Static approximate self-consistent GW or better starting points for G_0W_0)

→ S. V. Faleev, M. van Schilfgaarde, and T. Kotani, PRL 93, 126406 (2004).
QP self-consistent GW; see also Ferdi A.

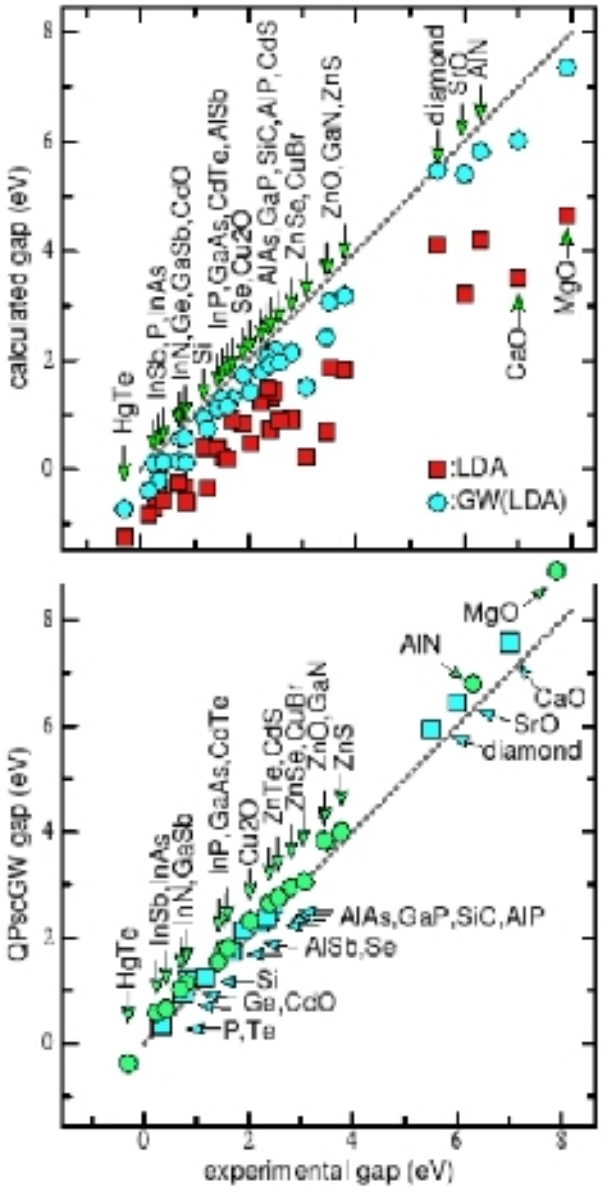
→ F. Bruneval, N. Vast, and L. Reining, Phys. Rev. B 74, 045102 (2006).
COHSEX

→ F. Fuchs, et al., Phys. Rev. B 76, 115109 (2007).
Hybrids

→Hong Jiang et al., , Phys. Rev. Lett. 102, 126403 (2009)
LDA+U

→P. Rinke et al., New J. Phys. 7, 126 (2005)
V_{EXX}

QP sc GW



van Schilfgaarde, Kotani, Faleev, Phys. Rev. Lett. 96, 226402 (2006)

