The GW approximation in GPAW!

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DFT vs. MBPT

Density Functional Theory

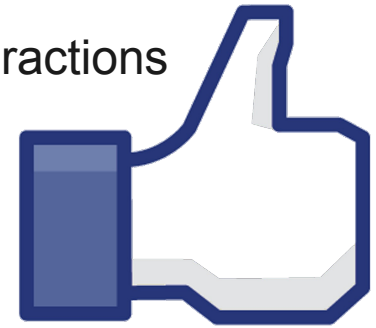
$$E^{\mathrm{XC}}[\rho]$$

- exchange-correlation Functional
- (semi-) empirical
- Effectively non-interacting electrons
- Interpretation of states and energies
- Band gaps
- van-der-Waals interactions
- Screening effects

Many-Body Perturbation Theory

$$\Sigma^{\mathrm{XC}}$$

- Self Energy
- Systematic expansion
- Quasiparticles
- Excitation energies
- Band gaps
- van-der-Waals interactions
- Screening effects



GW approximation

- self energy expanded to first order in *W*
- no vertex corrections
- corresponds to Hartree-Fock with screened potential *W*

$$\Sigma^{\mathrm{HF}} = iGV$$

$$\Sigma^{\mathrm{GW}} = iGW \qquad W = V^{\mathrm{screened}} = \epsilon^{-1} \cdot V^{\mathrm{Coulomb}}$$

Green's Function

dielectric response function

- static limit: COHSEX approximation
- model dielectric response function: Plasmon Pole Approximation
- fully dynamical GW: frequency-dependent dielectric response function

G_0W_0

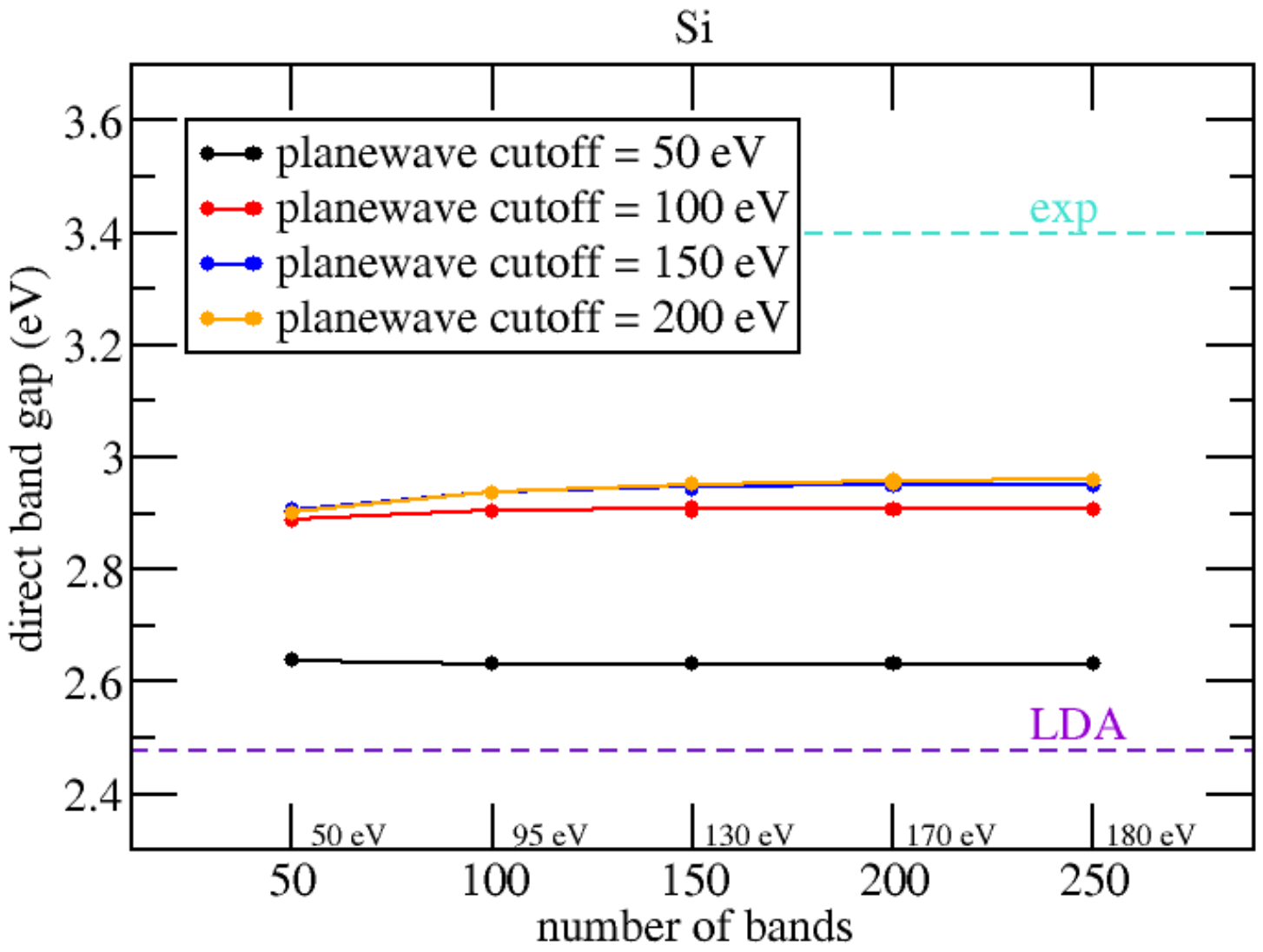
- Construct Green's Function from DFT energies and wavefunctions.
- Obtain energy corrections.

