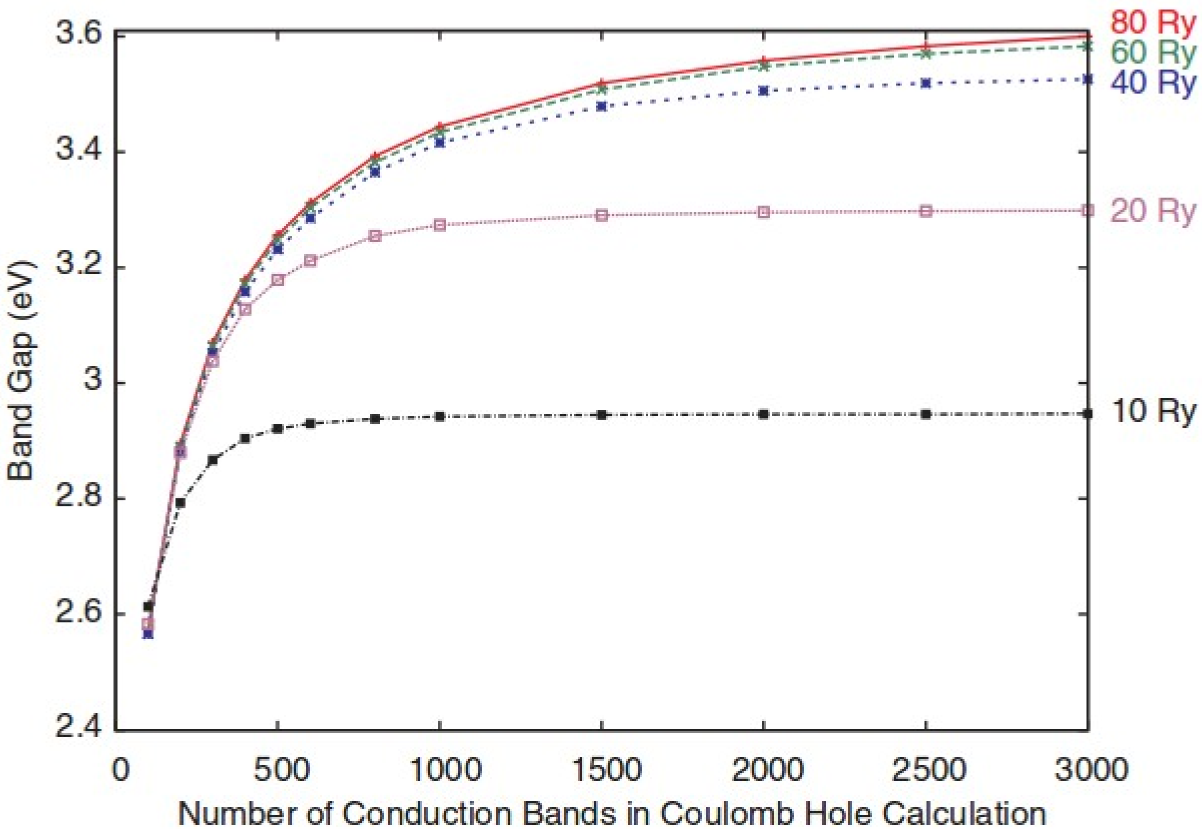
Convergence using BerkeleyGW



Derek Vigil-Fowler

11/22/13
BerkeleyGW Workshop 2013

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- People don't want to waste time/resources doing proper convergence tests
- Many calculations are under-converged
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- Unconverged calculations can cloud understanding

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$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0) = \sum_{n}^{\mathrm{occ}} \sum_{n'}^{\mathrm{emp}} \sum_{\mathbf{k}} M^*_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}') \frac{1}{E_{n\mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}}$$

$$\langle n\mathbf{k}| \Sigma_{\mathrm{CH}}(E) |n'\mathbf{k}\rangle = \frac{1}{2} \sum_{n''} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G}) M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}') \times \frac{\Omega^2_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(1 - i\tan\phi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}))}{\tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(E - E_{n''\mathbf{k}-\mathbf{q}} - \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}))}\, v(\mathbf{q}+\mathbf{G}')$$