COHSEX

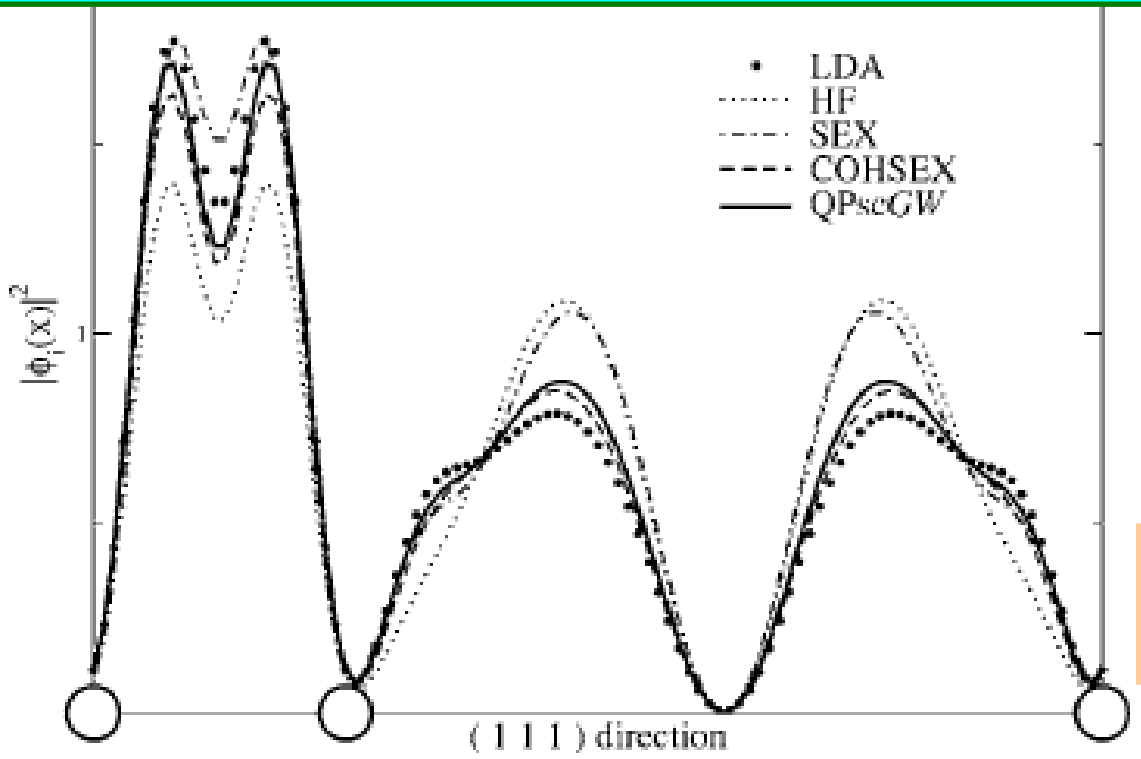


FIG. 8. First conduction band of silicon: squared modulus of the wave function along the direction (1 1 1) at $\mathbf{k}=(-1/8,-3/8,1/4)$. The white circles represent the location of the silicon atoms.

Bruneval, Vast, Reining, PRB 74, 045102 (2006)

Argon gap in Γ:

LDA 8.2 **G_0W_0** 12.98 **QpscGW** 14.84 **COHSEX+GW** 14.72

Expt. 14.2 [Haensel 1969]

Away from the LDA starting point!
...of practical importance: example photovoltaics