$$E_{n\vec{k}} = \varepsilon_{n\vec{k}} + Z_{n\vec{k}} \cdot \mathrm{Re}\left(\Sigma_{n\vec{k}} + \varepsilon_{n\vec{k}}^{\mathrm{EXX}} - V_{n\vec{k}}^{\mathrm{XC}}\right)$$

$$\begin{aligned}\Sigma_{n\vec{k}} = & \frac{1}{\Omega}\sum_{\vec{G}\vec{G}'}\sum_{\vec{q}}^{1.\mathrm{BZ}}\sum_{m}^{\mathrm{all}}\frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega'\, W_{\vec{G}\vec{G}'}(\vec{q},\omega') \cdot \\ & \left\langle n\vec{k}\middle| e^{i(\vec{q}+\vec{G})\vec{r}}\middle| m\,\vec{k}+\vec{q}\right\rangle \left\langle m\,\vec{k}+\vec{q}\middle| e^{-i(\vec{q}+\vec{G}')\vec{r}}\middle| n\vec{k}\right\rangle \cdot \\ & \frac{1}{\omega+\omega'-\varepsilon_{m\,\vec{k}+\vec{q}}+i\eta\,\mathrm{sgn}(\varepsilon_{m\,\vec{k}+\vec{q}}-\mu)}\end{aligned}$$

