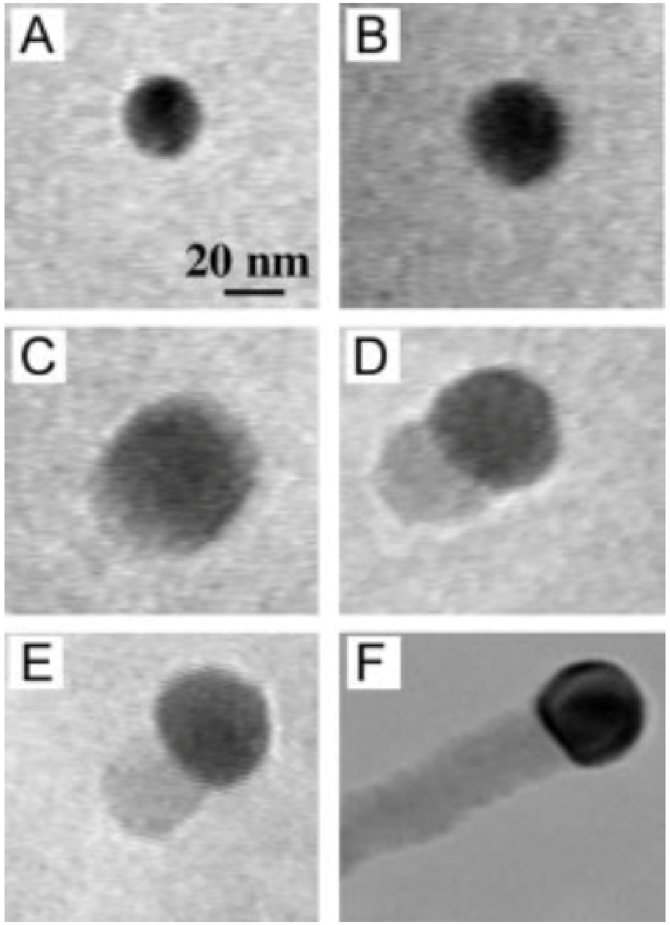
Overview

- General introduction on nanowires
- Results and discussion
  - Convergence issues and solutions
  - Wannier interpolation
  - Effective masses
- Conclusions

Growth of nanowires: VLS

Schematic representation of VLS growth





Y. Wu and P. Yang, J. Am. Chem. Soc. **123**, 3165 (2001)

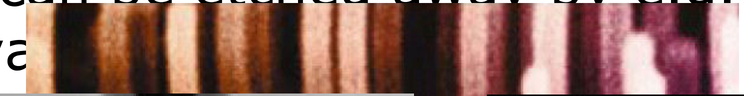
Growth of a Ge nanowire

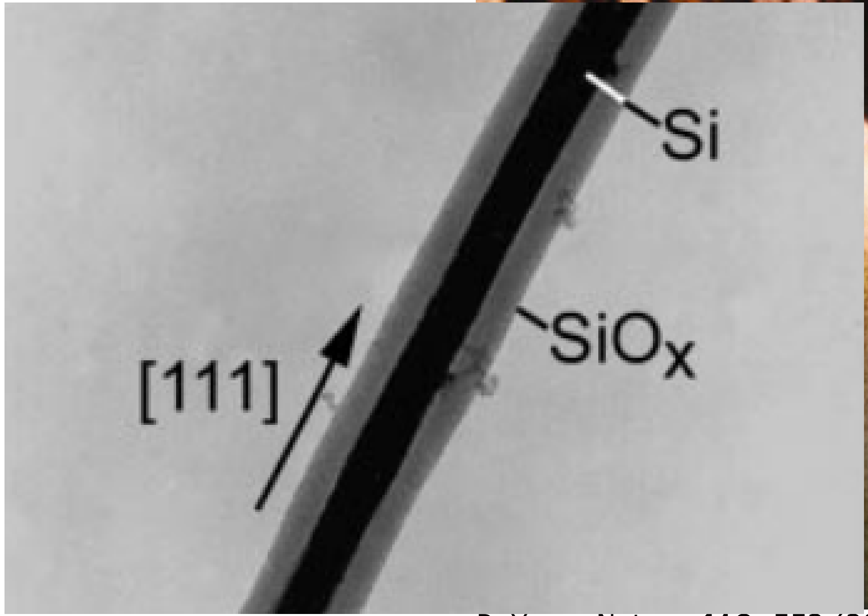
Growth of nanowires: VLS

The growth process can be controlled → several types of structures are possible

Arrays of nanowires can be readily grown

The oxide layer can be etched away by e.g. HF to obtain hydrogen passiva

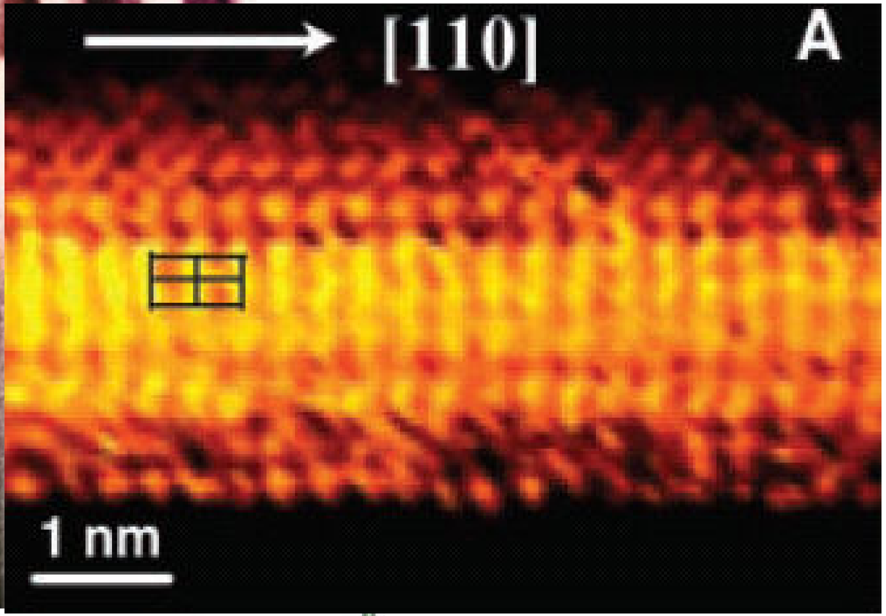




A.M. Morales and C.M. Lieber, Science **279**, 208 (1998)

P. Yang, Nature **419**, 553 (2002)

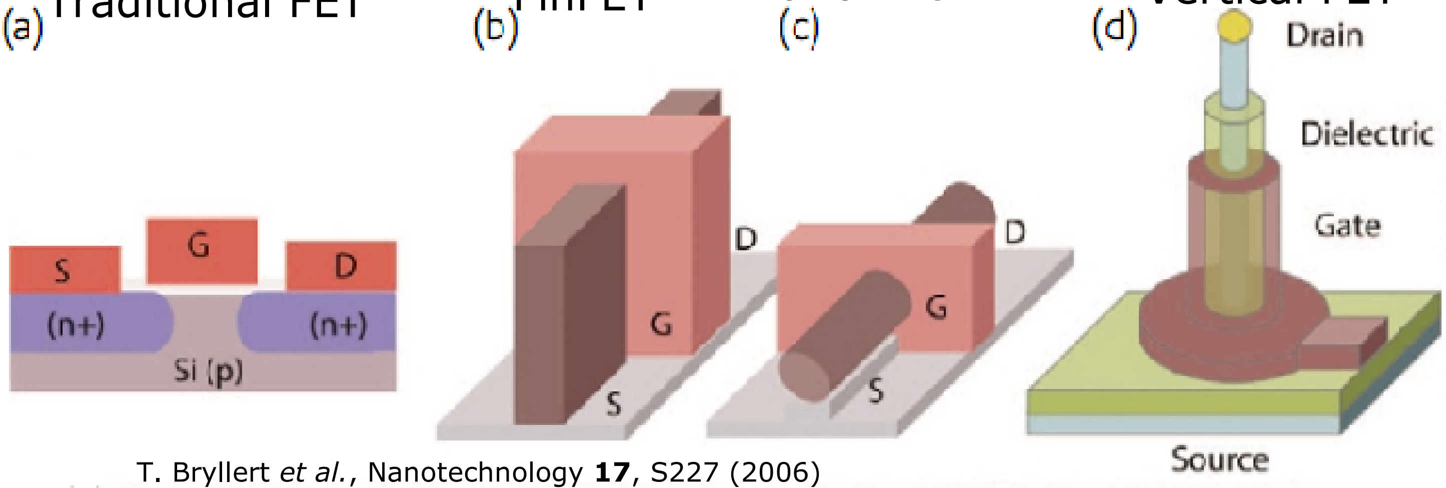
C.M. Lieber and Z.L. Wang, MRS Bull. **32**, 99 (2007)