Quasiparticle energies within sc-GW for CIS

$CuInS_2$

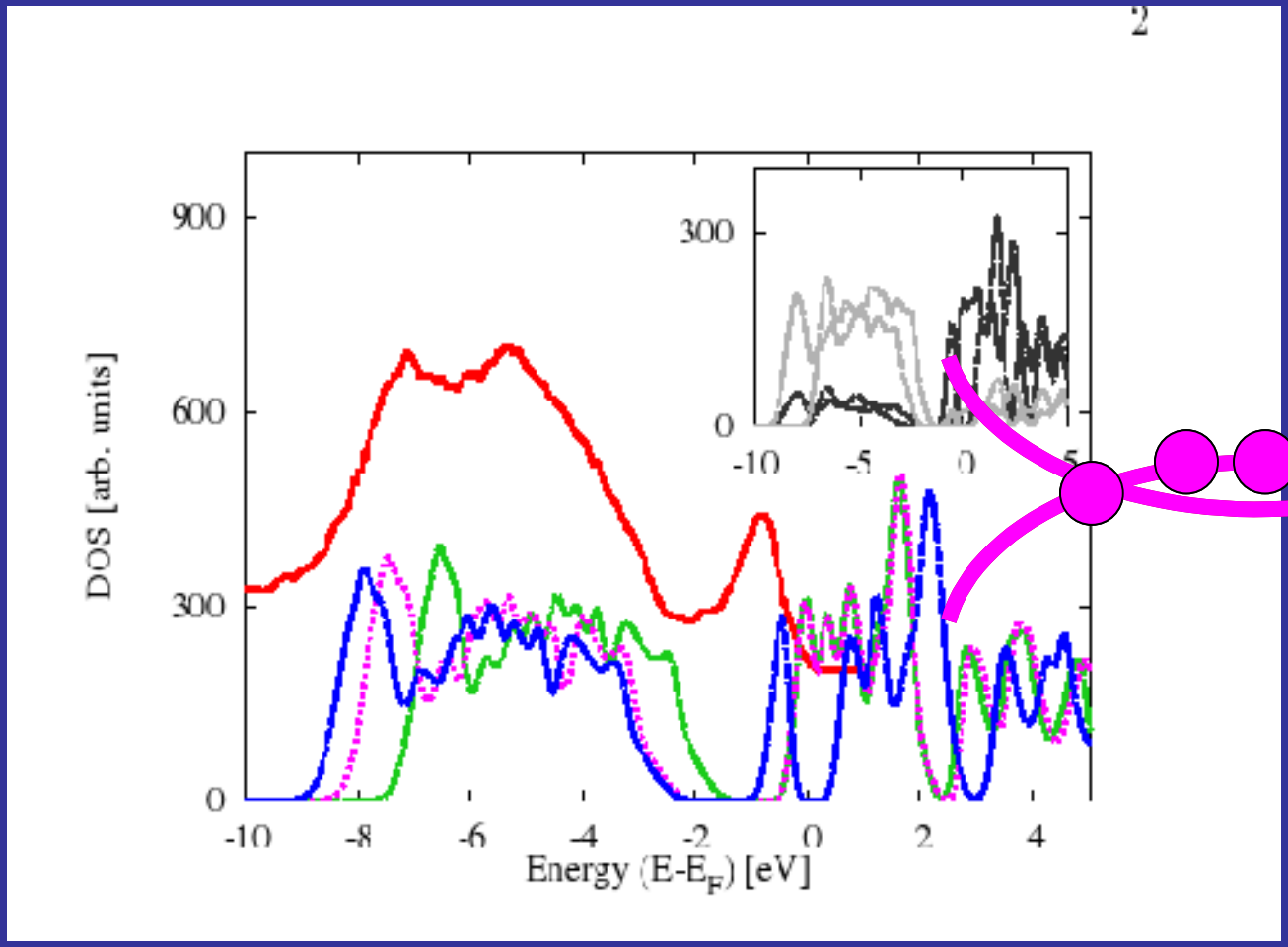
	DFT-LDA	G_0W_0	sc-GW	exp.
E_g	-0.11	0.28	1.48	1.54
In-(S,Se)	6.5	6.9	7.0	6.9
(Se,S) s band	12.4	13.0	13.6	12.0
In 4 d band	14.6	16.4	18.2	18.2

$CuInSe_2$

	DFT-LDA	G_0W_0	sc-GW	exp.
E_g	-0.29	0.25	1.14	1.05 (+0.2)
In-(S,Se)	5.8	6.15	6.64	6.5
(Se,S) s band	12.6	12.9	13.6	13.0
In 4 d band	14.7	16.2	17.8	18.0

