2012.03.17 東京大学本郷キャンパス工学部6号館2F63講義室

9:20-9:40

GW近似とその拡張による固体の電子状態計算

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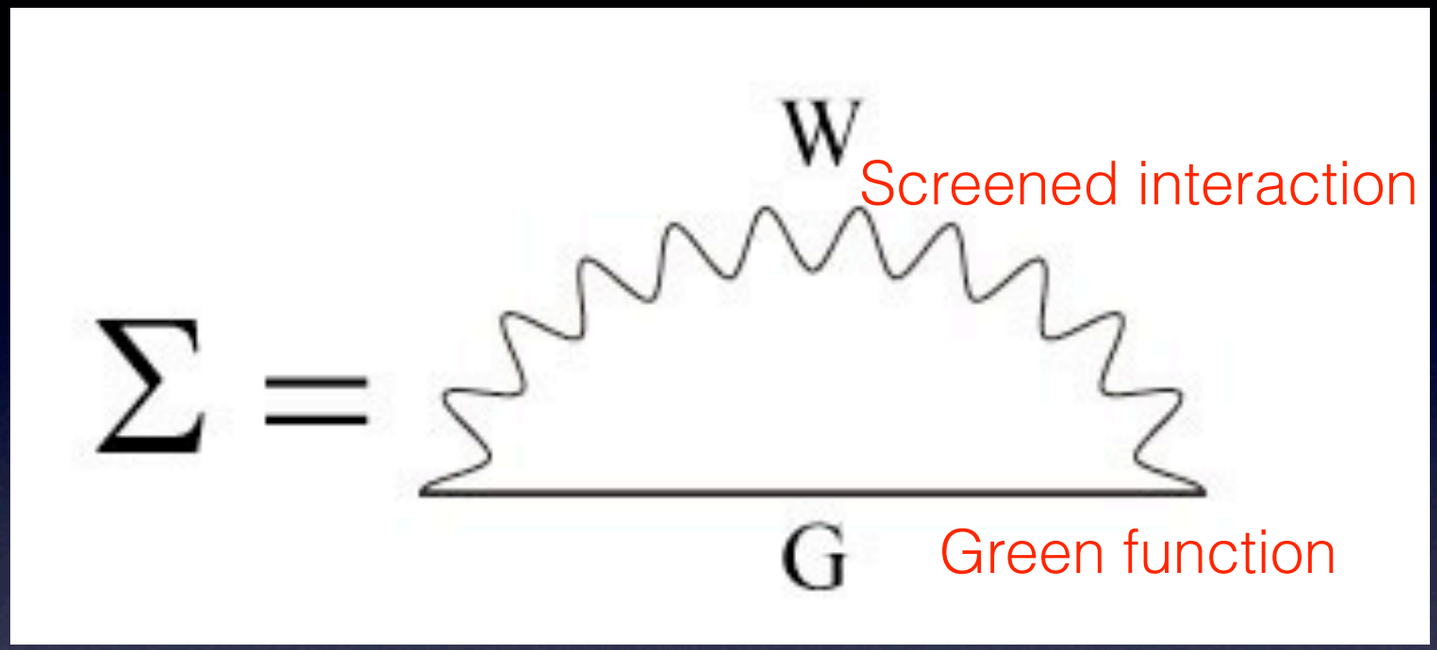
- GW approximation including spin-orbit coupling
- ~~GW approximation for localized states~~