D.D.D. Ma *et al.*, Science **299**, 1874 (2003)

Nanowires: prototype devices

Nanowires can be used as high performance FETs, in new types of geometries.



Traditional FET

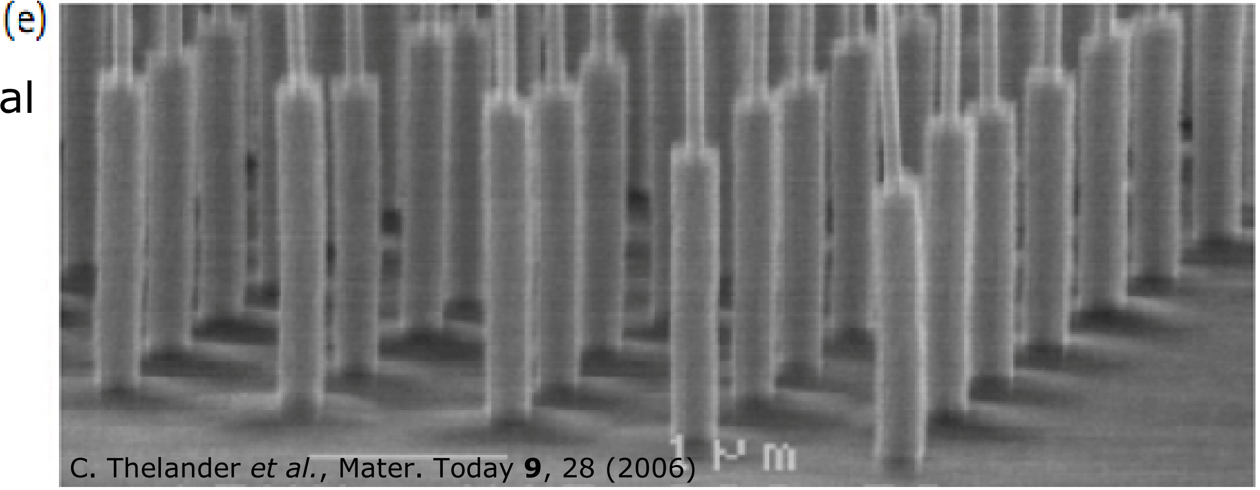
FinFET

Nanowire FinFET

Vertical FET

T. Bryllert *et al.*, Nanotechnology **17**, S227 (2006)

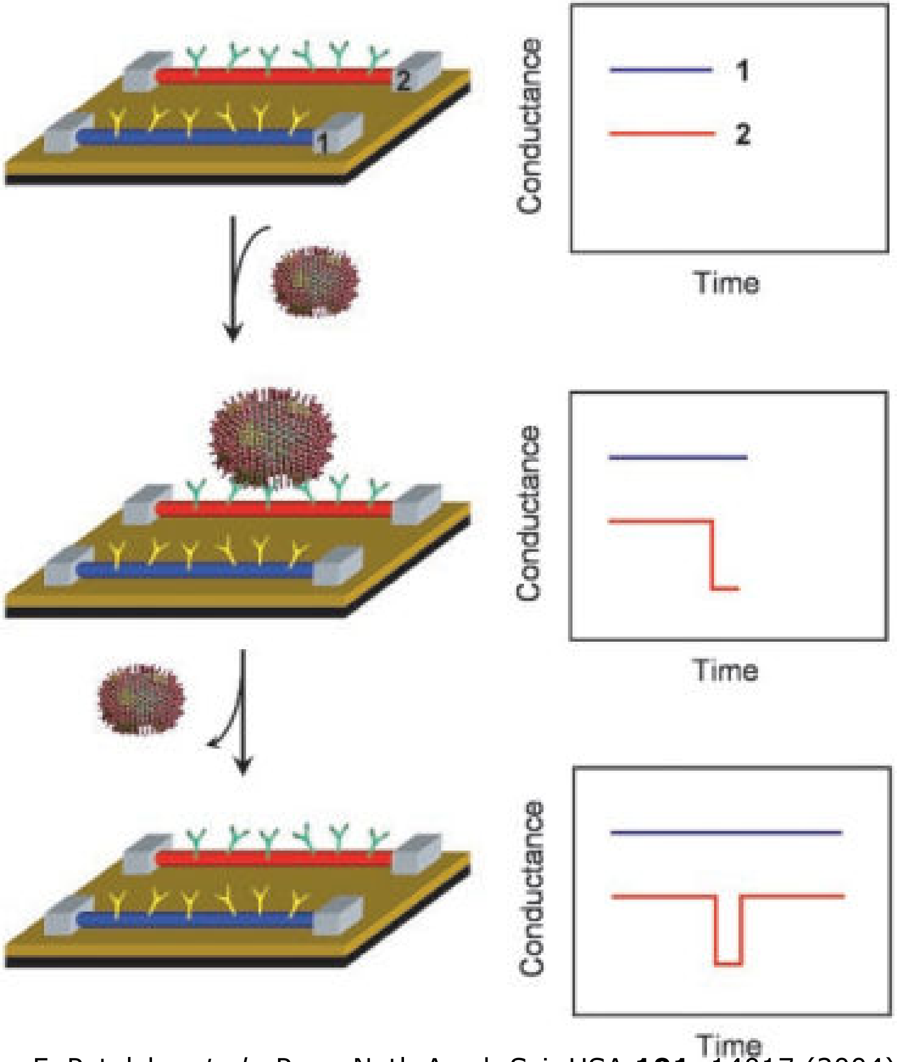
Array of vertical nanowire FETs



C. Thelander *et al.*, Mater. Today **9**, 28 (2006)

Nanowires: prototype devices

Due to the high performance of nanowire FETs and the large surface/volume ratio, they can be used as highly sensitive sensors.
Demonstrated examples include single virus detection and the simultaneous detection of different disease markers.