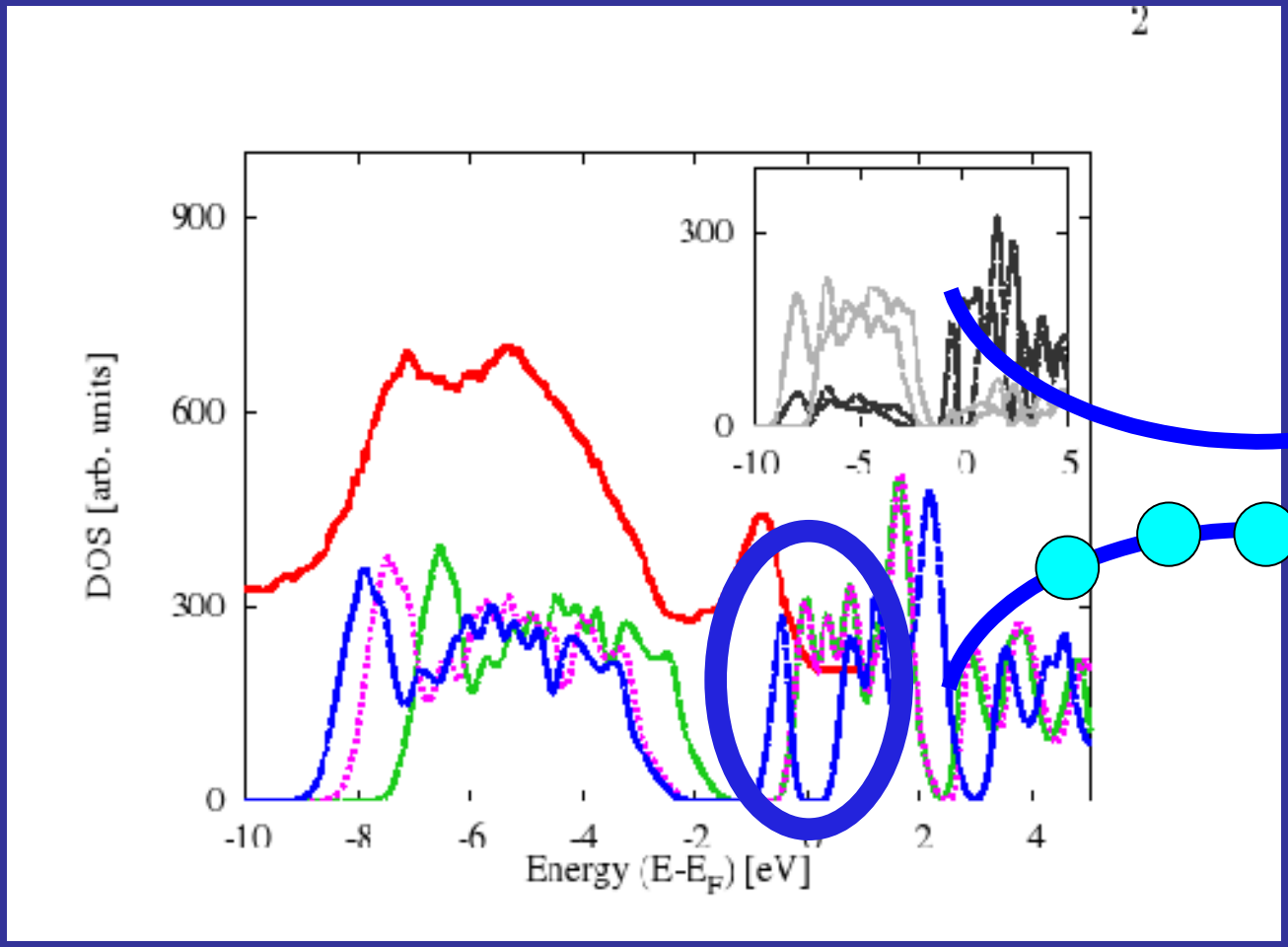
J. Vidal et al., collaboration EDF (2008)

G_0W_0 insulator → metal !!!!!



