QS$\boldsymbol{GW}_\Lambda$

INCLUDING LADDER DIAGRAMS IN THE SCREENING THROUGH THE BSE

3rd Daresbury Questaal school
15th May 2019

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Many Body Theory

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Eigenvectors and values of DFT/HF Hamiltonian can be used!

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LDA based GW VERY successful and widely used!

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- Limit of a quasiparticle picture?
- Limitations of basis set, time integration techniques, cut-offs, accurate experimental data, etc

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Self-consistent GW is the answer (possibly?)!
How to implement self-consistency?
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QSGW missing the effect of Λ
In both Pol. & S.E

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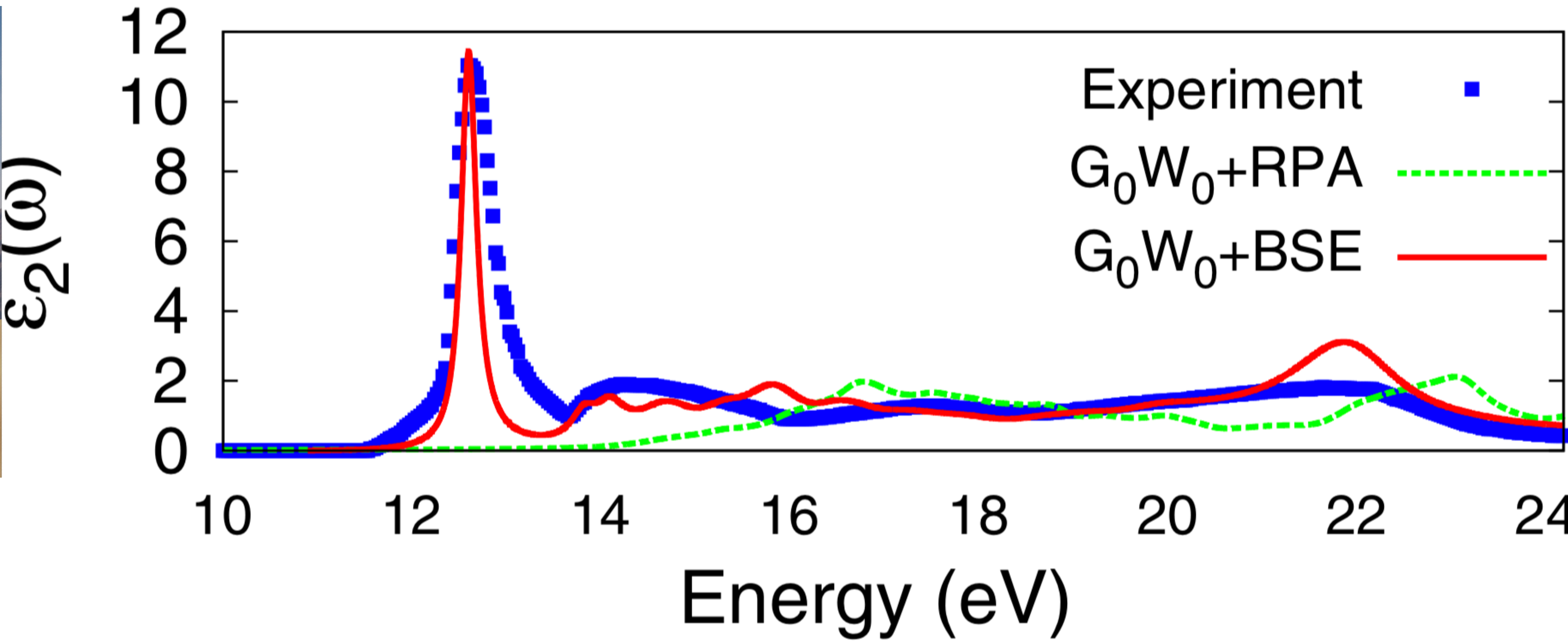
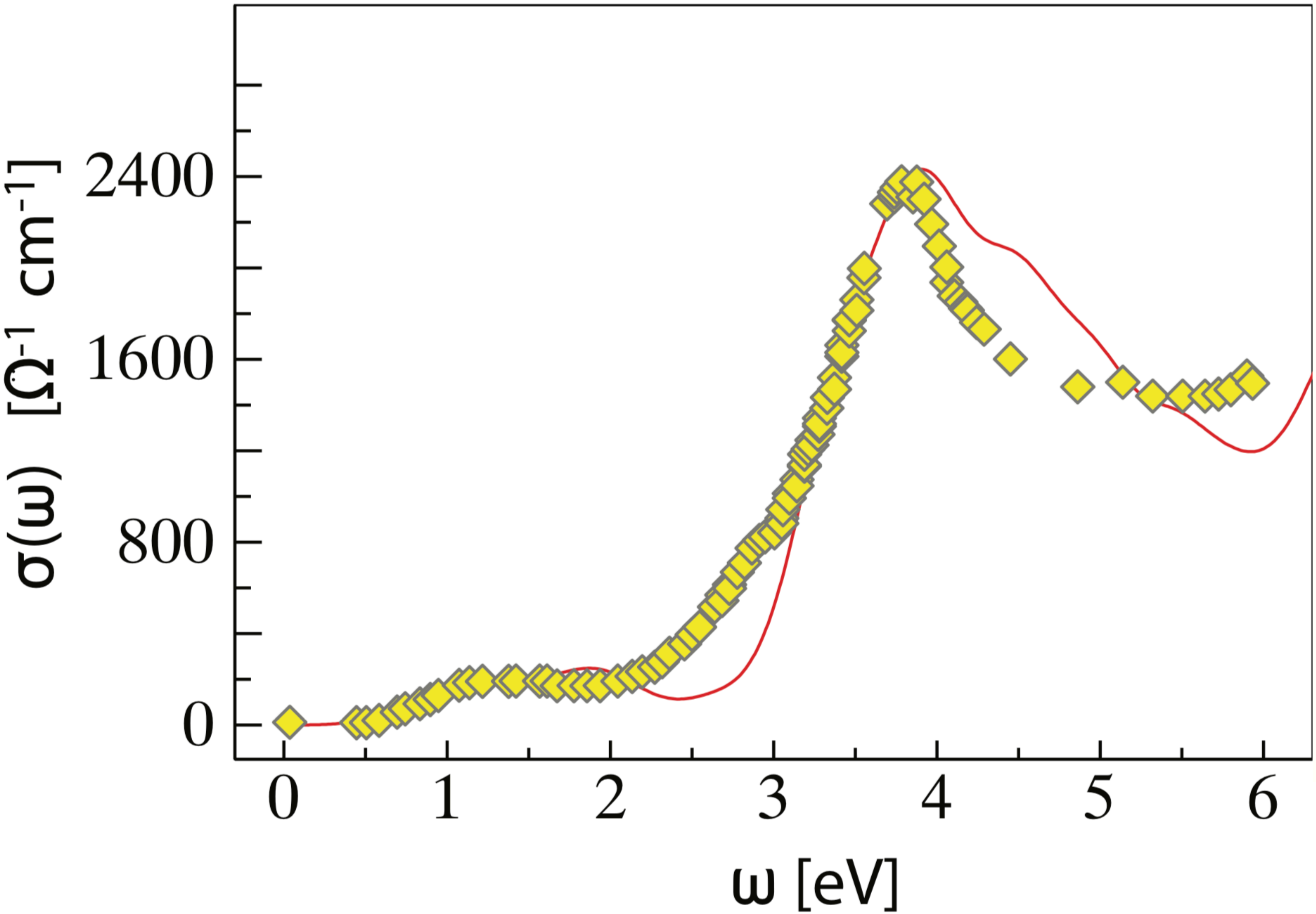
Using the GWA electronic structure in the BSE to produce the macroscopic dielectric function is a common technique and many codes do this Yambo, Vasp, Exciton,...**
This method, usually called, GW+BSE demonstrates the effect of Λ on the dielectric function

**** Note that the electronic structure here (i.e., Σ) does not include the effect of Λ at all!**

Excitons in LiF



Excitons in VO2



QSGW

Pros and Cons

- QSGW goes beyond single-shot GW and removes starting point dependence
- Significantly corrects electronic structure in correlated systems, e.g., NiO
- Band gaps overestimated by up to 2eV in LiF (GWA gets it almost exact); why?