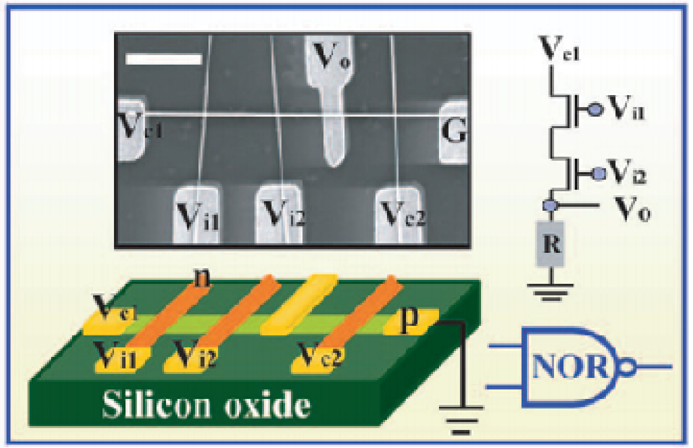


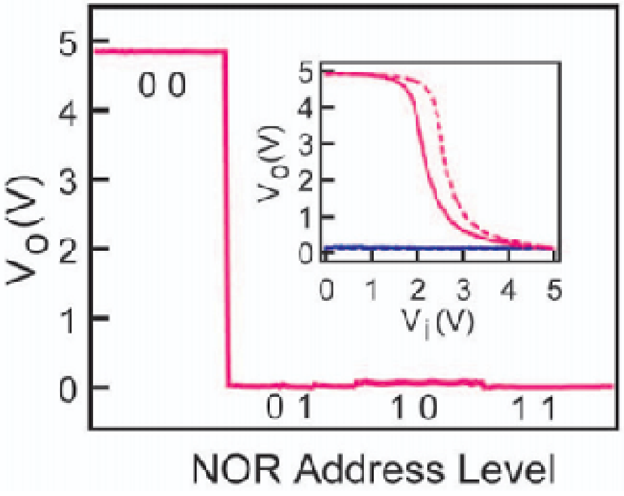
F. Patolsky *et al.*, Proc. Natl. Acad. Sci. USA **101**, 14017 (2004)

Nanowires: prototype devices

More advanced devices have also been demonstrated

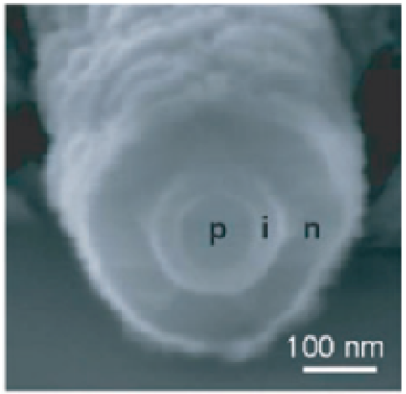
Crossed nanowire NOR gate



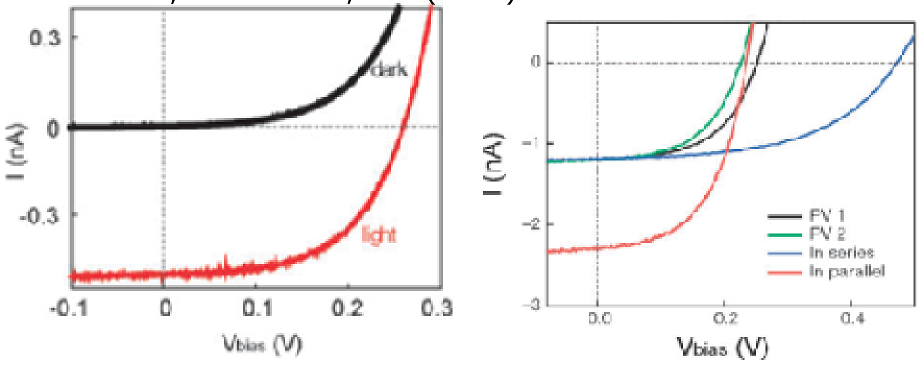


Y. Li *et al.*, Mater. Today **9**, 1442 (2008)

P-i-n type nanowire as solar cell



B. Tian *et al.*, Nature **449**, 885 (2007)



GW corrections to spectra

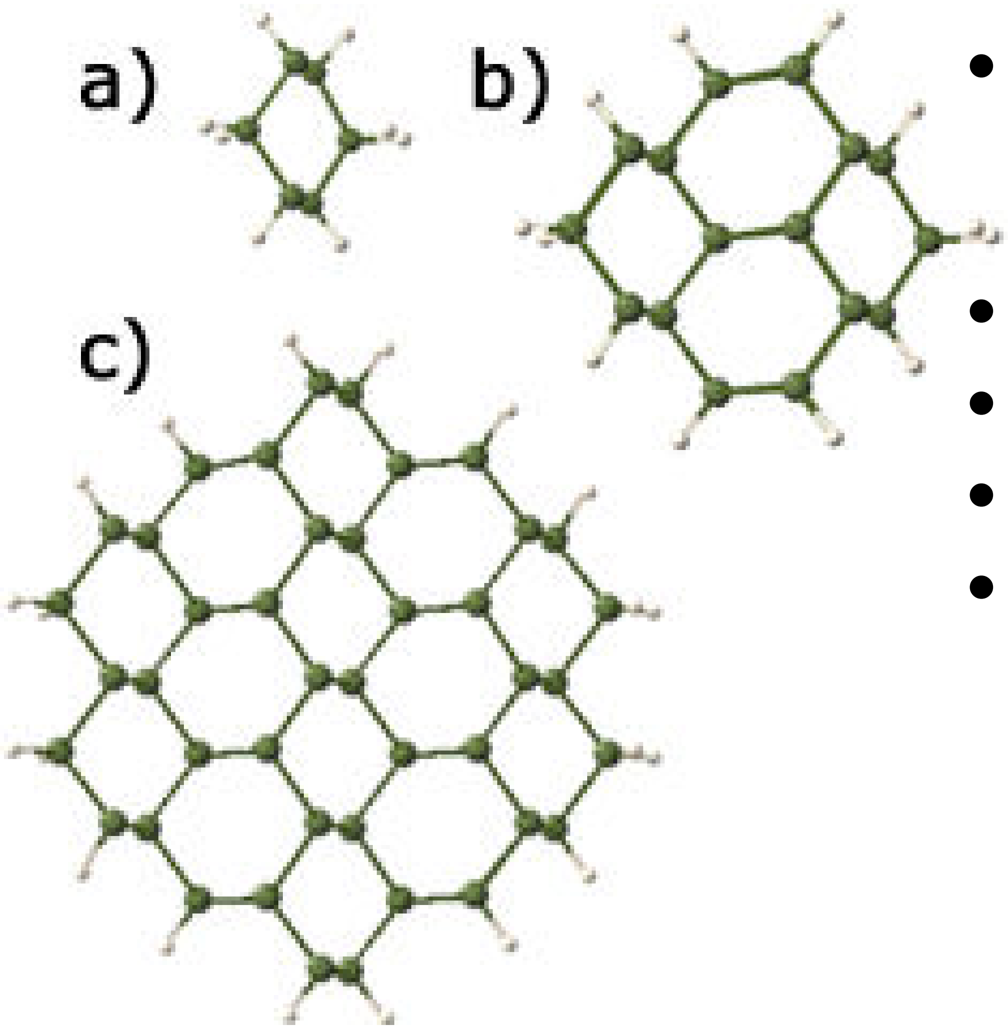
- LDA underestimates bandgap
- Solution: quasi-particle corrections: G_0W_0
- Traditionally GW correction at Gamma + uniform “scissor” shift

Is this accurate for nanowires (important for optical spectra)?