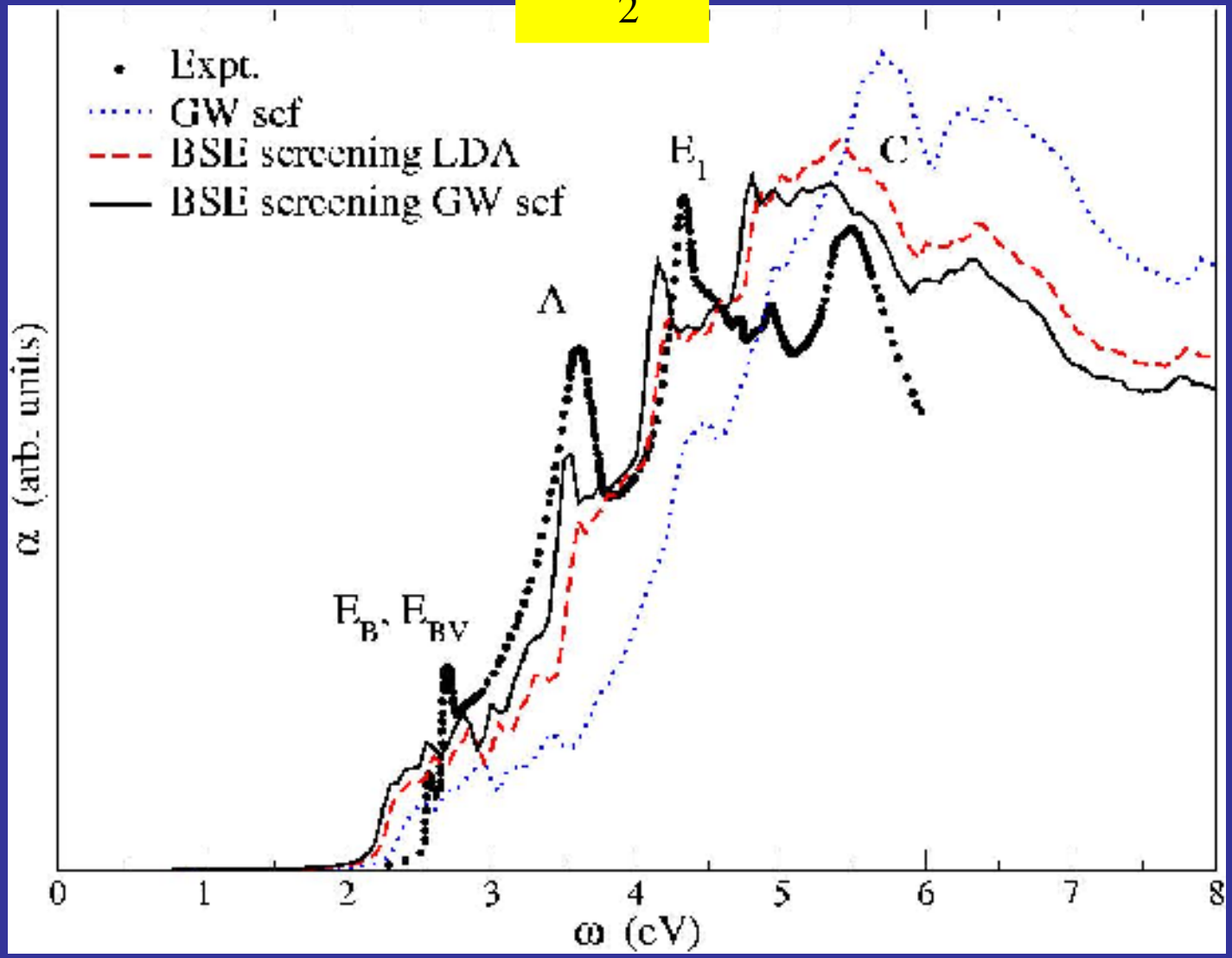
M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

sc GW insulator = insulator !!!



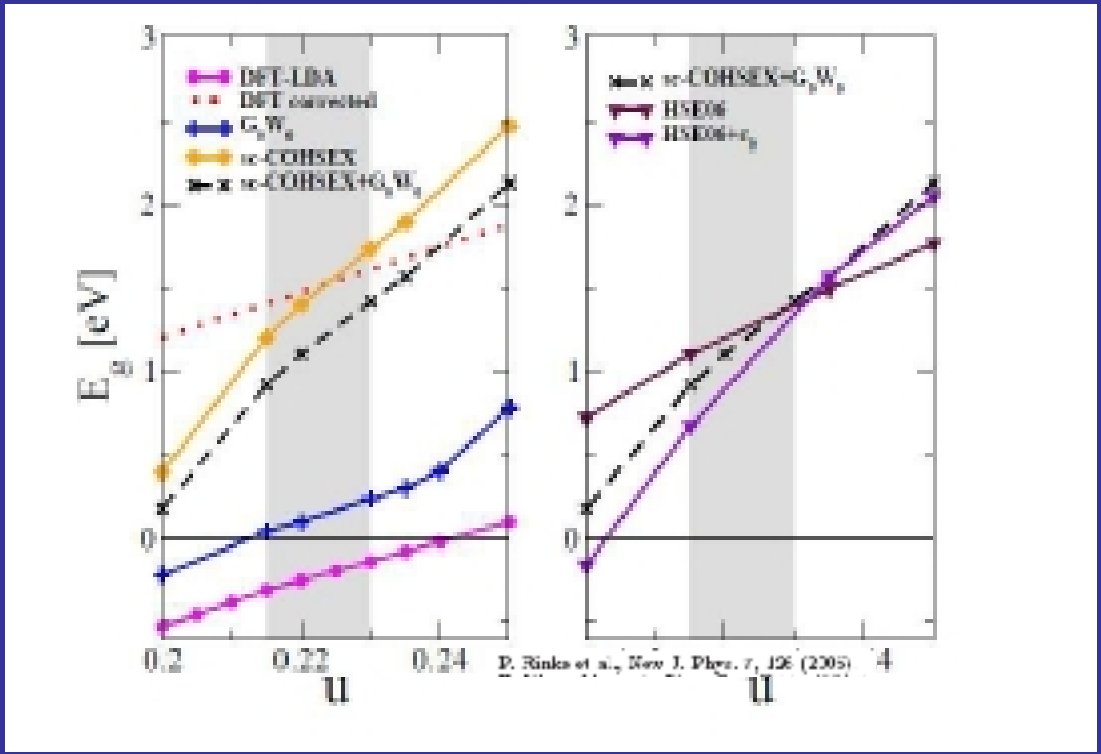
M. Gatti, F. Bruneval, V. Olevano and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007)