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There are 5 convergence parameters

- Screened cutoff
- Empty bands (dielectric matrix)
- Bands in CH summation (sigma)
- q-grid
- Wavefunction cutoff (matrix elements)

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- Convergence with screened cutoff and bands in sigma/epsilon inter-dependent

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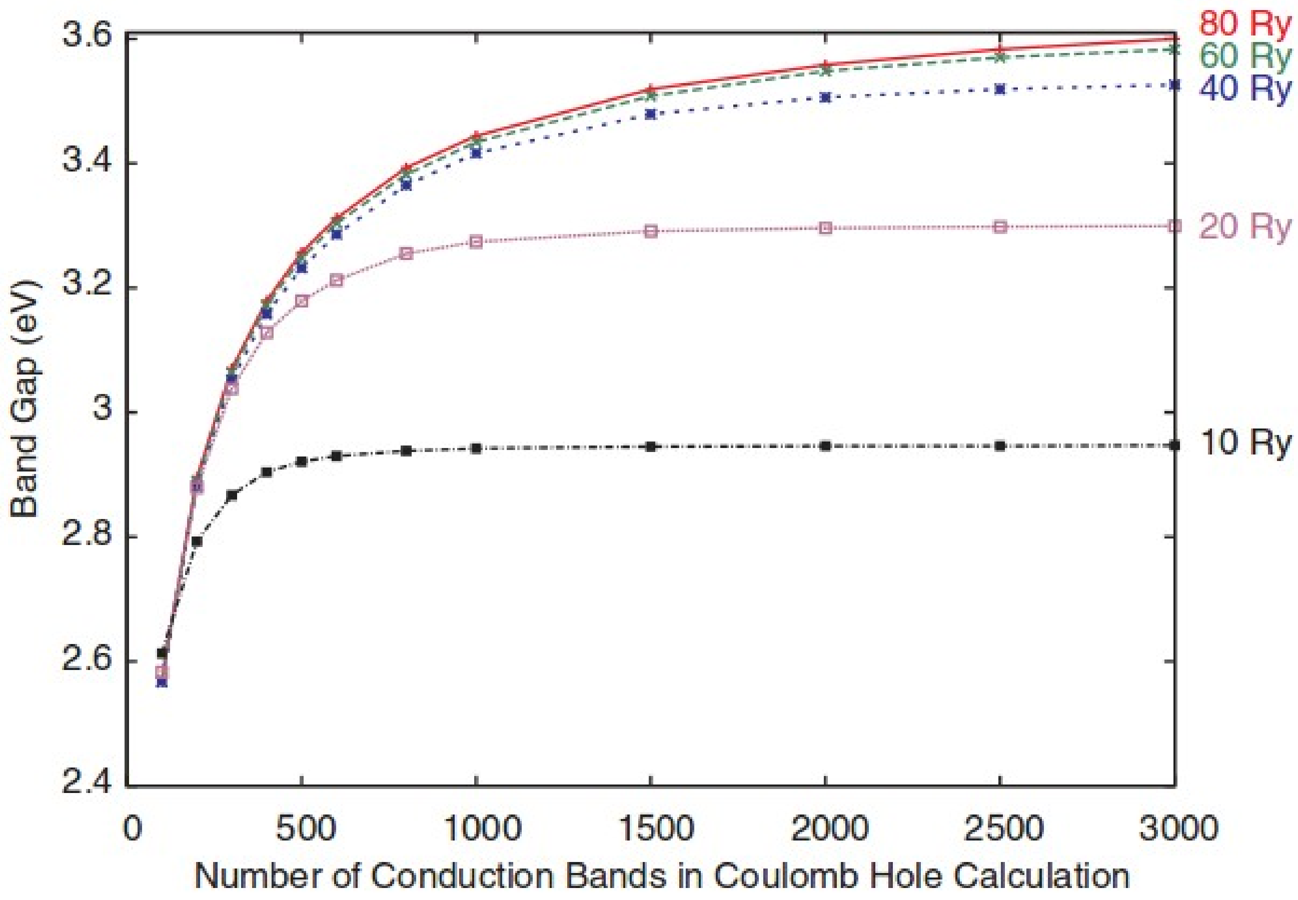