- GW computations are very resource intensive, especially in supercells with vacuum → new techniques are available in ABINIT to solve some of these problems

- Test these techniques on nanowires: example 0.5 nm Ge wire

Computational details



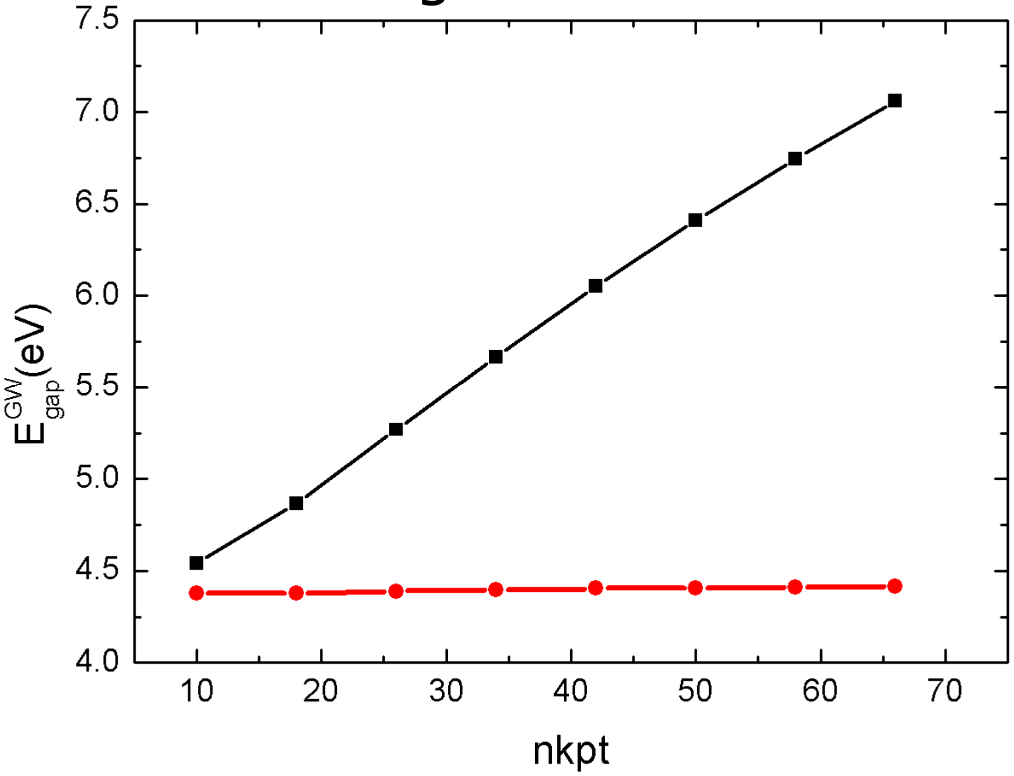
- 0.5, 1.2, and 1.6 nm nanowire in [110] direction
- Si or Ge
- H passivated
- G_0W_0 on top of LDA
- Model system: 0.5 nm nanowire: 6 Ge atoms, 8 H atoms, 16 occupied bands

Coulomb cutoff

Problem: Long range Coulomb interaction between neighbouring cells, as system is no longer neutral

→Apply a cutoff to this interaction, as the interaction itself is unphysical (done in reciprocal space)

Parameters:
icutcoul 1
vcutgeo 0 0 1



S. Ismael-Beigi, PRB **73**, 233103 (2006)

Extrapolar technique: GW gap

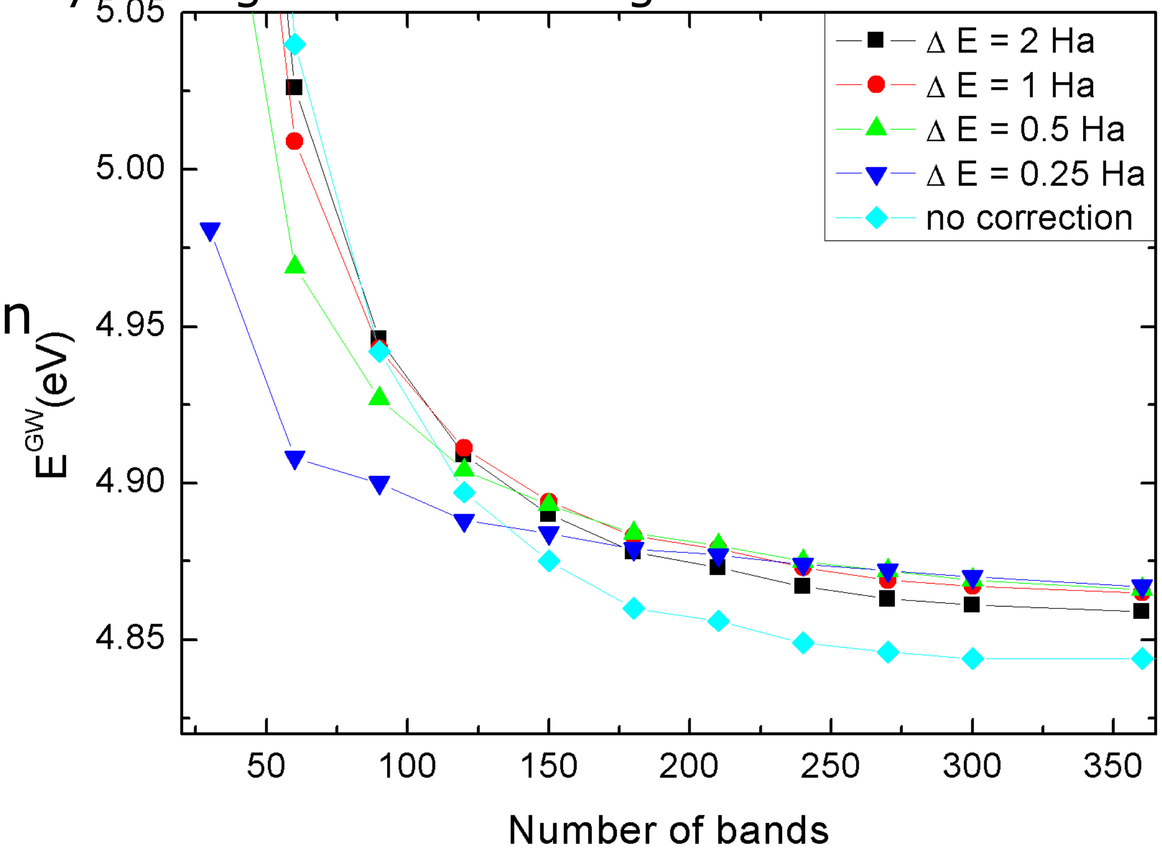
GW calculations require a lot of empty bands

