All-Electron, Conserving Investigation of the Band Gap of Si and Ge within the *GW* approximation

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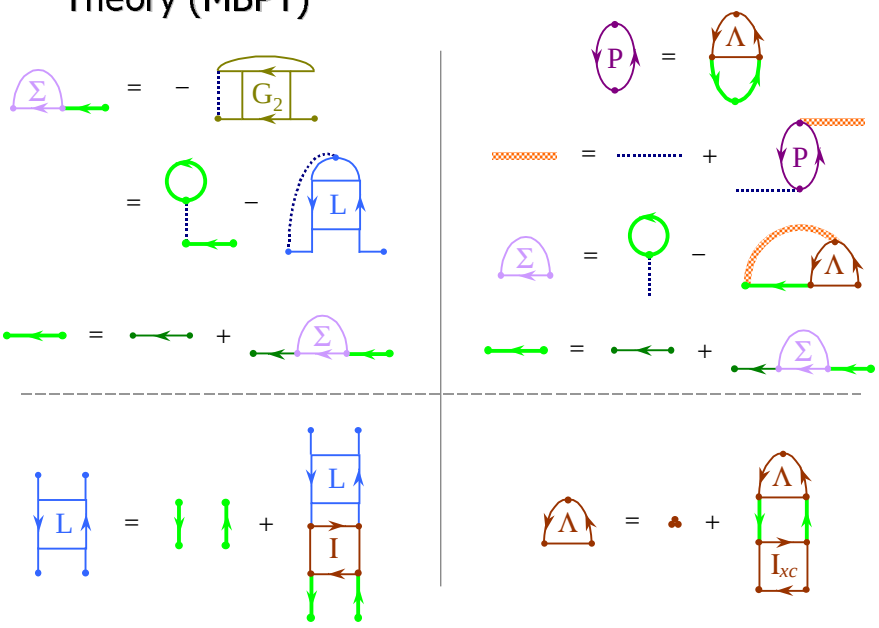
This work was supported by NSF-DMR and NERSC

Motivation

- Non-conserving $G^{LDA}W^{LDA}$ has been successful in calculating quasi-particle (QP) band gap: Why?
  - Schindlmayr : $G^{LDA}W^{LDA}$ violates particle number conservation. [PRB 56, 3528 (1997)]
  - Schöne and Eguiluz : conserving *GW* overshoots the gap by the amount LDA underestimates it. [PRL 85, 2410 (2000)]
  - Do we have a conserving theory capable of producing good gap?
- Deep core electrons play almost no role: True?
- Polarization from 3d core states is responsible to switch Ge from direct gap (no gap) to indirect gap: True?
- Is pseudo-potential designed for performing QP calculation?

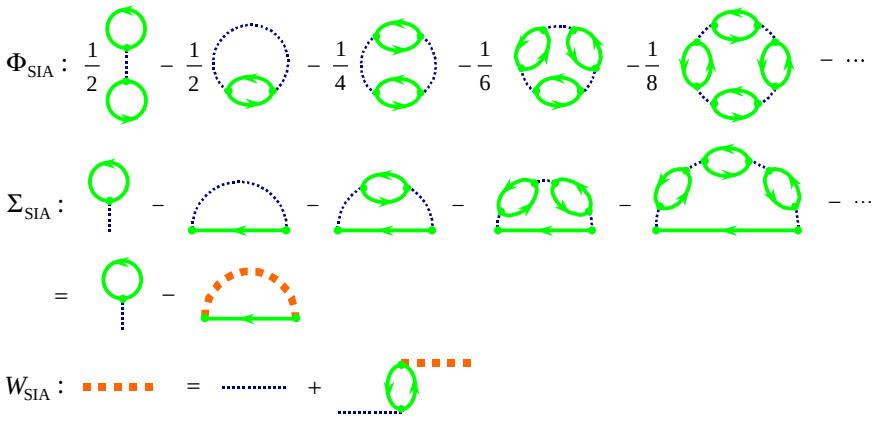
Finite Temperature Many-Body Perturbation Theory (MBPT)



Baym-Kadanoff Conserving Scheme :