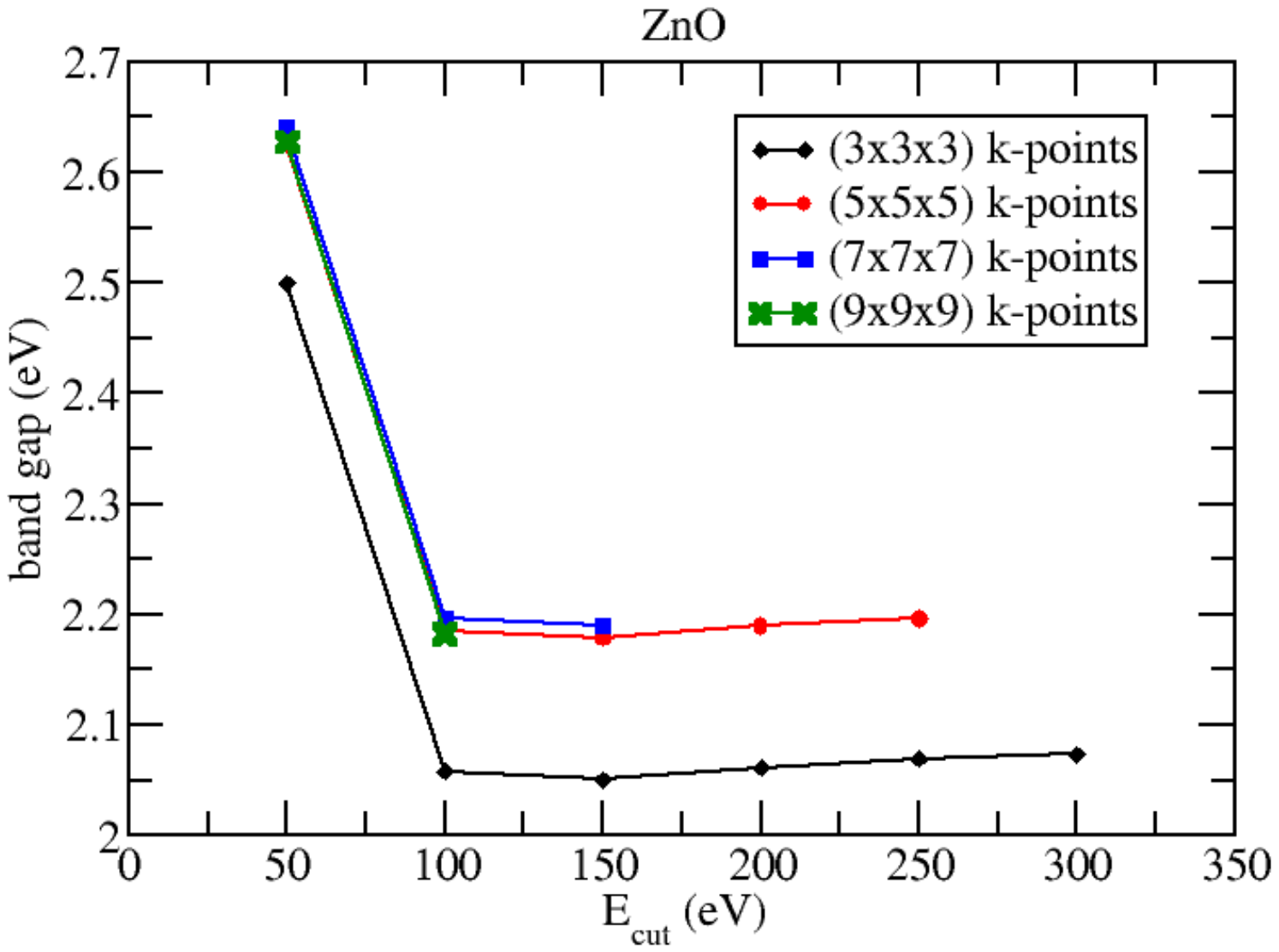
convergence tests

- Convergence with respect to number of bands and plane waves



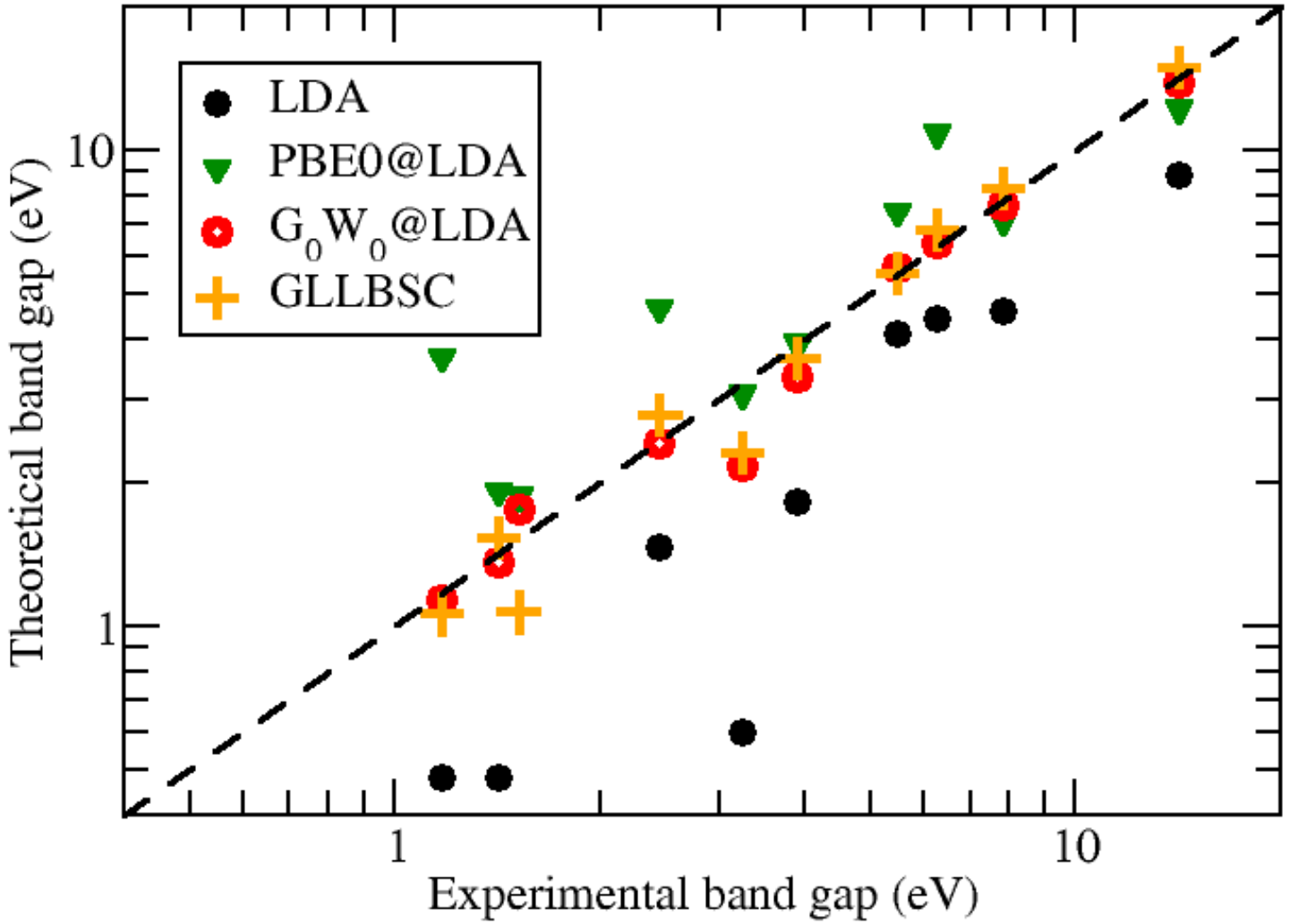
convergence tests

- Convergence with respect to number of k-points