Goal: reduce this number → extrapolar technique

➔ Explained in detail yesterday during the talk of Berger

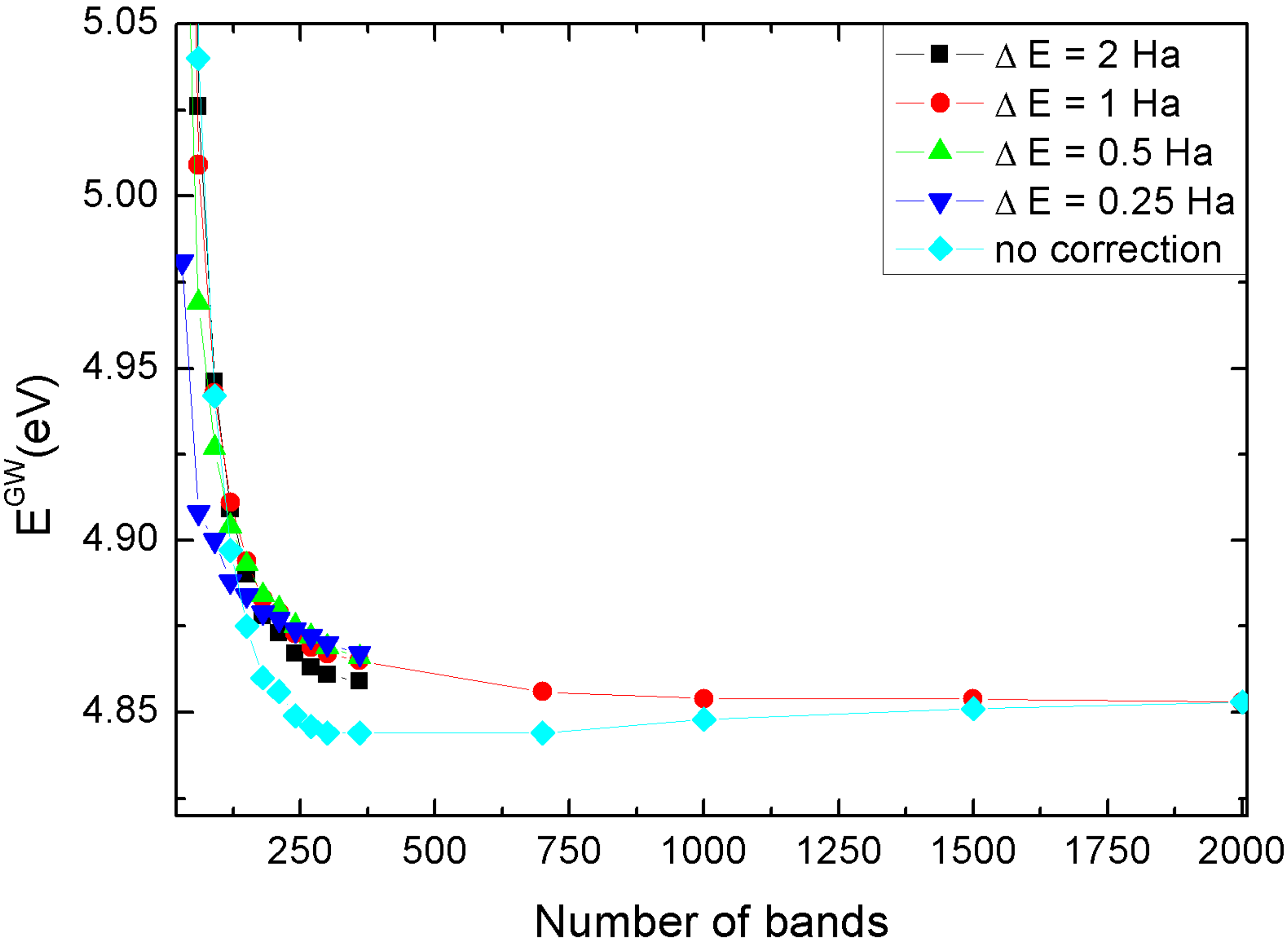
Replace the contributions of higher bands that are not treated explicitly with a common energy + application closure relation

Parameter: gwencomp



F. Bruneval and X. Gonze, PRB **78**, 085125 (2005)

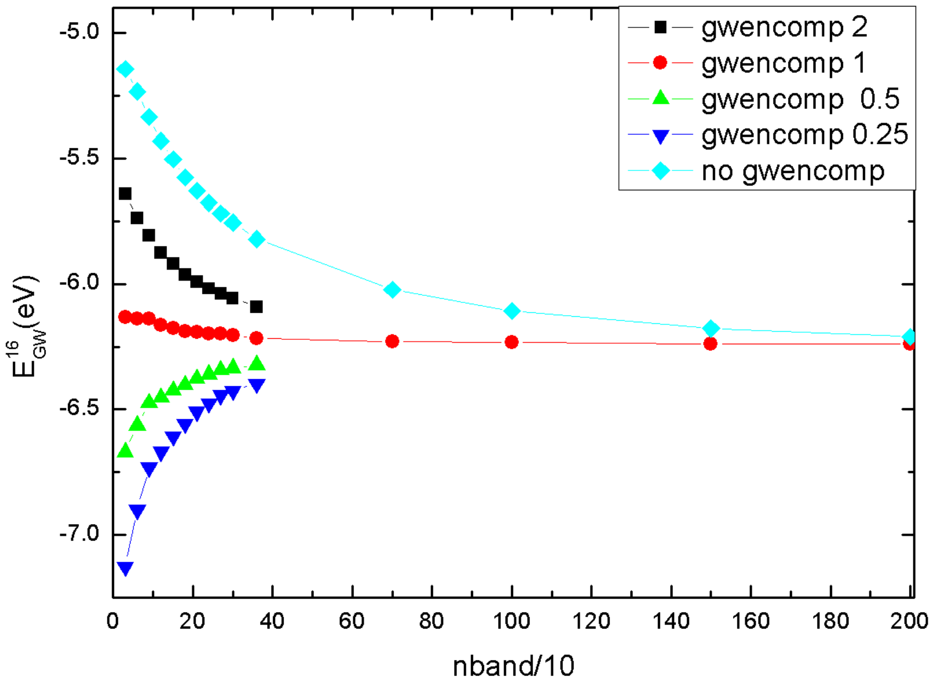
Extrapolar technique: GW gap



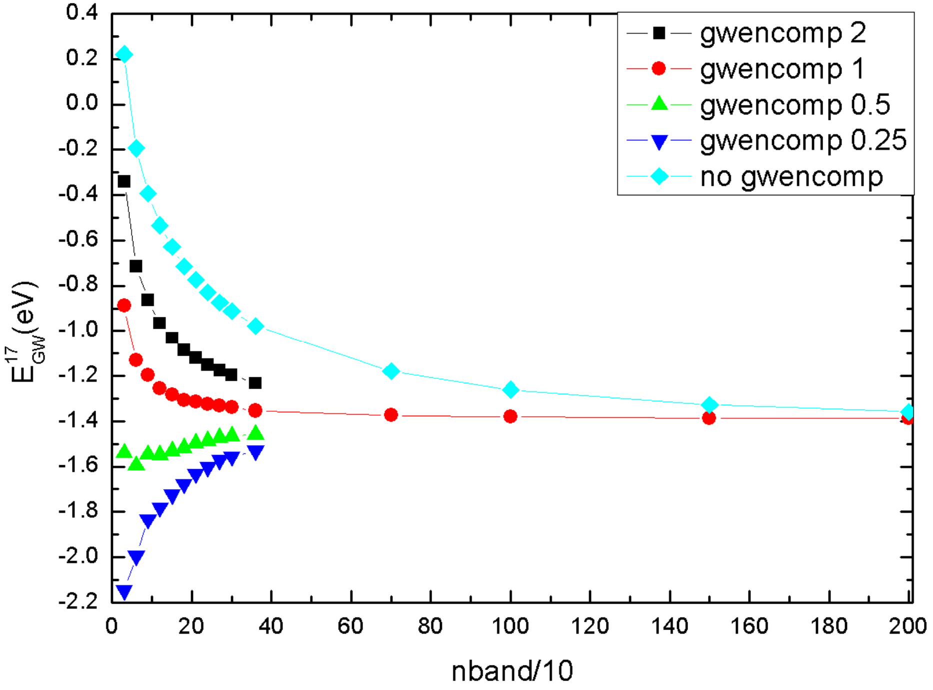
F. Bruneval and X. Gonze, PRB **78**, 085125 (2005)