GW approximation



$$\Sigma = GW$$

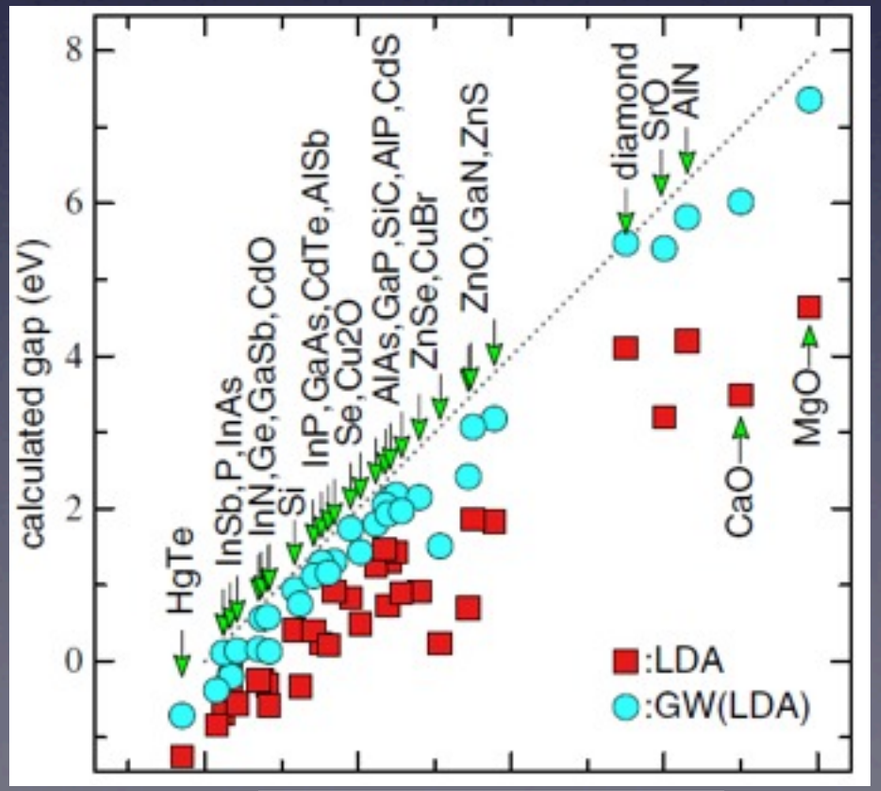
$$W = \varepsilon^{-1}V$$

$$\varepsilon = 1 - VP$$

$$P = GG$$

$$G = G_0 + G_0\Sigma G$$

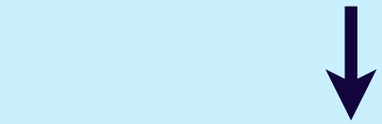
- Tool for the quantitative description of quasiparticle band structures
- Starting point for (first-principles) many-body theory
  - GWΓ (Y. Takada)
  - GW+DMFT (S. Biermann et al.)



Schilfgaarde *et al.* (2006)

Flow-chart of G_0W_0

Self-consistent DFT calculation



$$P(r,r';\omega) = 2\sum_{i}^{occ.}\sum_{j}^{unocc.} \psi_i^*(r)\psi_j(r)\psi_j^*(r')\psi_i(r')$$

$$\times\left[\frac{1}{\omega-\Delta_{ij}+i\eta}-\frac{1}{\omega+\Delta_{ij}-i\eta}\right]$$

$$\varepsilon(r,r';\omega) = \delta(r-r') - \int V(r,r'')P(r'',r';\omega)d^3r''$$

$$W(r,r';\omega) = \int \varepsilon^{-1}(r,r'';\omega)V(r'',r')d^3r''$$

$$\Sigma(r,r';\omega) = \frac{-1}{2\pi i}\int_{-\infty}^{+\infty} G_0(r,r';\omega+\omega')W(r,r';\omega')d\omega'$$

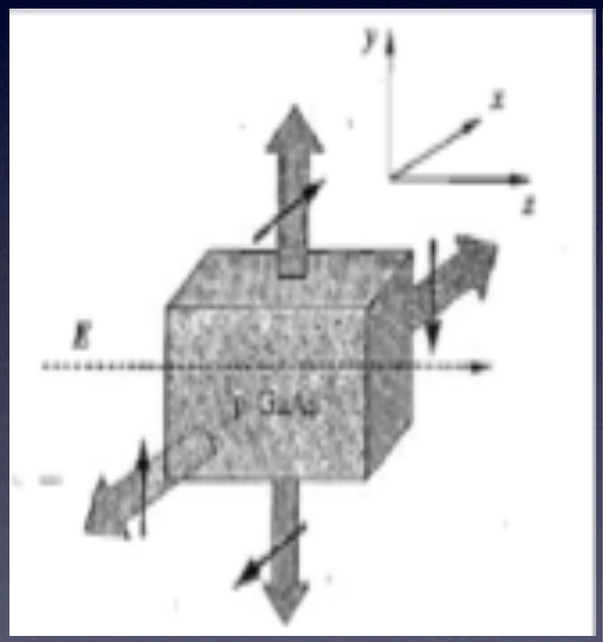
$$E_n^{QP} = E_n^{DFT} + \langle\psi_n|\Sigma(E_n^{QP}) - V_{xc}|\psi_n\rangle$$

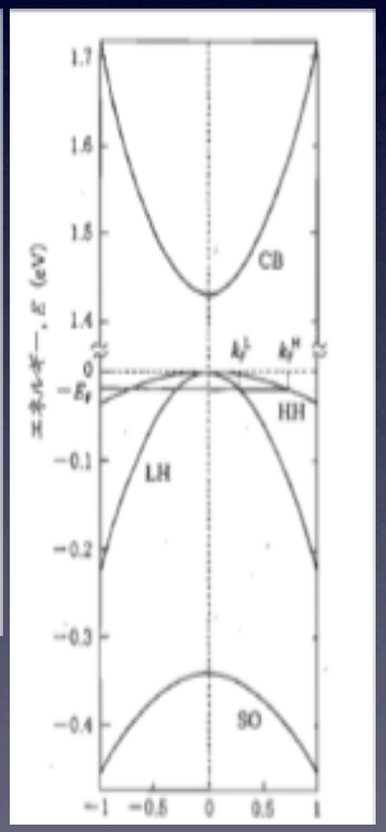
GW approximation including spin-orbit coupling

Collaborators: C. Friedrich (FZ-Juelich)
S. Bluegel (FZ-Juelich)
T. Miyake (NRI-AIST)