semiconductors

calculated vs. experimental band gaps



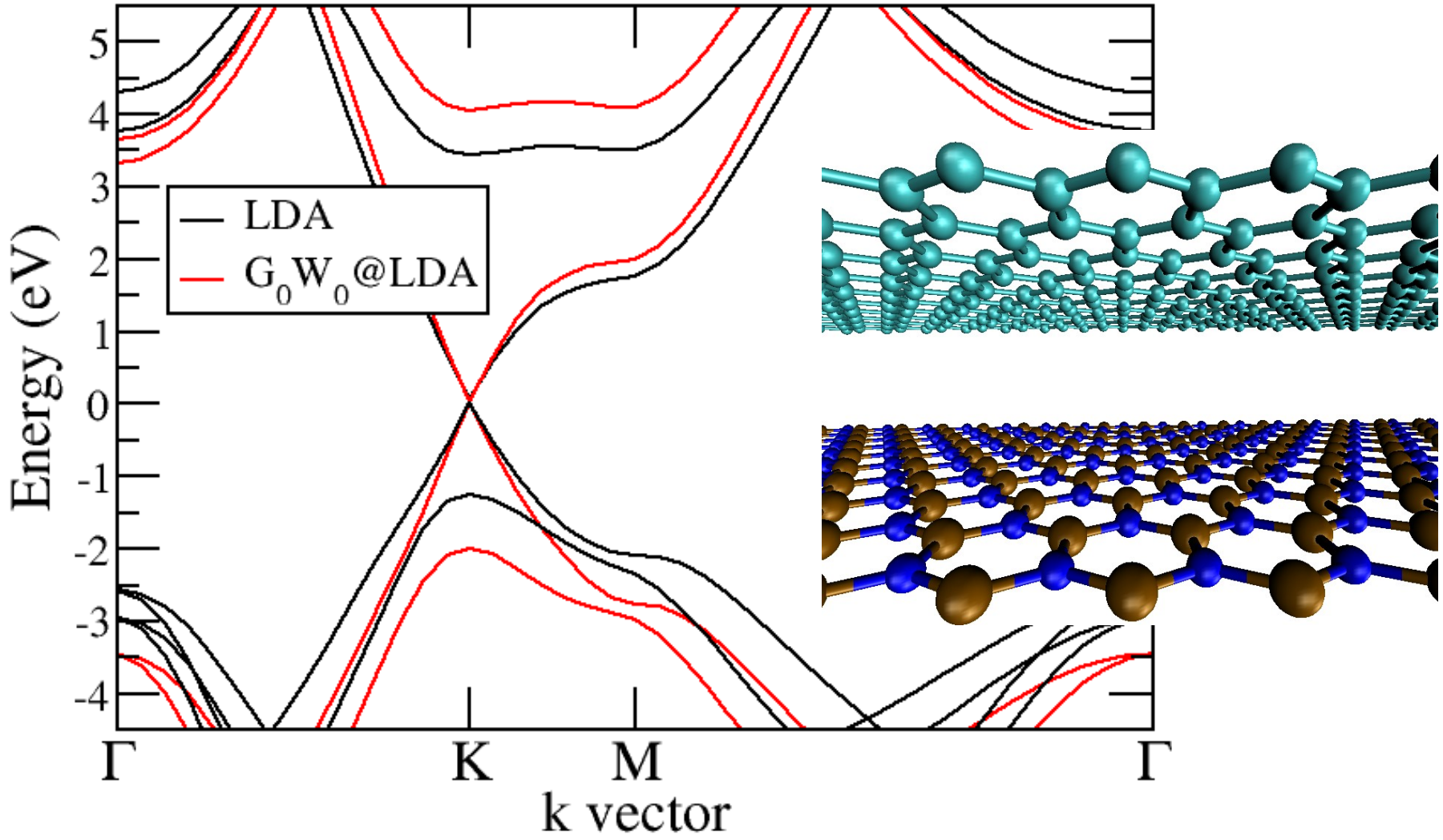
semiconductors

	LDA	HF	COHSEX	GW (PPA)	GW (dyn)	GLLBSC	Expt.
C	4.12	11.83	6.46	5.59	5.67	5.52	5.48
GaAs	0.38	5.46	3.77 (0.97)	1.76	1.75	1.23	1.52
InP	0.48	5.51	1.99 (1.53)	1.38	1.36	1.63	1.42
LiF	8.83	21.86	16.02	13.64	13.84	14.94	14.20
MgO	4.59	14.84	10.30	7.44	7.61	8.32	7.83
Si	0.48	5.26	0.52	1.09	1.13	1.09	1.17
MAE	*2.12*	*5.52*	*1.46*	*0.24*	*0.18*	*0.31*	