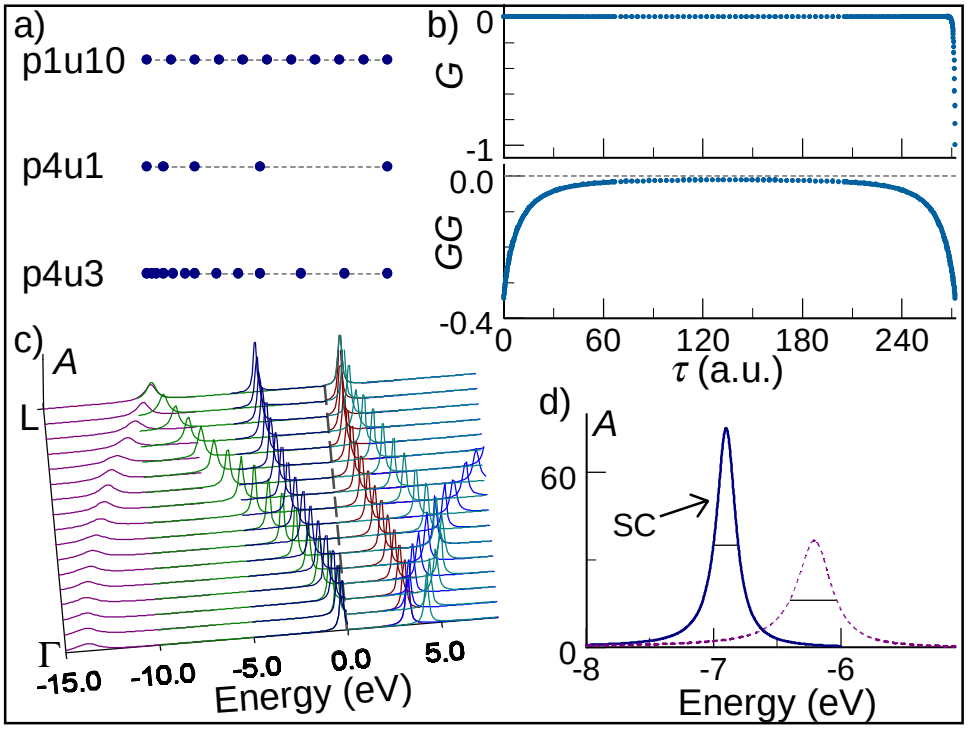
- Σ is Φ derivable.
- Dyson equation is solved self-consistently. (Σ=Σ[*G*])
- All microscopic conservation laws are guaranteed!

Ex: Shielded Interaction Approximation (SIA) : (*GW* form)



New Implementation

- All-electron and full-potential:
  - Realistic wave functions (oscillations near atomic sites)
  - Core (and semi-core) states explicitly included in Σ
  - Applicable to systems with localized *d*-states (Physical temperature effect → finite temperature formalism)
- Matsubara time :
  - Bounded and continuous → cutoff- and modeling-free
  - Capable of treating shallow core states or highly excited states (no exponential growth)
  - Applicable beyond *GW*
  - real algorithms → ~ 5 times more efficient