Extrapolar technique: E_{16} and E_{17}

E_{16}



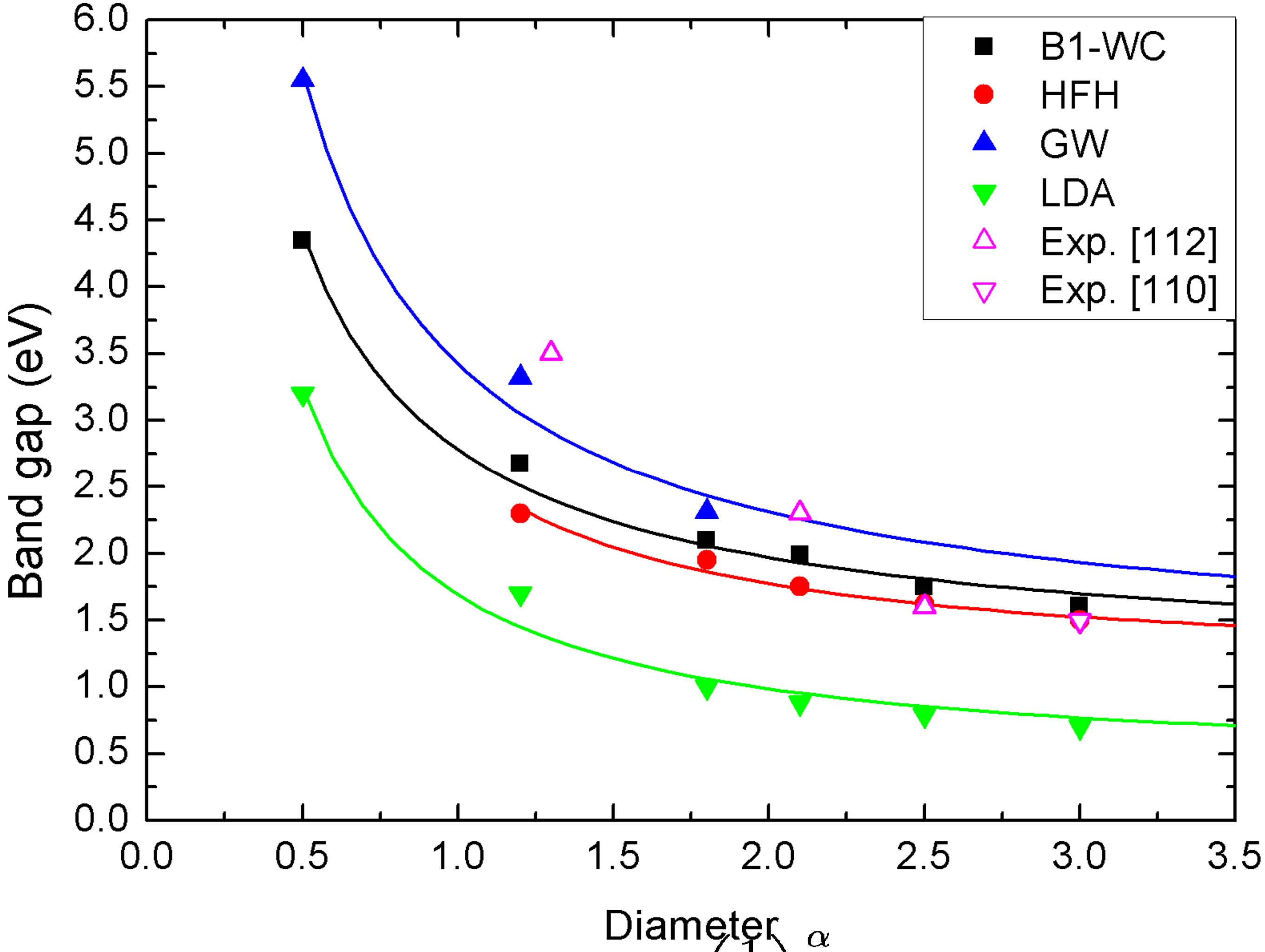
E_{17}



Results: GW gaps

Wire diameter	E_{gap}^{LDA}	ΔE_{gap}^{GW}	E_{gap}^{GW}	Literature
Ge:				
0.5 nm	2.76	2.11	4.87	4.5[a]
1.2 nm	1.57	1.41	2.98	3.01[b]
Si:				
0.5 nm	3.20	2.35	5.55	5[c]
1.2 nm	1.70	1.62	3.32	3.12[d]-3.2[c]-3.4[e]
1.6 nm	1.14	1.18	2.31	2.2[c]-2.32[d]-2.33[e]

Results: GW gap



Lines are fitted to $E_{gap} = E_{gap,bulk} + C \left(\frac{1}{d} \right)^{\alpha}$

With thanks to E. Durgun and Ph. Ghosez for the B1-WC hybrid calculations

Wannier interpolation

- Full band structure, based on a limited number of GW corrected k points → need of a smart interpolation

- Not needed for LDA calculations: nscf calculations possible

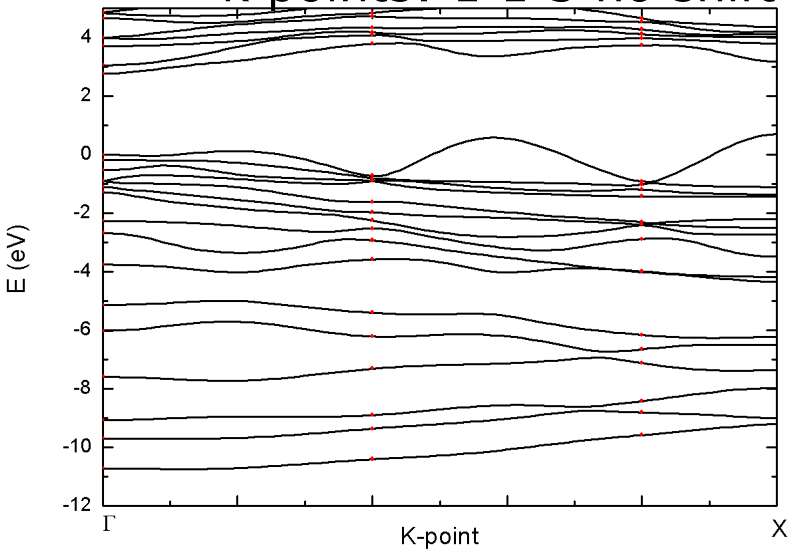
- Construction of basis of Wannier functions using all available information
  - wave functions from LDA
  - eigenvalues of GW

- Use this basis to do the interpolation

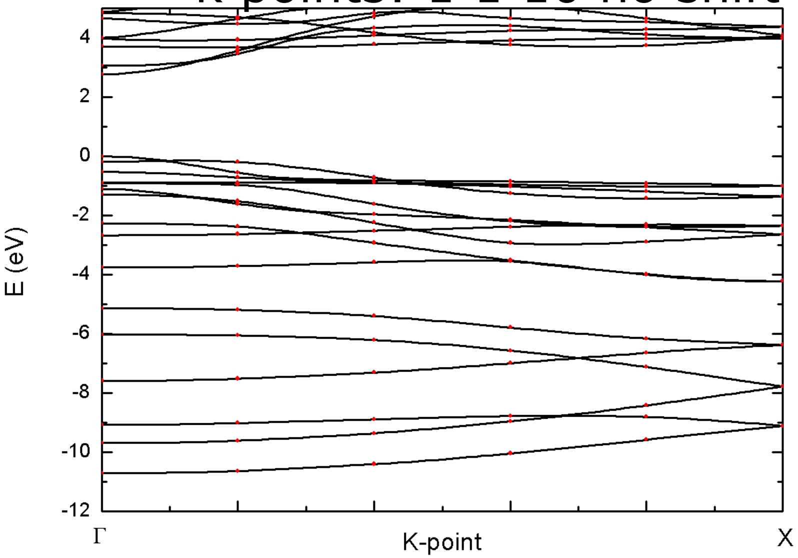
I. Souza, N. Marzari and D. Vanderbilt, PRB **65**, 035109 (2002)