band gaps for bulk systems and mean absolute error in eV

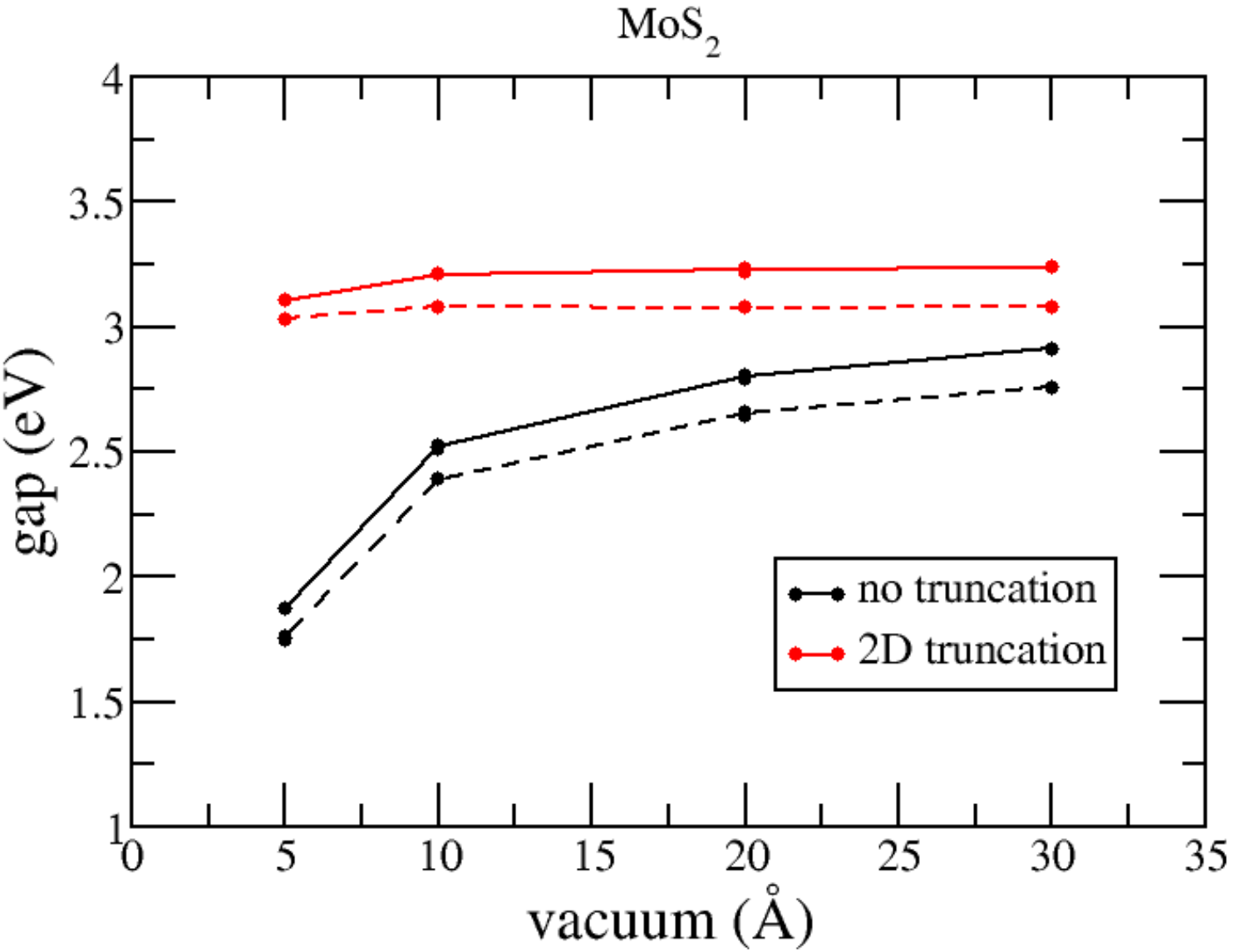
2D materials

Bandstructure of graphene / *h*-BN