B.-C. Shih, et. al., Phys. Rev. Lett. **105**, 146401 (2010)

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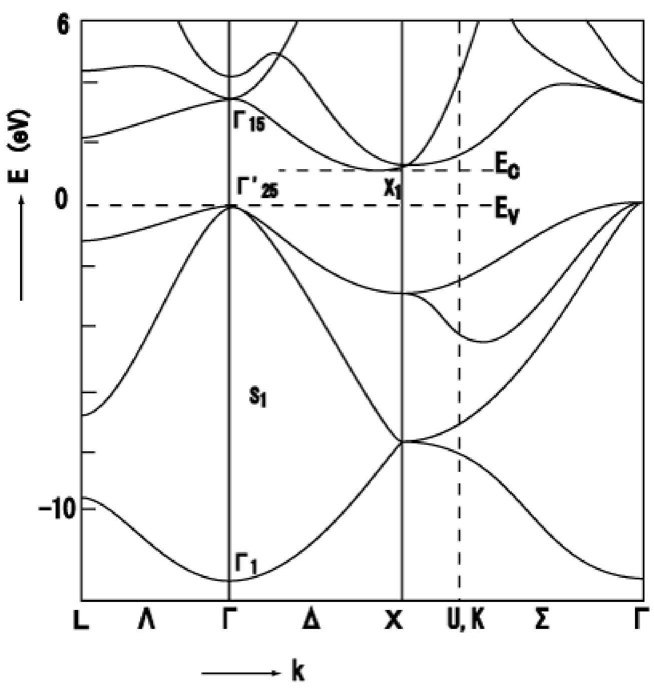

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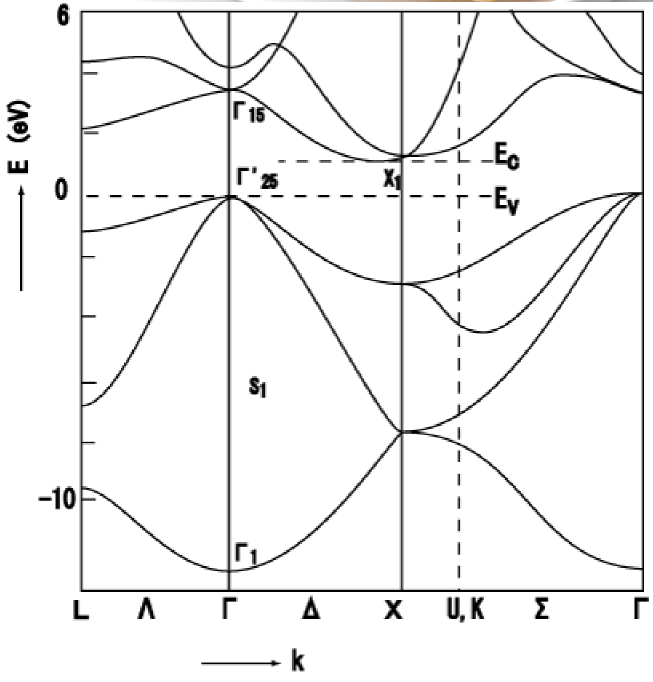