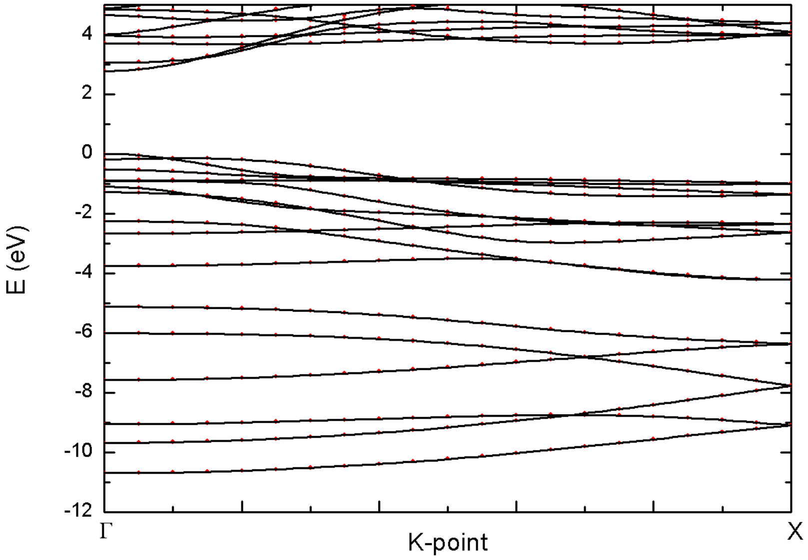
Wannier interpolation

k points: 1 1 5 no shift



k points: 1 1 10 no shift



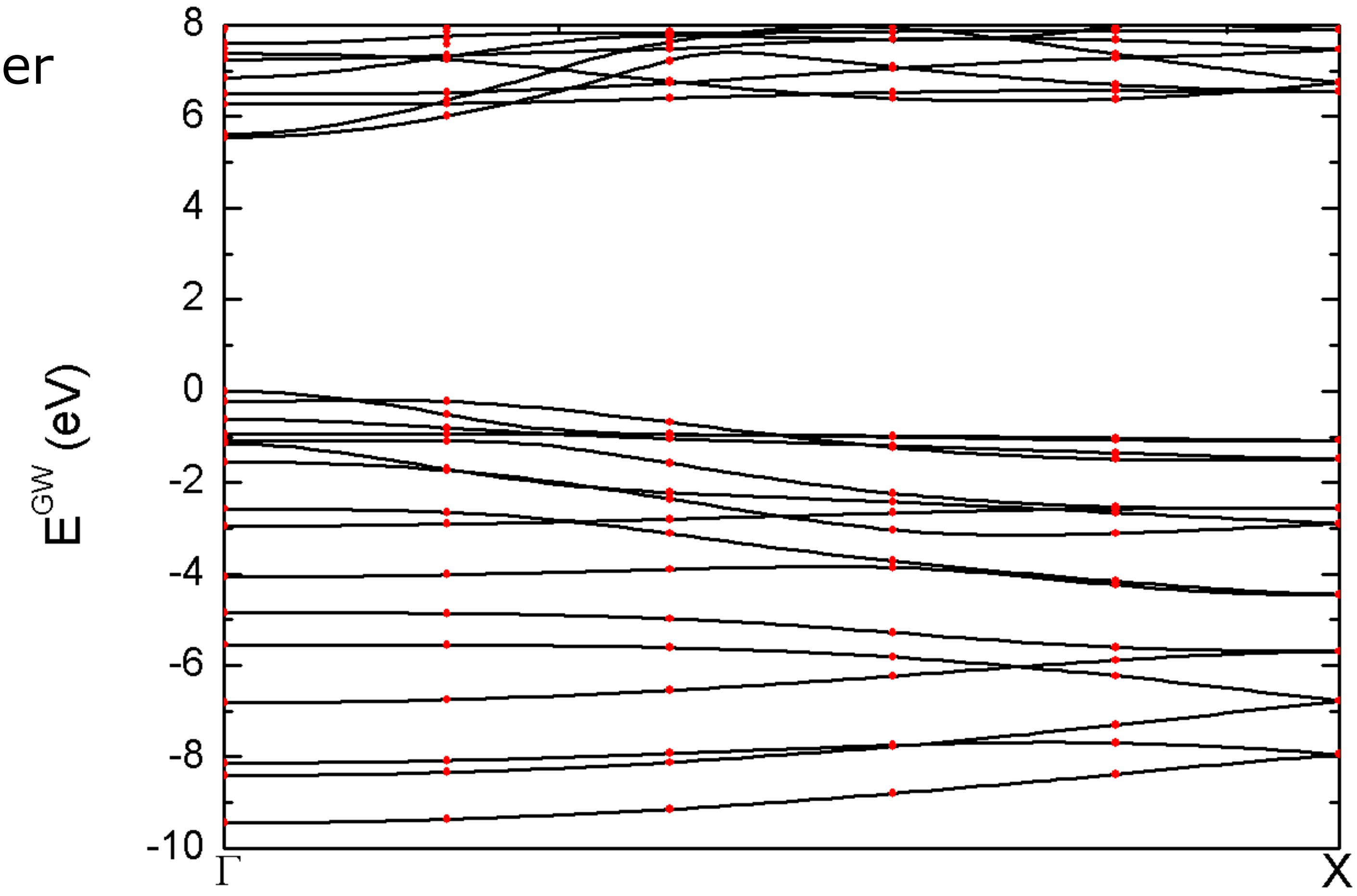


LDA as test

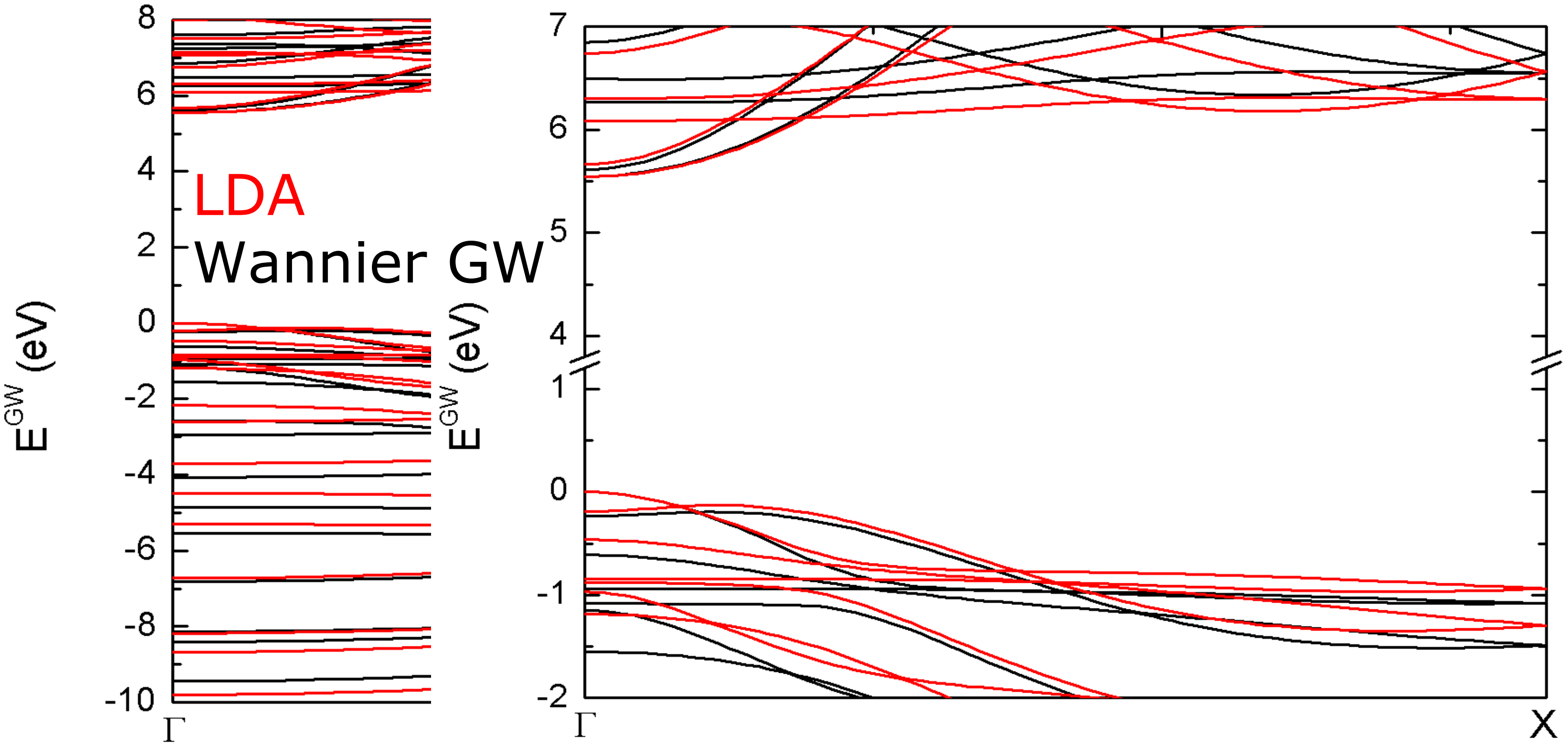
Wannier interpolation

Full quasi particle band structure

Diameter
0.5 nm

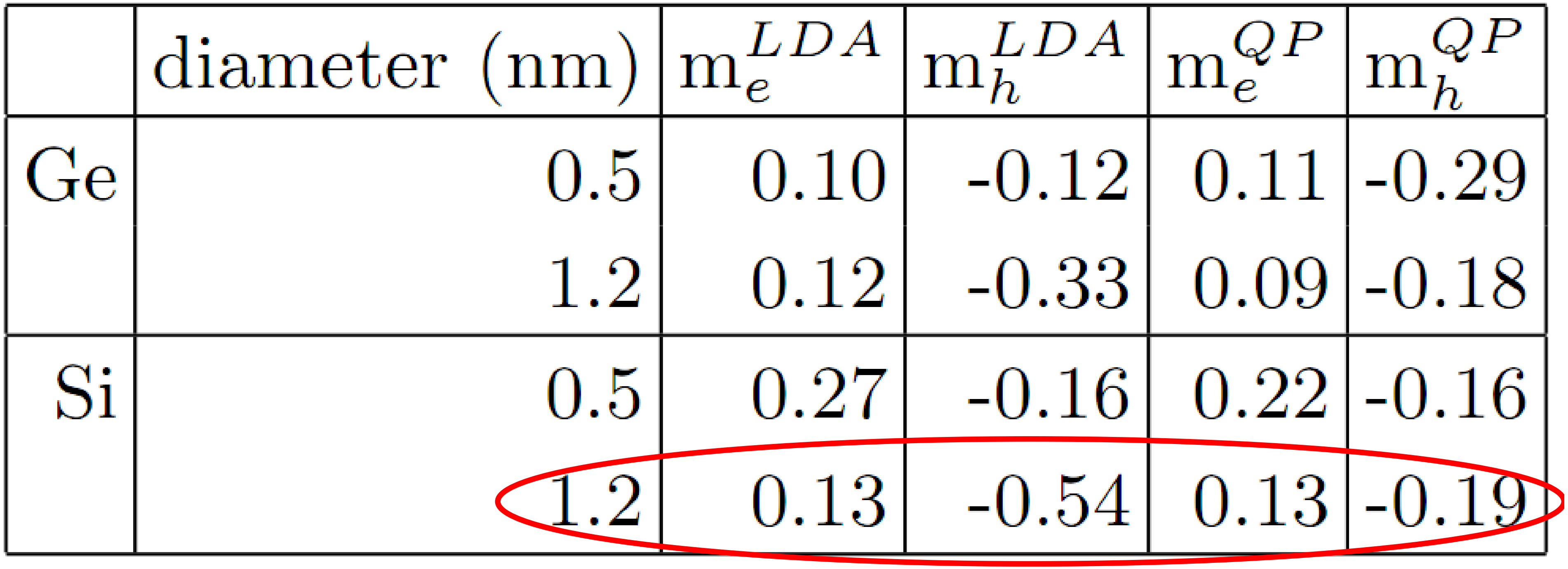


Wannier interpolation



Scissor operation works good around Γ for highest valence and lowest conduction band, but not for other k points and bands!

Effective masses



	diameter (nm)	m_e^{LDA}	m_h^{LDA}	m_e^{QP}	m_h^{QP}
Ge	0.5	0.10	-0.12	0.11	-0.29
	1.2	0.12	-0.33	0.09	-0.18
Si	0.5	0.27	-0.16	0.22	-0.16
	1.2	0.13	-0.54	0.13	-0.19

- QP corrections to electron effective masses are small