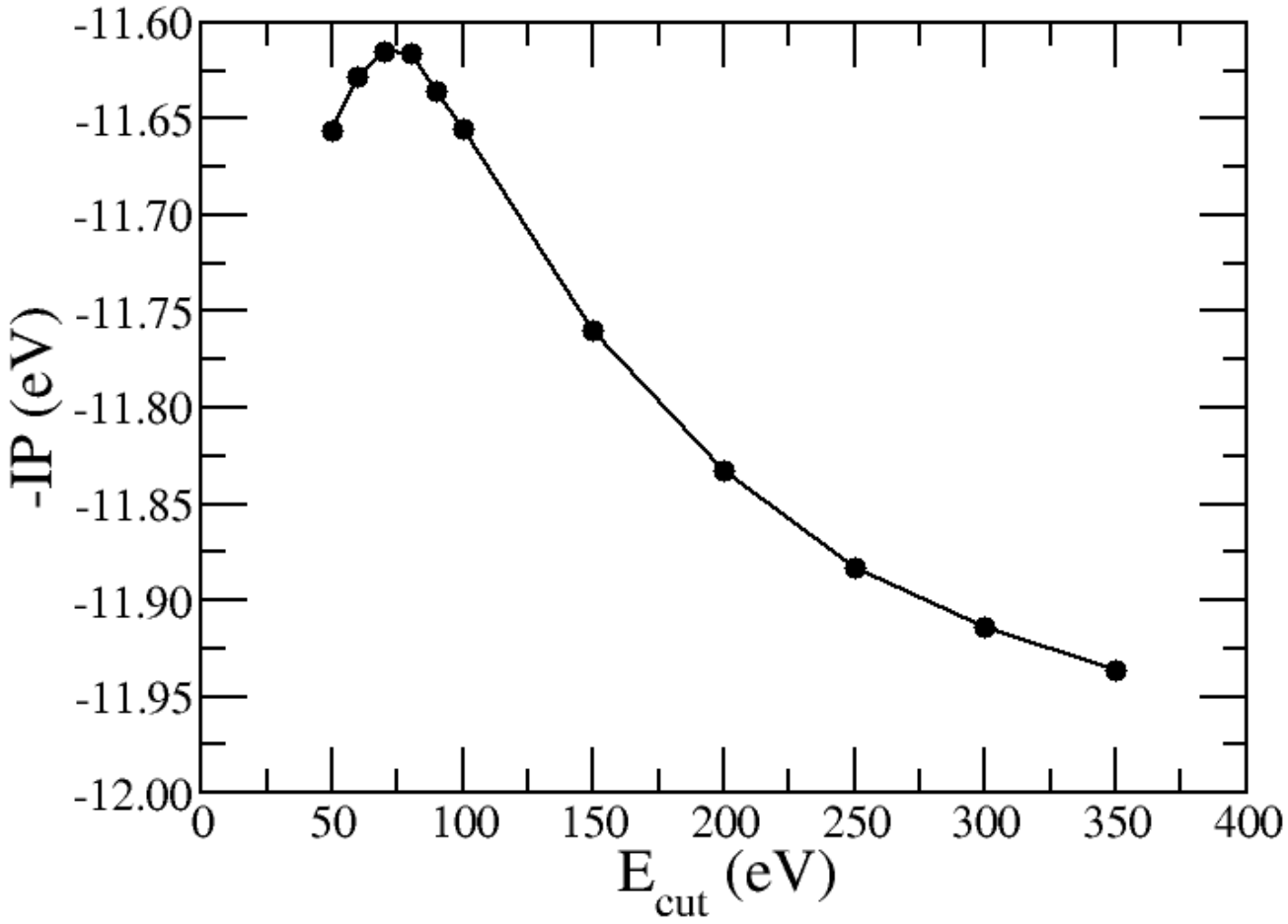
2D materials

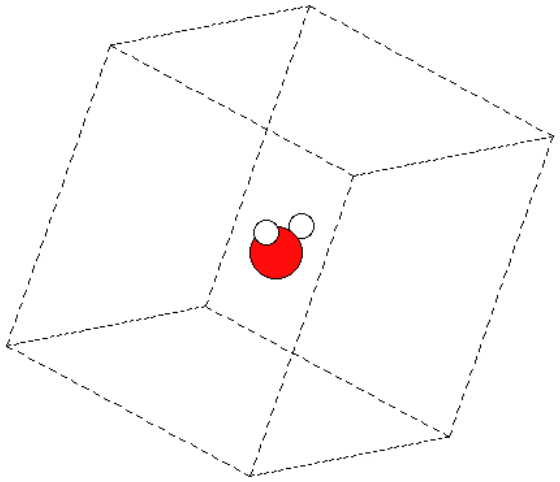
- Convergence with respect cell size and Coulomb truncation