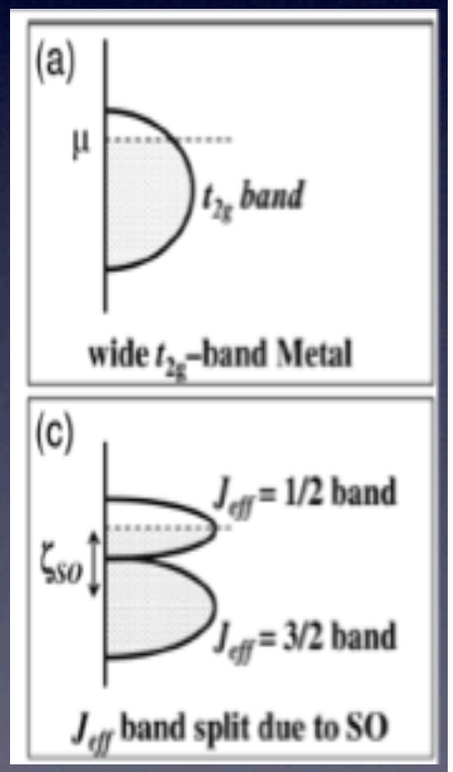
Motivation

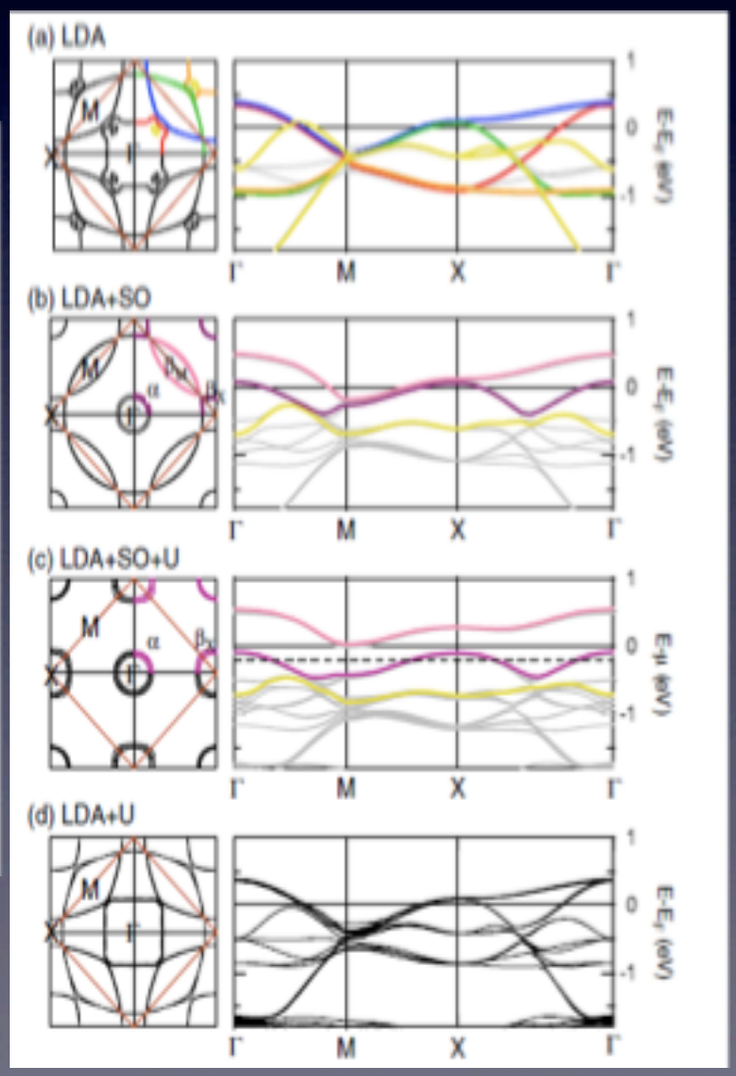
Intrinsic spin-Hall effect:
(Murakami et al., Science 2003)





J-insulator: Sr_2IrO_4
(Kim et al., PRL 2009)





Spin-dependent GW

Spin-dependent many-body Hamiltonian

$$H = \int \psi_\alpha^+(r) h^0_{\alpha\beta}(r) \psi_\beta(r) d^3r$$
$$+ \frac{1}{2}\int \psi_\alpha^+(r)\psi_\beta^+(r') v_{\alpha\delta;\beta\gamma}(r,r')\psi_\gamma(r')\psi_\delta(r) d^3r d^3r'$$

Spin-dependent GW approximation

F. Aryasetiawan and S. Biermann,
Phys. Rev. Lett. 100, 116402(2008);
J. Phys. : Condens. Matter 21, 064232(2009)

$$\Sigma_{\alpha\beta}(1,2) = i\sigma^I_{\alpha\gamma} G_{\gamma\eta}(1,2) W_{JI}(2,1)\sigma^J_{\eta\beta}$$
$$= iG_{\gamma\eta}(1,2) W_{\eta\beta,\alpha\gamma}(2,1)$$
$$W_{IJ}(1,2) = v_{IJ}(1,2) + \int d(34) v_{IK}(1,3) P_{KL}(3,4) W_{LJ}(4,2)$$
$$P_{IJ}(1,2) = -i\sigma^I_{\alpha\beta} G_{\alpha\gamma}(1,2)\sigma^J_{\gamma\eta} G_{\eta\beta}(2,1)$$
$$(I = 0, x, y, z, \quad \sigma^0 = 1)$$

Spin-dependent GW

Special case: (one-particle) spin-orbit coupling + Coulomb interaction

$$h^0_{\alpha\beta}(r) = h^0(r)\delta_{\alpha\beta} + v^{SOC}_{\alpha\beta}(r)$$

$$V_{\alpha\beta;\gamma\eta}(r,r') = \frac{1}{|r-r'|}\delta_{\alpha\beta}\delta_{\gamma\eta}$$

GW + SOC

$$\Sigma_{\alpha\beta} = G_{\alpha\beta}W$$

$$\varepsilon = 1 - VP$$

$$P = \sum_{\alpha\beta} G_{\alpha\beta}G_{\beta\alpha}$$

$$W = \varepsilon^{-1}V$$

- The self-energy and Green's function now have off-diagonal matrix elements.
- The polarization P is calculated from the band dispersion including SO splitting