Cu_2O



F. Bruneval et al., PRL 97, 267601 (2006))

Hybrids
Bandgaps in function of structure (Cu-S)



LDA+U (Hong Jiang et al.)

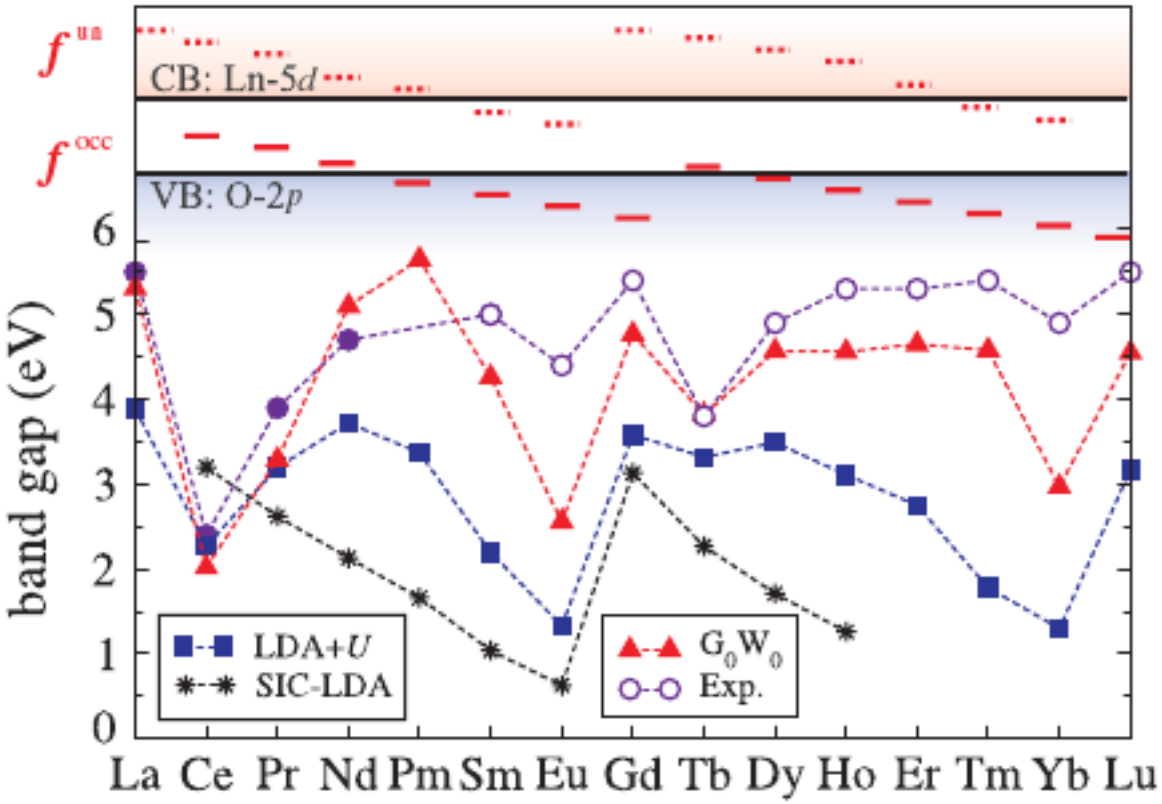


FIG. 3 (color online). Band gaps of the Ln_2O_3 series from LDA + U and G_0W_0 ($U = 5.4$ eV) are compared to SIC-LDA results [10] and experimental optical gaps [8]. The schematic in the upper part of the figure illustrates the position of the f^{occ} and f^{un} states extracted from the G_0W_0 @ LDA + U calculations in relation to the valence and conduction band edge (VB and CB).