Results: QP Band Gap of Si within *GW* Effect of Self-consistency

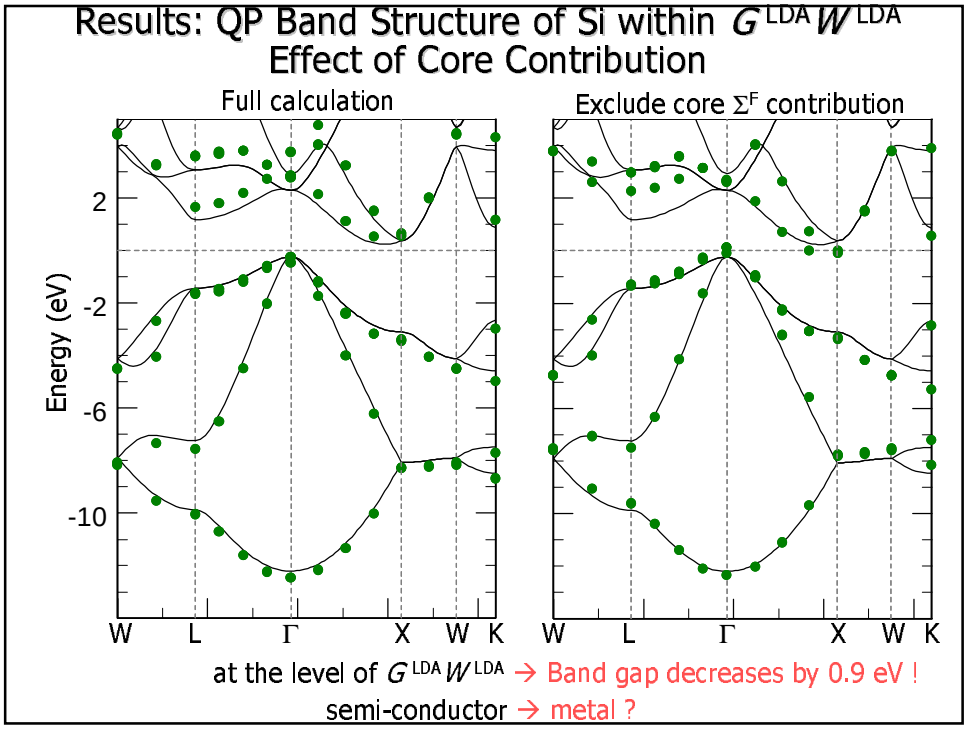
	abs. gap (eV)	direct gap (eV)	occupied bandwidth (eV)
Landolt-Börnstein (exp)	1.17	3.4	12.5 ± 0.6
present work (LDA, FLAPW)	0.52	2.53	12.22
Hybertsen and Louie	1.29	3.35	12.04
Schöne and Eguiluz	1.34	3.27	11.65
Schöne and Eguiluz (SC)	1.91	4.02	13.10
present work (all e^-)	0.85	3.12	12.15
present work (all e^-, SC)	1.03	3.48	13.53

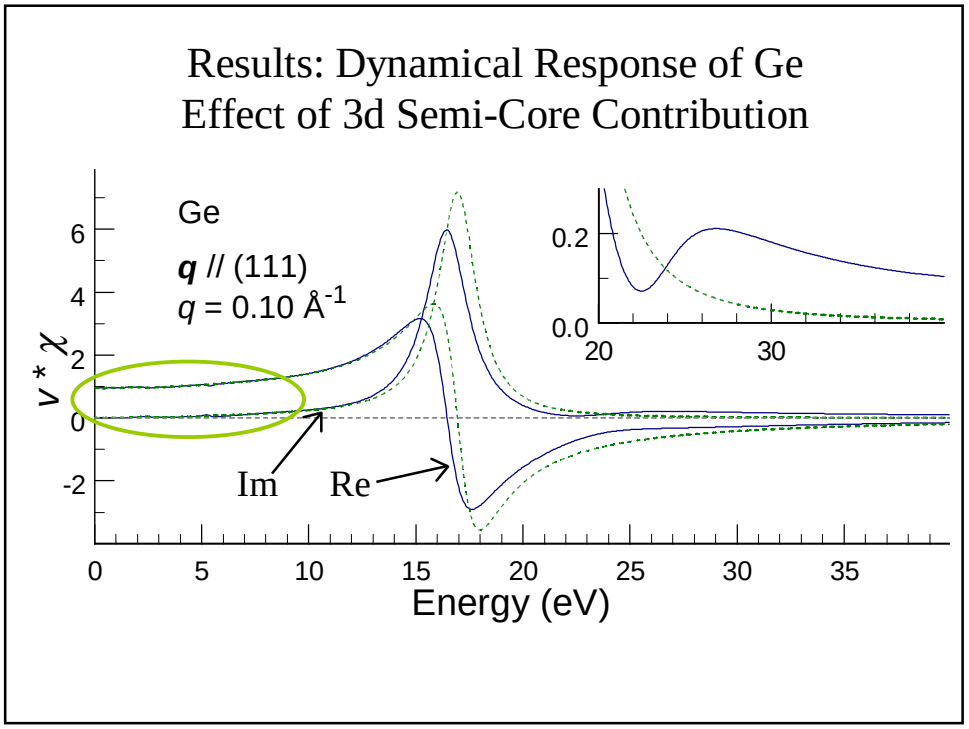
Results: QP Band Gap of Si within $G^{LDA}W^{LDA}$ All-electron vs. Pseudo-potential

	absolute gap (eV)
Landolt-Börnstein (exp)	1.17
present work (LDA, FLAPW)	0.52
Hybertsen and Louie	1.29
Rohlfing, Krüger, and Pollmann	1.17
Rojas, Godby, and Needs	1.29
Fleszar and Hanke	1.19
Schöne and Eguiluz *	1.34
Arnaud and Alouani (~all e^-, PAW)	1.00
Hamada, Hwang, and Freeman (~all e^-, LAPW)	1.01
present work (all e^-, LAPW)	0.85