Hg Chalcogenides (HgX, X=S, Se, Te)

Motivation

Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells

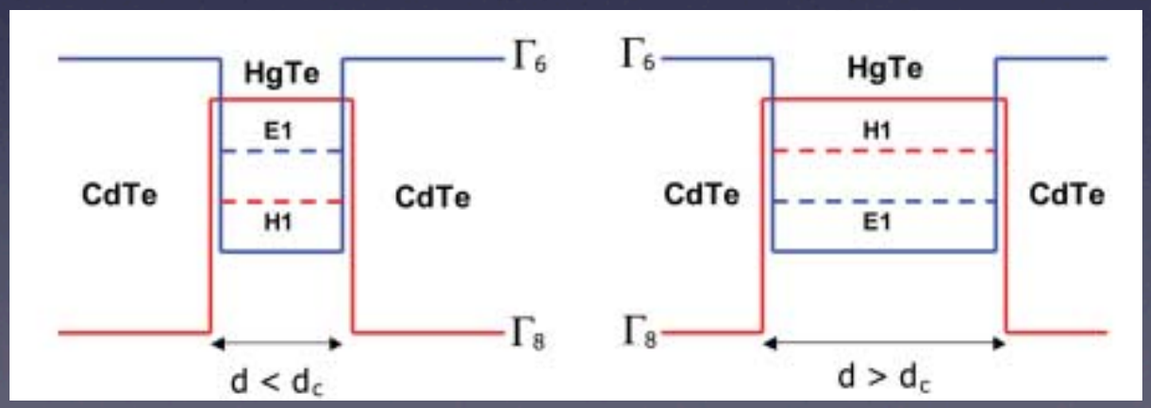
B. Andrei Bernevig,[1,2] Taylor L. Hughes,[1] Shou-Cheng Zhang[1]*

