Quasiparticle study of the bulk TIs Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃ including spin-orbit coupling

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Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, Stefan Blügel
Peter Grünberg Institute and Institute for Advanced Simulation
Density functional theory (DFT)

DFT and the LDA approximation:

- Most widely used *ab-initio* approach.
- Good for ground-state properties: total energies, structural properties…
- Allows calculations of big systems like surfaces or defects.

BUT…
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BUT…

- Not appropriate for excited-state properties like excitation energies, optical properties, …

![Graph showing theoretical vs. experimental band gap](image)

- **$\text{Bi}_2\text{Se}_3$:** 0.2-0.35 eV
- **$\text{Bi}_2\text{Te}_3$:** 0.13-0.17 eV
- **$\text{Sb}_2\text{Te}_3$:** 0.17-0.28 eV
GW-SOC: Hg chalcogenides

- $GW$ corrects LDA band gaps
- Excitation energies as measured in PE experiments.
- BUT very time-consuming, only affordable for small systems (bulk)
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Theoretical value [eV] vs. experimental value [eV]

- $E_g(\Gamma)$
- $E_g(L)$
- $E_g(X)$

Spin-orbit splitting

R. Sakuma, C. Friedrich, T. Miyake, S. Blügel, and F. Aryasetiawan, PRB 84 085144 (2011)
**GW-SOC: Bi$_2$Se$_3$**

**LDA-VBM**

**GW-VBM(Γ)**

**E - E$_F$ (eV)**

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**Gaps**

- **LDA gap (I)**: 0.27 eV
- **GW gap (D)**: 0.23 eV (0.30*)
- **EXP. (D**): 0.2-0.35 eV

**References**

- Kioupakis et al.
  PRB 82, 245203 (2010)
- Yazyev et al.
  PRB 85, 161101(R) (2012)

**Authors**

GW-SOC: Bi$_2$Te$_3$

I. Aguilera, C. Friedrich, G. Bihlmayer, S. Blügel, in preparation
GW-SOC: Sb$_2$Te$_3$

LDA gap (I) 0.11 eV
GW gap (I) 0.17 eV
EXP. (I) 0.17-0.28 eV

I. Aguilera, C. Friedrich, G. Bihlmayer, S. Blügel, in preparation
**GW-SOC: Sb$_2$Te$_3$**

- **LDA gap (I)**: 0.11 eV
- **GW gap (I)**: 0.17 eV
- **EXP. (I)**: 0.17-0.28 eV

I. Aguilera, C. Friedrich, G. Bihlmayer, S. Blügel, *in preparation*
Topological $Z_2$ invariants do not change in GW.

Perturbative (pSOC) vs. full SOC

\[
GW - pSOC \rightarrow GW \text{ calculation without SOC} \\
\text{SOC calculated within LDA and added } a \text{ posteriori} \\
\text{(Approx. 4 times faster than full SOC)}
\]

\[
\text{Pert. SOC} \rightarrow LDA + GW + SOC(LDA) \\
\text{Full SOC} \rightarrow LDA + SOC + G^{SOC}W^{SOC}
\]

**MOTIVATION:**

- FULL-SOC calculations very time-consuming
- Two references recently published for Bi$_2$Se$_3$ and Bi$_2$Te$_3$ with GW-pSOC:
  
  Kioupakis, Tiago, Louie
  PRB 82, 245203 (2010)

  Yazyev, Kioupakis, Moore, Louie
  PRB 85, 161101(R) (2012)
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\[ E - E_F \text{(eV)} \]

I. Aguilera, C. Friedrich, G. Bihlmayer, S. Blügel, \textit{in preparation}
Summary and conclusions

- **GW** calculations change significantly the dispersion of the highest VB and the lowest CB. The „M-shape“ of the VB flattens or disappears.

- The band inversion is present in **GW** even in the case of Sb₂Te₃ in which the „M-shape“ disappears completely.

- A perturbative approach to SOC does not predict the dispersion of the VB and CB correctly.
Thank you!

DFT calculations  →  FLEUR: www.flapw.de

GW calculations  →  SPEX: www.flapw.de/spex

Virtual Institute for Topological Insulators (VITI): www.vi-ti.de

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