Why the large overestimation?

- Electron-phonon interactions and ladder diagrams are missing in the SELF-ENERGY
- Can we use the BSE to improve on W?

Ladders in the Self Energy

Macroscopic dielectric function for optical spectra & EELS calculate

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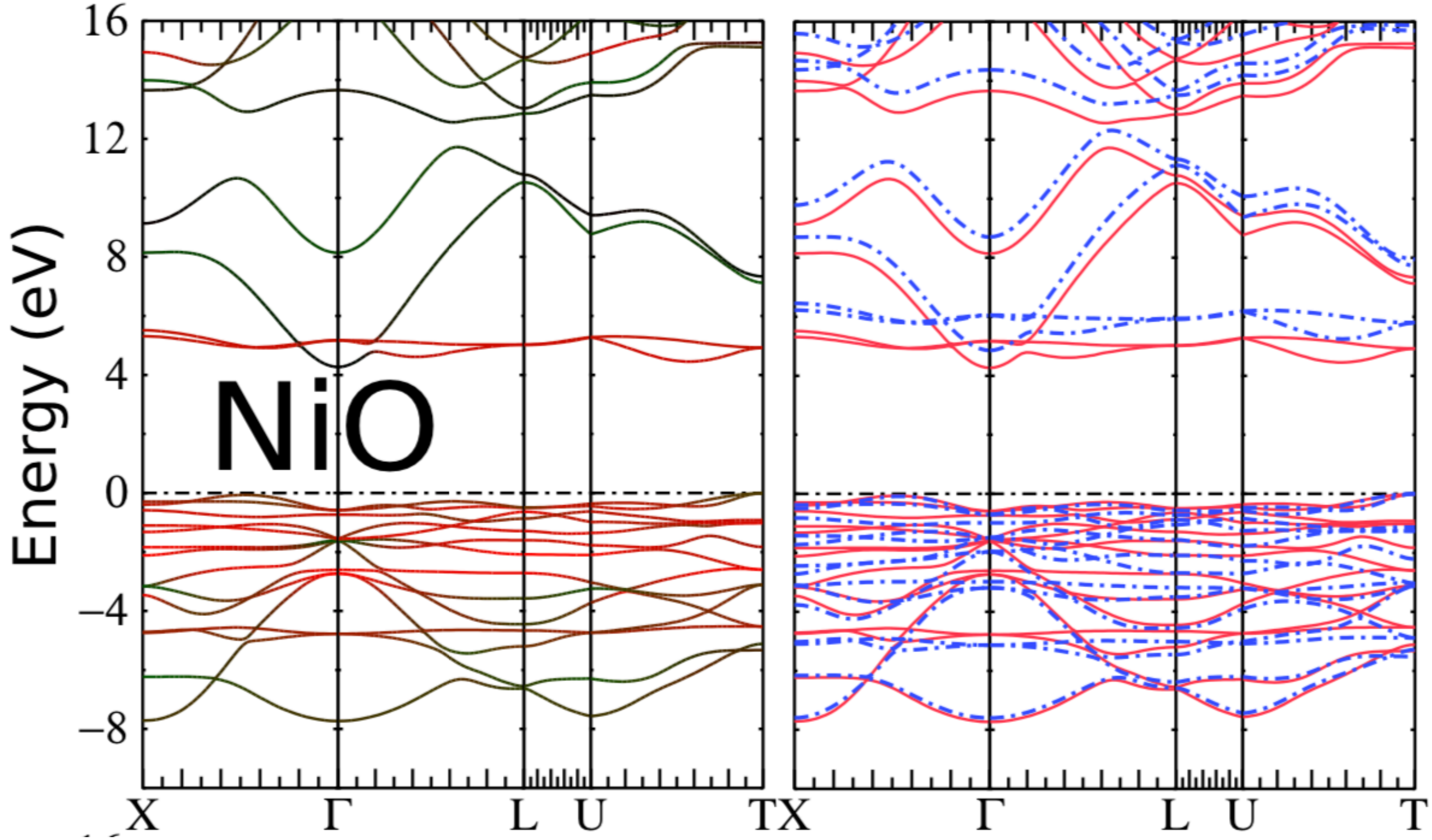
Role of Λ in the expression for Σ not as important as in P!