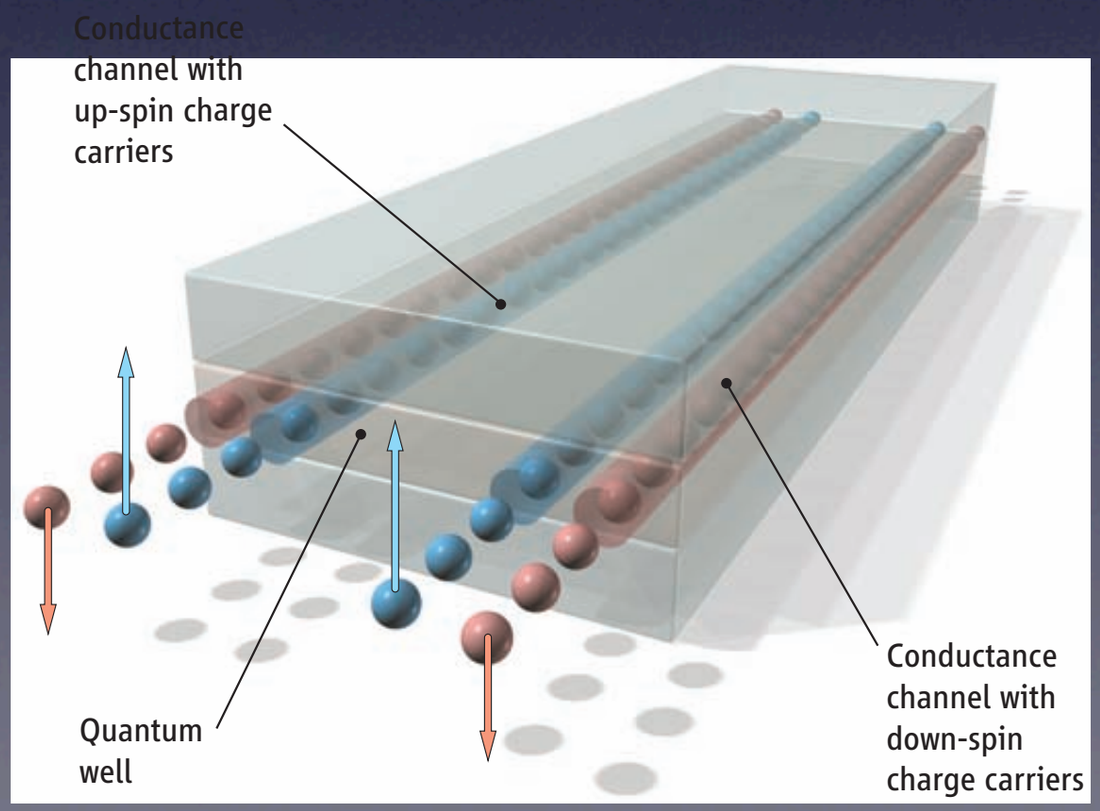
Science 2006

Quantum Spin Hall Insulator State in HgTe Quantum Wells

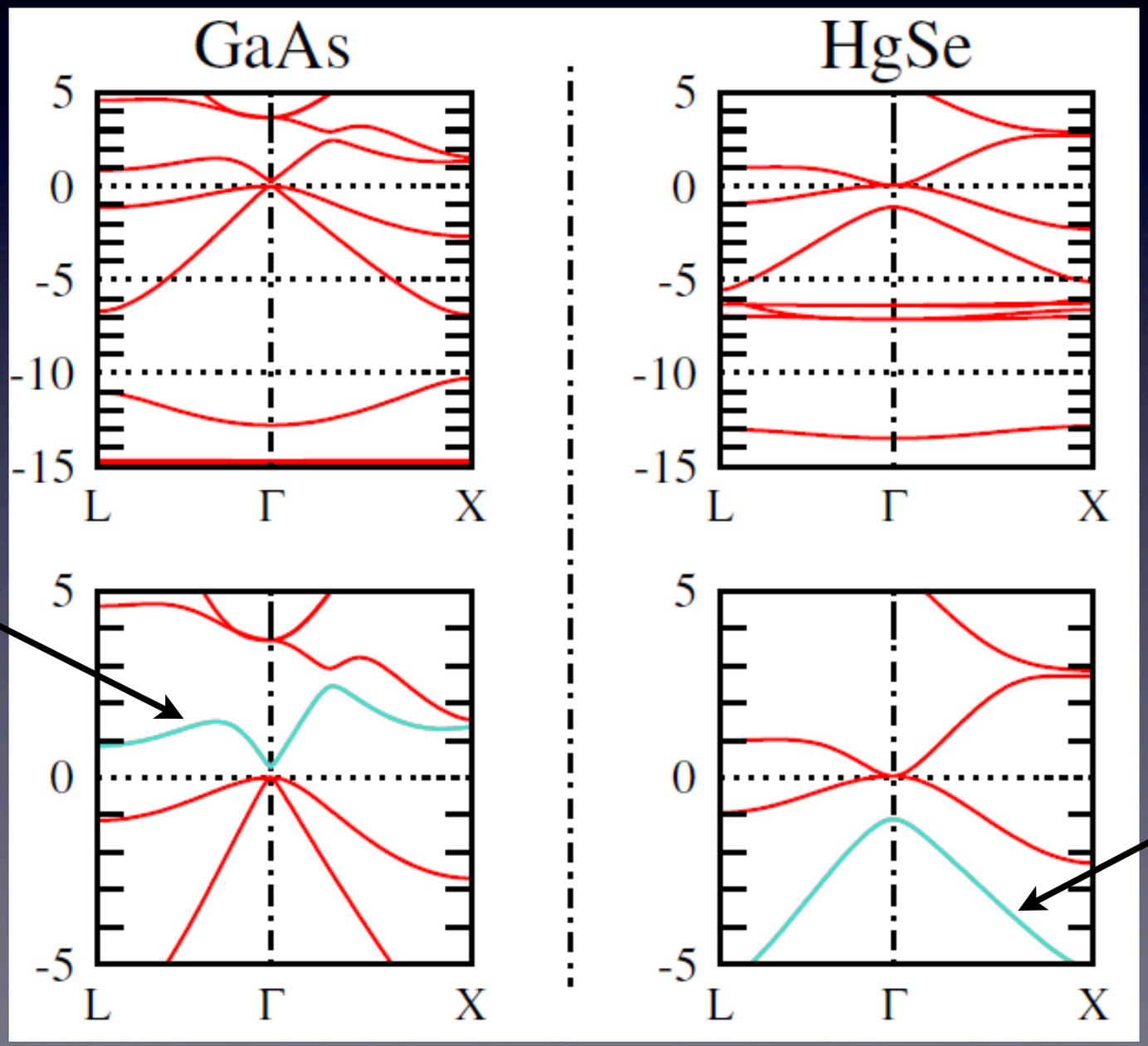
Markus König,[1] Steffen Wiedmann,[1] Christoph Brüne,[1] Andreas Roth,[1] Hartmut Buhmann,[1] Laurens W. Molenkamp,[1]* Xiao-Liang Qi,[2] Shou-Cheng Zhang[2]

Science 2007





Inverted band structure (without SOC)