molecules

Ionization Potential of water molecule

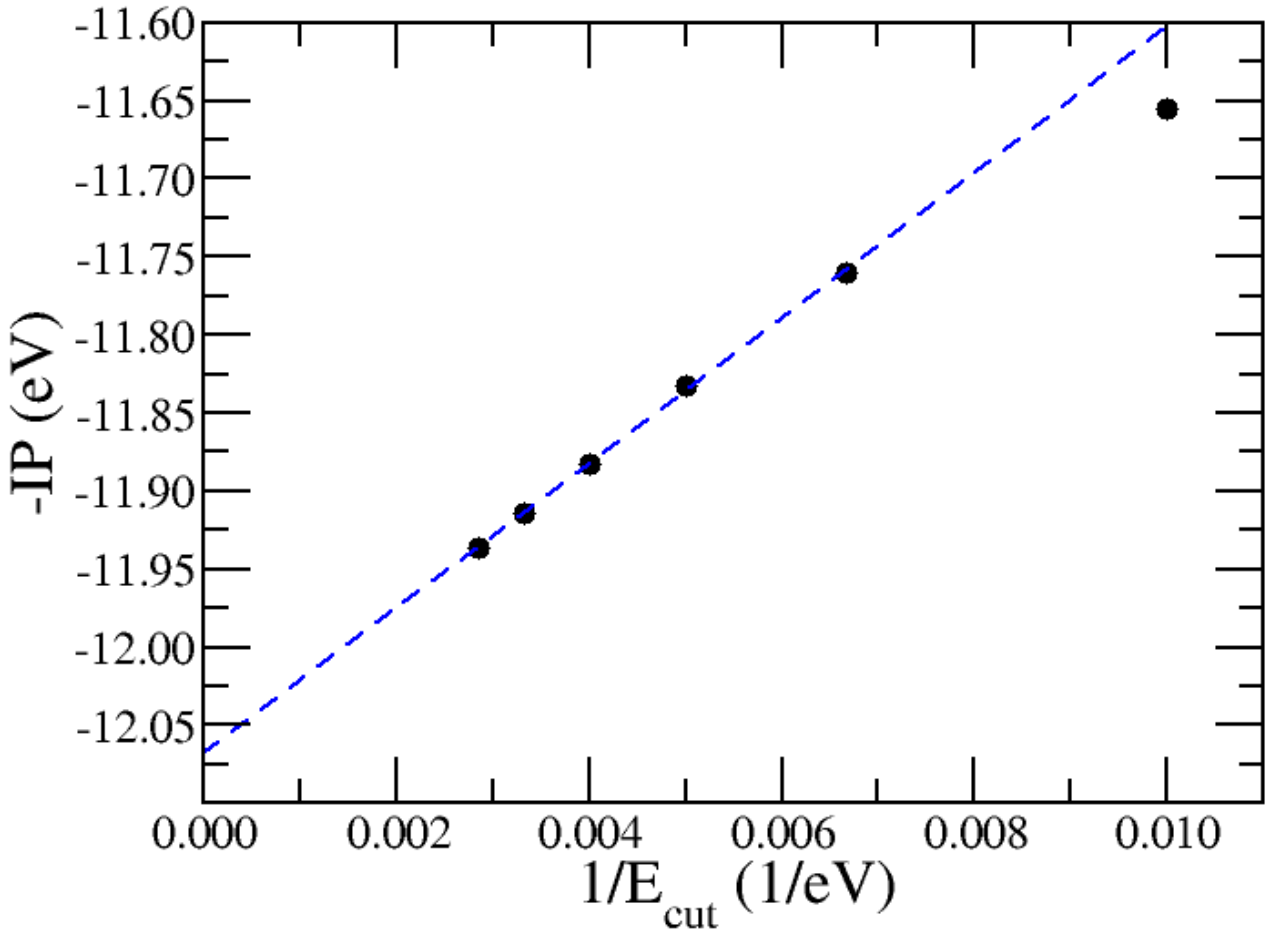




- 7 Å vacuum
- planewave basis
- PPA
- G_0W_0 (LDA)

molecules

extrapolation to infinite number of bands



Expt.	12.6
PBE	7.2
HF	13.9
GW	12.3
G_0W_0	12.1
PBE total	12.9

C. Rostgaard et al., PRB **81**, 085103 *(2010)*

getting started

```
import numpy as np
from gpaw.response.gw import GW

gw = GW(
        file='MoS2_groundstate.gpw',
        nbands=200,
        bands=np.array([11,12,13,14,15,16]),
        kpoints=np.array([1012,1058,1104,1150,1196,1242,1288,1334,1380,1426,1472,1518,1564,1610,1656, \
                          1702,1613,1524,1435,1346,1257,1168, \
                          1034,1033,1032,1031,1030,1029,1028,1027,1026,1025,1024, \
                          1023,1022,1021,1020,1019,1018,1017,1016,1015,1014,1013,1012]),
        w=np.array([100., 400., 0.05]),
        ecut=50.,
        eta=0.2,
        ppa=True,
        E0=None,
        hilbert_trans=False,
        wpar=1,
        vcut='2D',
        txt='GW_ppa.out'
       )

gw.get_exact_exchange()

gw.get_QP_spectrum()
```

Summary & Outlook

features:

- fully parallelized over k-points, bands and frequencies
- supports grid and planewave mode
- frequency integration, plasmon pole approximation, static COHSEX
- spin polarized
- data post-processing (e.g. BSE)

to do:

- full LCAO support
- QP lifetimes
- self-consistent GW
- GPU

thank you:

Jun Yan & Jens Jørgen Mortenson

The Plasmon Pole Approximation

$$\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \sum_s \left\{ \frac{R^*_{s\mathbf{G}\mathbf{G}'}(\mathbf{q})}{\omega - \epsilon_s + i\eta} - \frac{R_{s\mathbf{G}\mathbf{G}'}(\mathbf{q})}{\omega + \epsilon_s - i\eta} \right\}$$

$$\approx \frac{R_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{\omega - \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) + i\eta} - \frac{R_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{\omega + \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) - i\eta}$$

$$\mathrm{Im}\left\{\varepsilon^{-1}\right\} = -\pi R\left(\delta(\omega - \tilde{\omega}) + \delta(\omega + \tilde{\omega})\right)$$

$$\mathrm{Re}\left\{\varepsilon^{-1}\right\} = R\left(\frac{1}{\omega - \tilde{\omega}} - \frac{1}{\omega + \tilde{\omega}}\right)$$

The Plasmon Pole Approximation