Results: NiO (1)

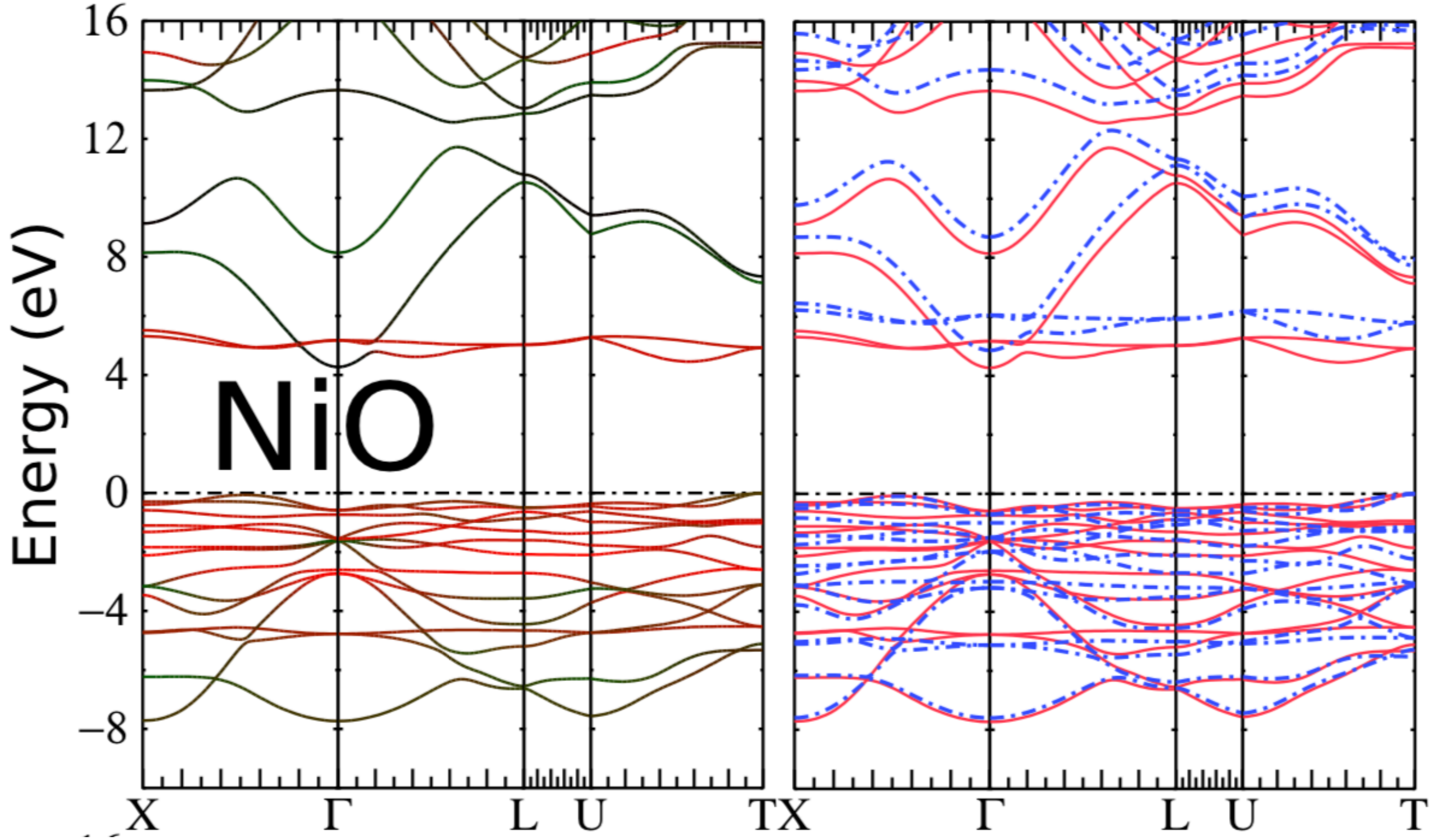


Right panel: blue dashed lines are QSGW and the red lines are QSGW

Orbital character weights on left: red are Ni d bands and green are O p bands

d-bands shifted down in energy further than the s and p bands

RESULTS: NIO (1)