conduction band

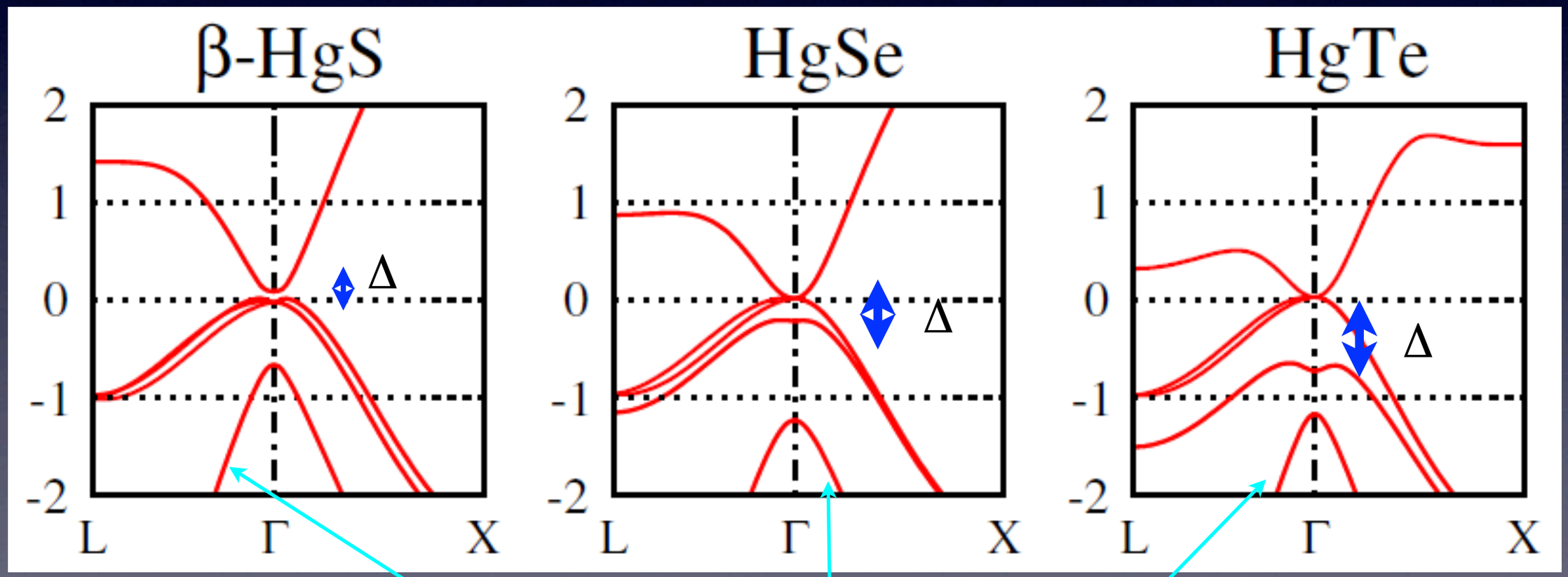
$E_{gap} > 0$

← Hg 5d

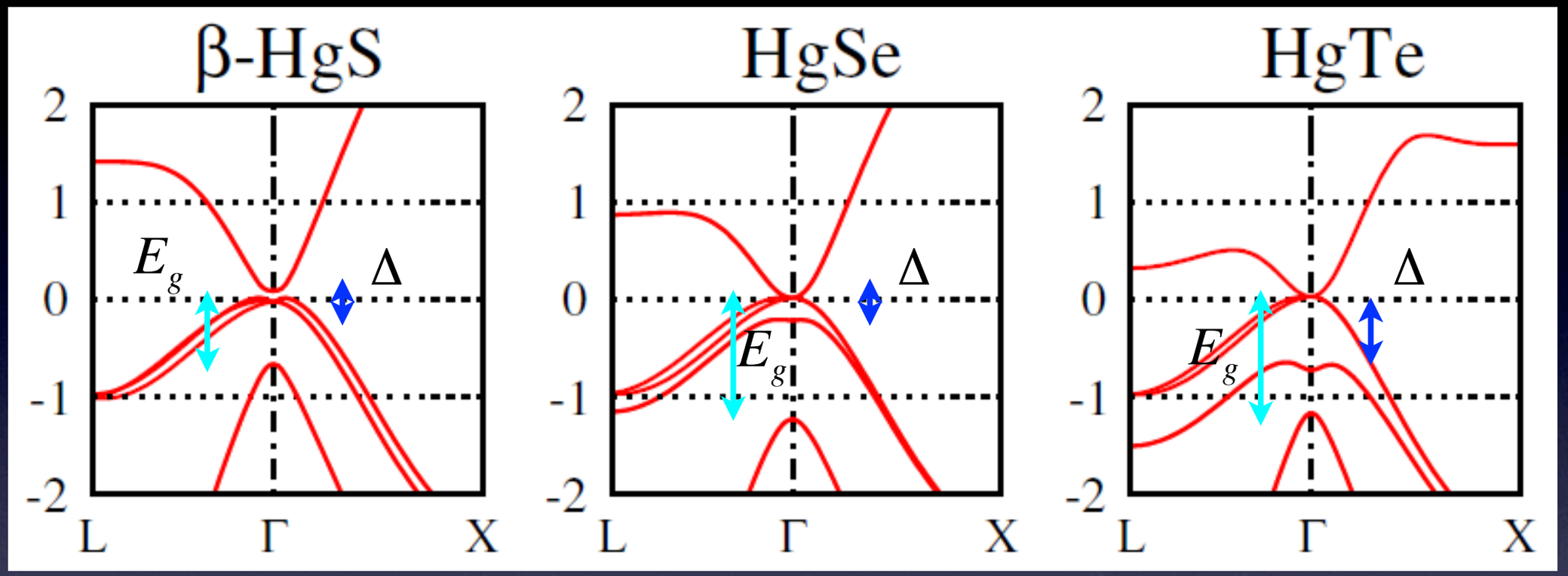
"conduction" band

$E_{gap} < 0$

Inverted band structure (with SOC)