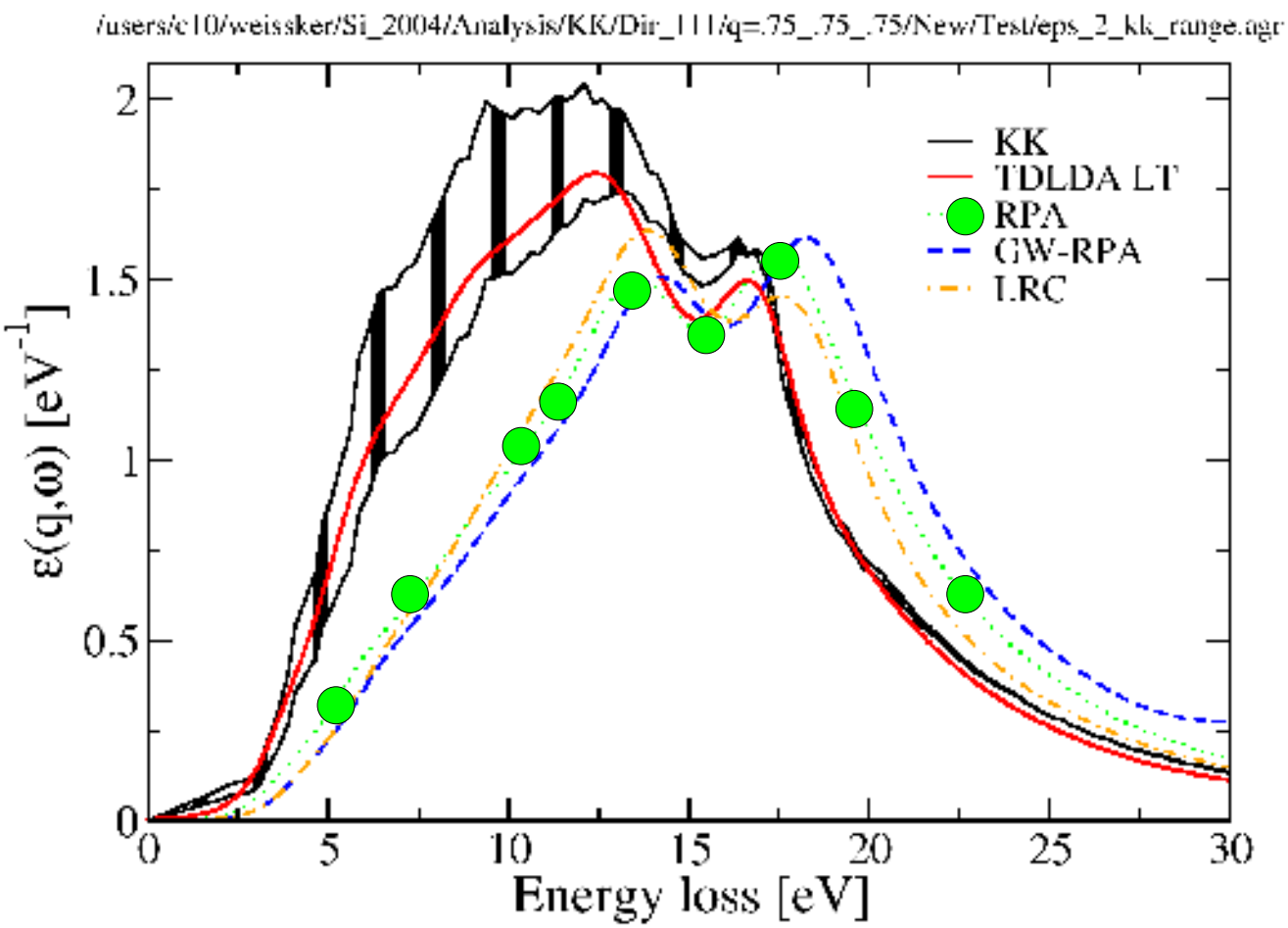
What about W from P=-iGG?

* too low screening

* ....compared to TC-TC, but TC-TE needed!

Γ in P : →

Γ in Σ =iGWΓ: ←



H. Weissker et al., Phys. Rev. Lett. **97**, 237602 (2006)
Collaboration LSI – ESRF (ID16)