Right panel: blue dashed lines are QSGW and the red lines are $QSGW_{\Lambda}$

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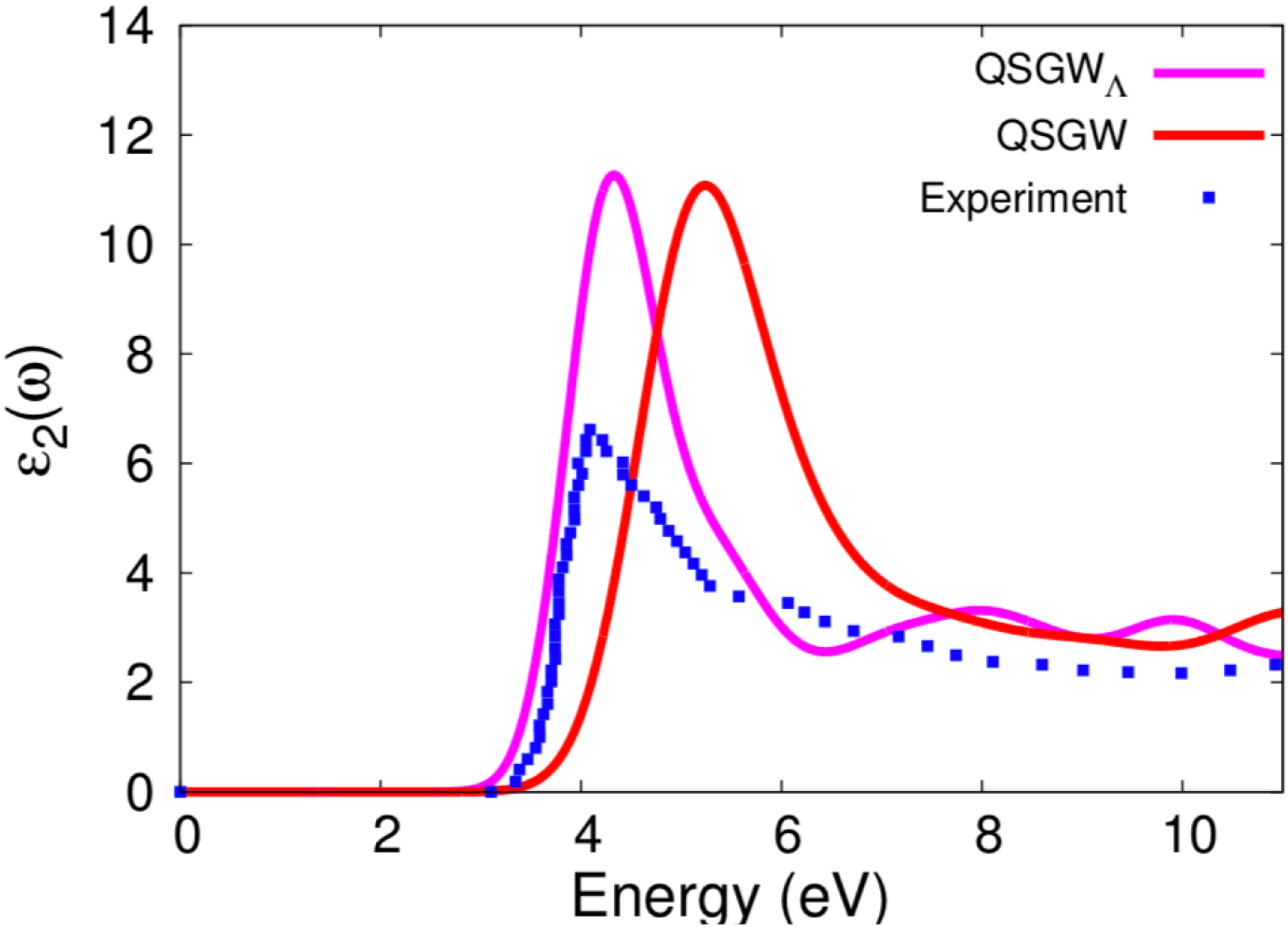
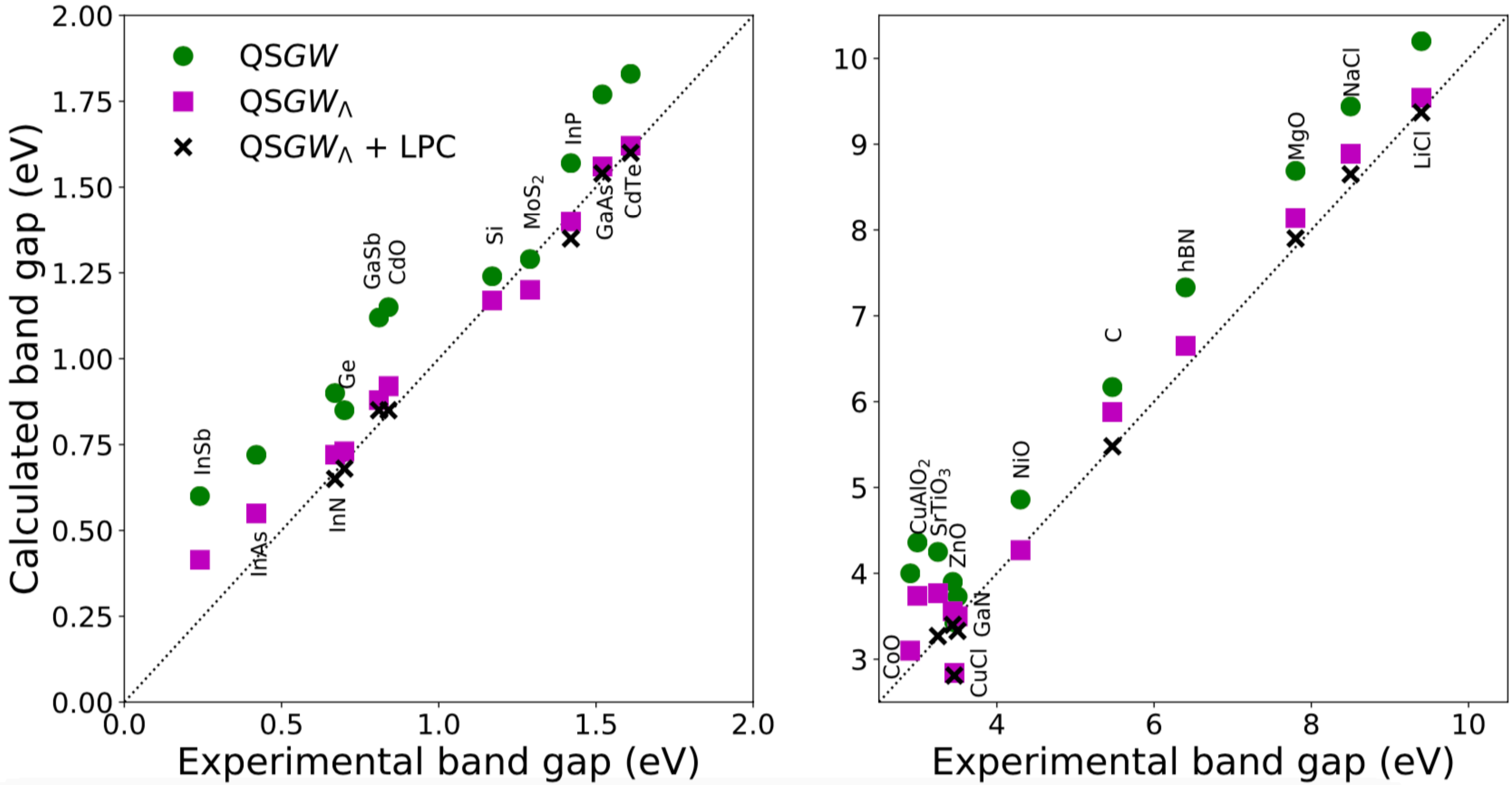
RESULTS: NIO (2)