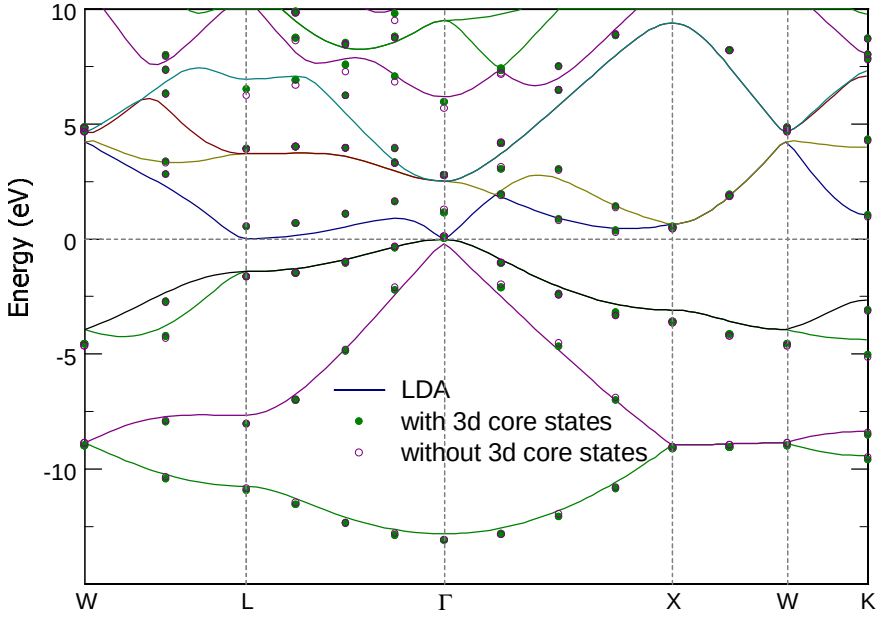
~all e^- : $\Sigma^{\text{from core}} \approx V^{LDA}\left[n^{\text{valence + core}}\right] - V^{LDA}\left[n^{\text{valence}}\right] \Rightarrow \sim -0.15eV$ error

* discrepancy due to oscillation of WF is also found in dynamical response. (N31.008, Z13.010)


Results: QP Band Structure of Si within $G^{LDA}W^{LDA}$
Effect of Core Contribution
Full calculation
Exclude core Σ^F contribution
Energy (eV)
2
-2
-6
-10
W L Γ X W K
W L Γ X W K
at the level of $G^{LDA}W^{LDA}$ → Band gap decreases by 0.9 eV !
semi-conductor → metal ?


Results: Dynamical Response of Ge
Effect of 3d Semi-Core Contribution
Ge
q // (111)
q = 0.10 Å-1
v * χ
6
4
2
0
-2
0.2
0.0
20
30
Im
Re
0 5 10 15 20 25 30 35
Energy (eV)

Results: QP Band Structure of Ge within $G^{LDA}W^{LDA}$ Effect of 3d Core Contribution



Conclusion

- The success of non-conserving $G^{LDA}W^{LDA}$ calculations is helped by large compensation between effects from Lack of:
  - core contribution to self-energy
  - oscillations in wave functions when evaluating $\langle k,j|\Sigma|k,j\rangle$
  - self-consistency
- Deep core states play an important role in defining the QP band gap through exchange process with the valence states.
- Omission of oscillations of the wave functions near the the atomic sites have sizeable impact on the QP band gap.
- Self-consistency is necessary in our conserving calculation to produce satisfactory gap.
- Polarization from 3d core states in Ge has almost no effect on the QP band structure within *GW* approximation.
- Further improvement requires processes beyond *GW* diagram.