- Hole effective masses are corrected significantly

Effective masses

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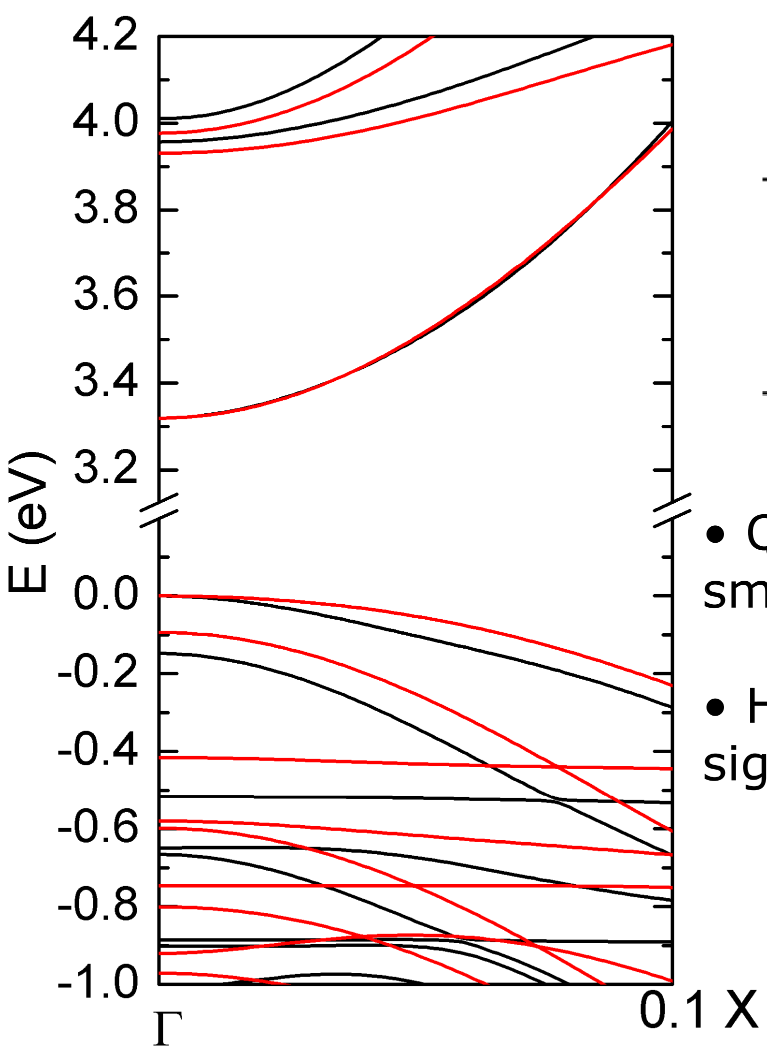

- QP corrections to electron effective masses are small

- Hole effective masses are corrected significantly

Conclusions

- A Coulomb cutoff is necessary to achieve convergence
- The extrapolar technique can be used to speed up the calculations
- Full QP corrected band spectra can be obtained using a Wannier interpolation
- QP corrections are larger for smaller wires
- Corrections to hole effective masses can be large

H. Peelaers, B. Partoens, M. Giantomassi, T. Rangel, E. Goossens, G.-M. Rignanese, X. Gonze, and F. M. Peeters, Phys. Rev. B **83**, 045306 (2011)