RESULTS: BAND GAPS



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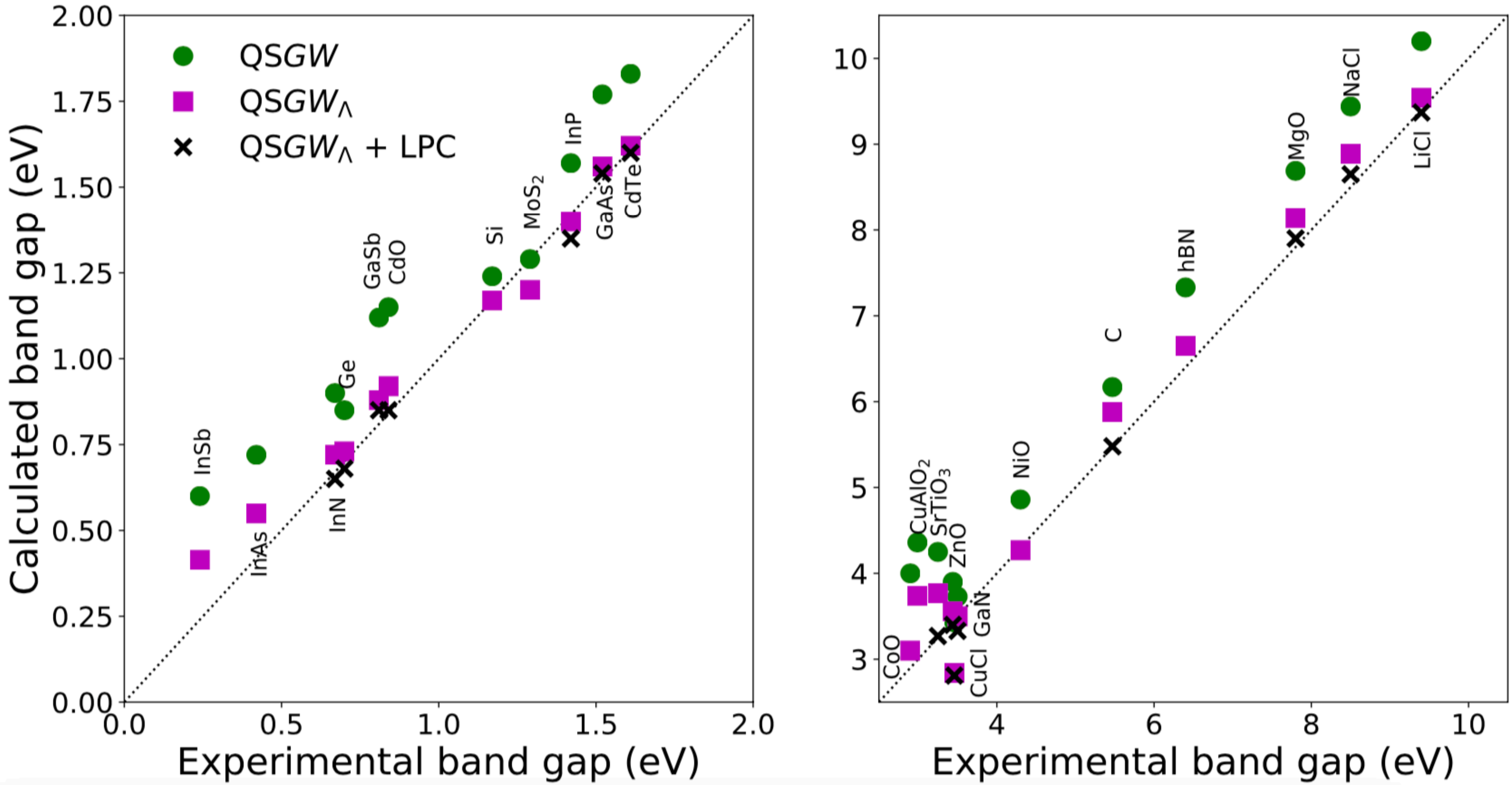
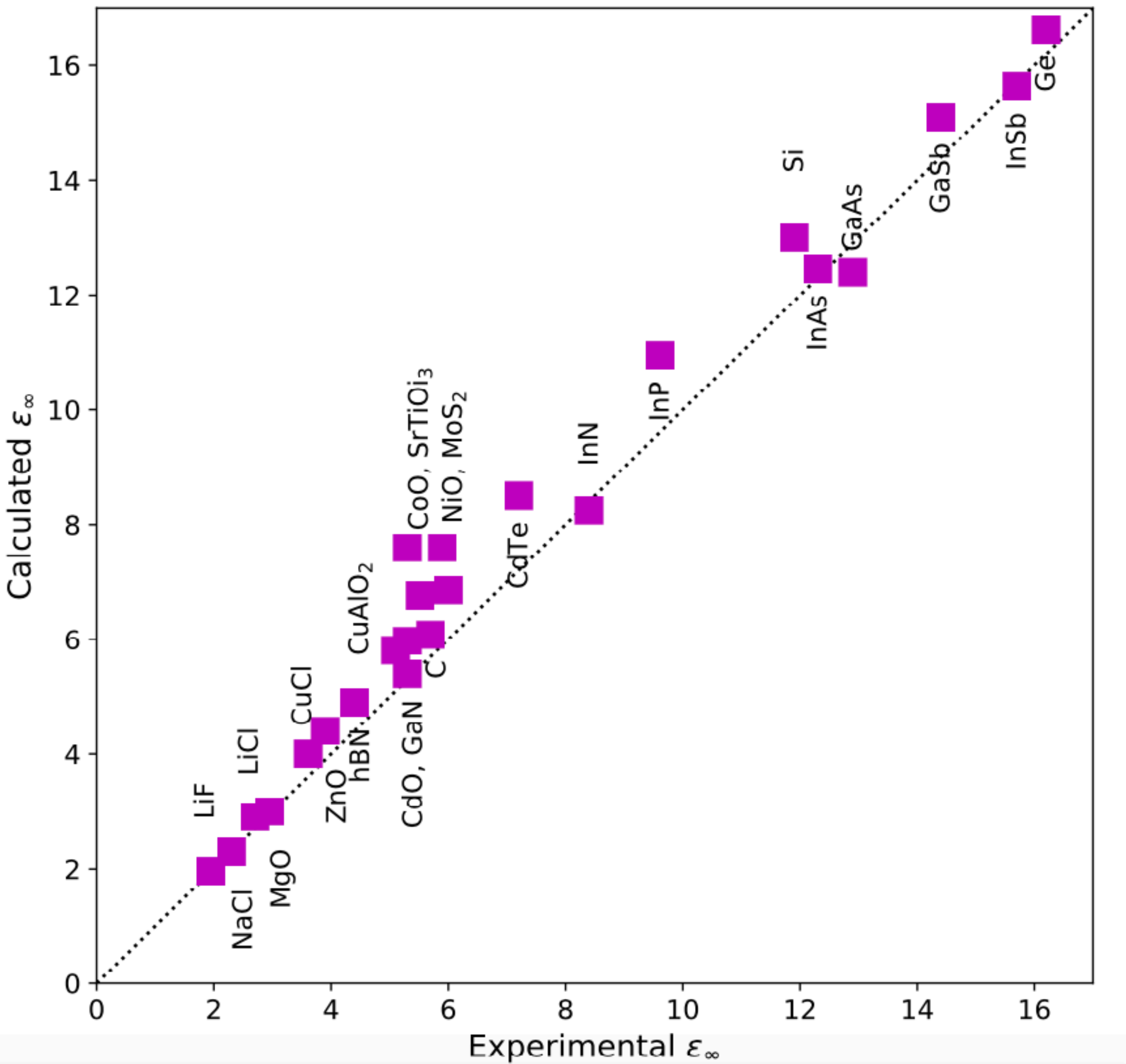


CuCl: too shallow Cu d state intermixes too strongly with the Cl p states, pushing them too high energy, reducing the gap. Vertex in S.E. may fix

RESULTS: OPTICAL CONSTANTS



Thank You!