LDA results

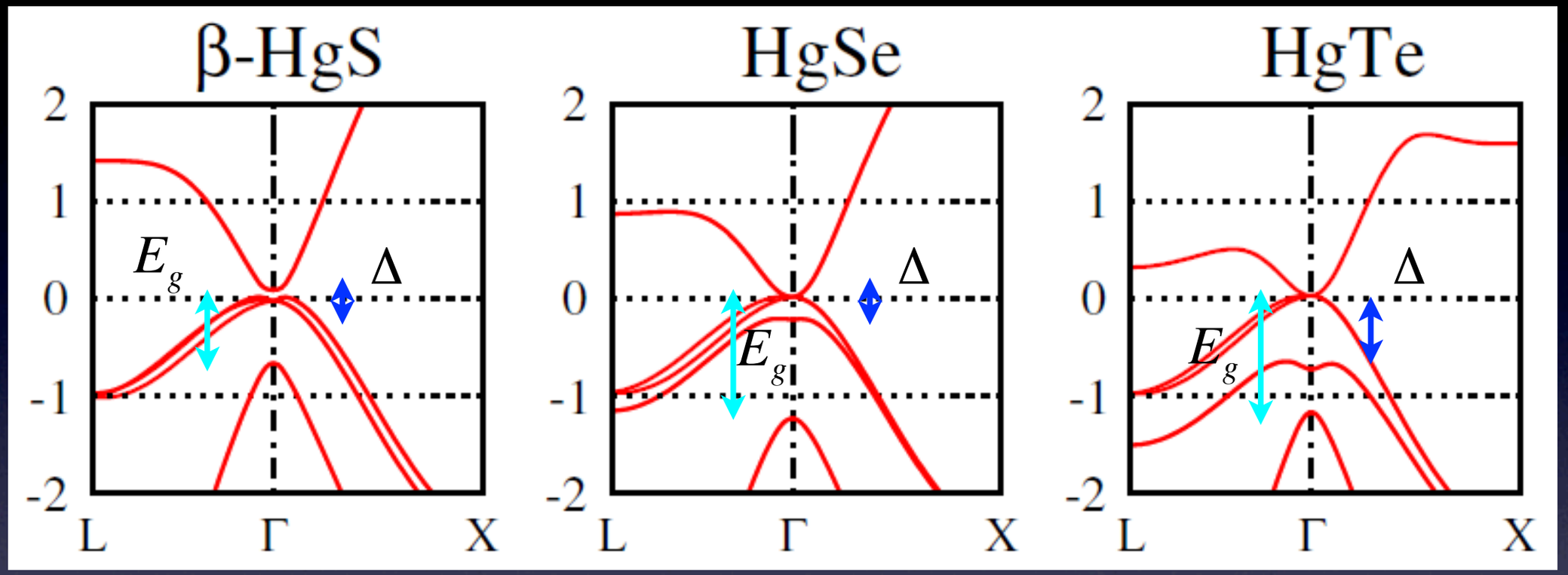


	HgS	HgSe	HgTe
LDA	-0.66	-1.27	-1.20
Expt.	-0.15, -0.11	-0.274	-0.29, -0.30
LDA	-0.12	+0.23	+0.78
Expt.		+0.39,+0.38	+0.91

E_g

Δ

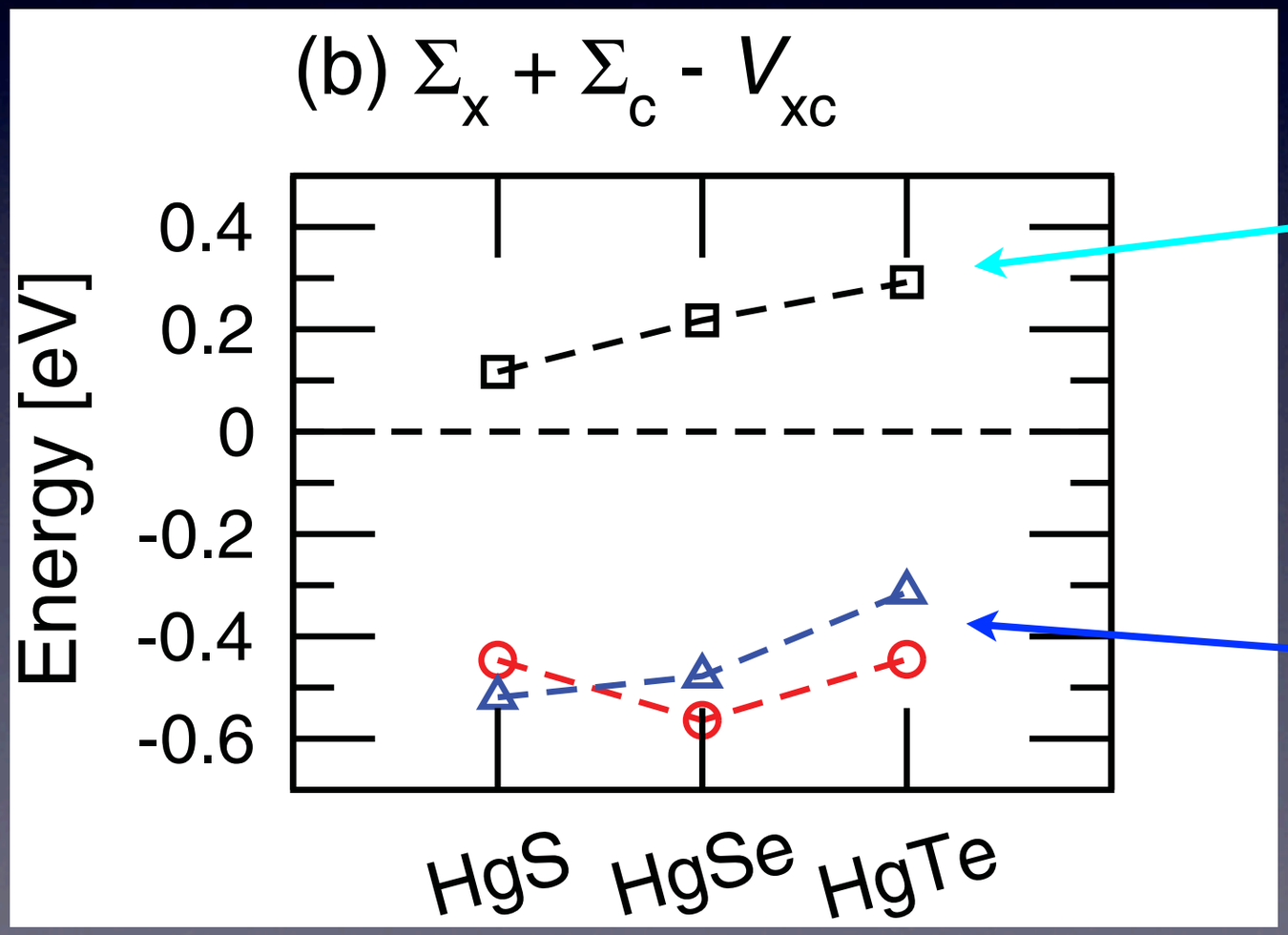
GW results



	HgS	HgSe	HgTe
E_g LDA	-0.66	-1.27	-1.20
E_g Expt.	-0.15, -0.11	-0.274	-0.29, -0.30
E_g GW	-0.02	-0.58	-0.60
Δ LDA	-0.12	+0.23	+0.78
Δ Expt.		+0.39,+0.38	+0.91
Δ GW	-0.19	+0.32	+0.91

Self-energy correction

$$\Delta E_n^{QP} \equiv E_n^{QP} - E_n^{DFT} = \langle \psi_n | \Sigma(E_n^{QP}) - V_{xc} | \psi_n \rangle$$

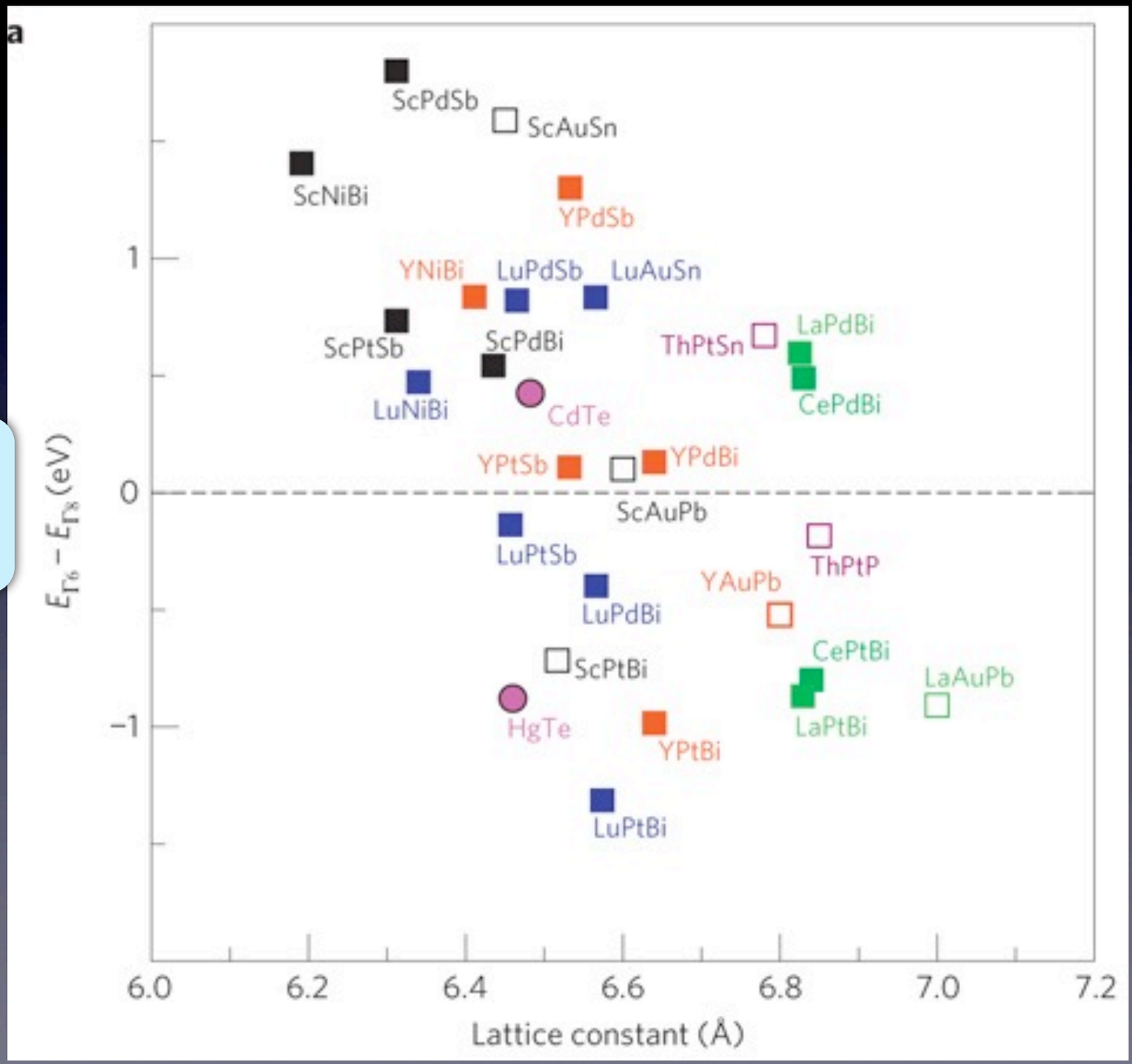


"conduction" bands

SO-splitted bands

Possible application: Searching new topological insulators

E_g



S. Chadov et al., Nature (2010)

Summary

- SOC-included GW approximation is proposed
- Application to Hg chalcogenides shows:
  - Improvement of the negative “band gap”
  - Enhancement of spin-orbit splitting
  - State-dependent self-energy correction