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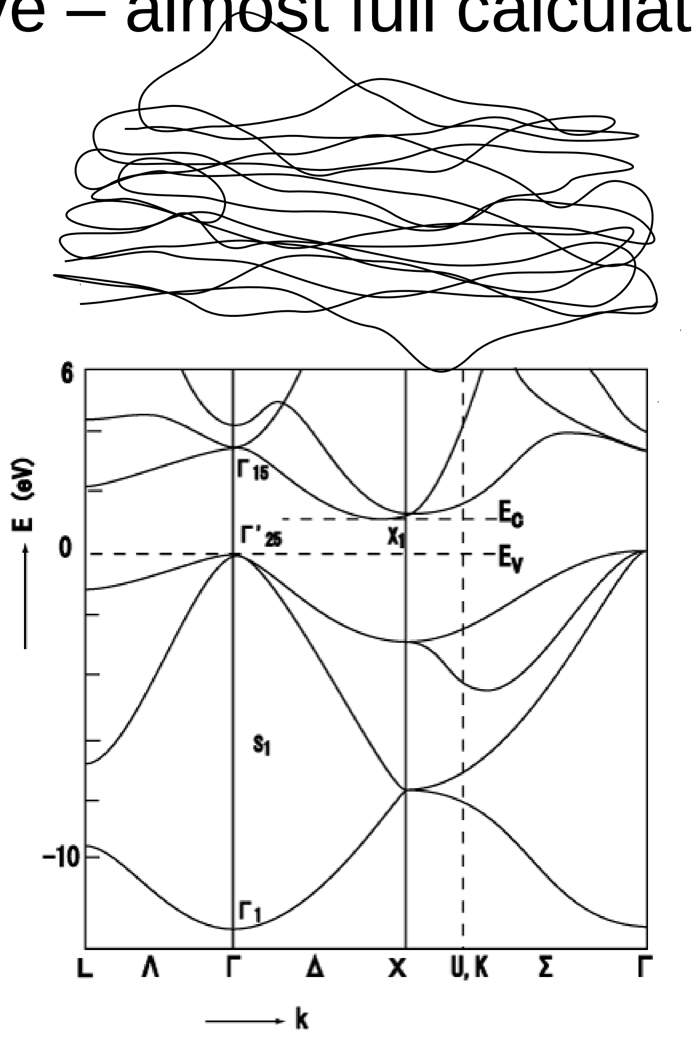
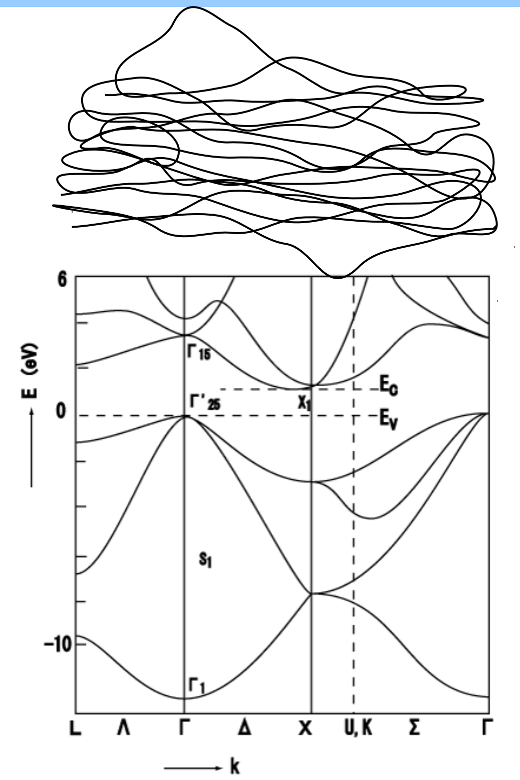


Weak kpoint dependence of conduction bands allows use of small q-grid when doing convergence wrt bands,cutoff

- 2x2x2 grid is usually sufficient
  - Allows you to check multiple gaps
  - Different gaps converge with different speed



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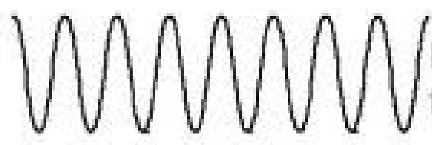
$\epsilon^{-1}($  $) = 1$

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B.D. Malone, M.L. Cohen, J. Phys.: Condens. Matter **25** 105503 (2013)

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- Infinite = very large number
  - Chosen from experience/physical considerations
  - Best to be conservative

- Error = deviation from value calculated with largest value for the parameter under consideration
  - In gaps because converge faster and physically relevant

- Step 2 cheap after step 1 because can set "screened cutoff" in sigma.inp

- Use close to final wavefunction cutoff

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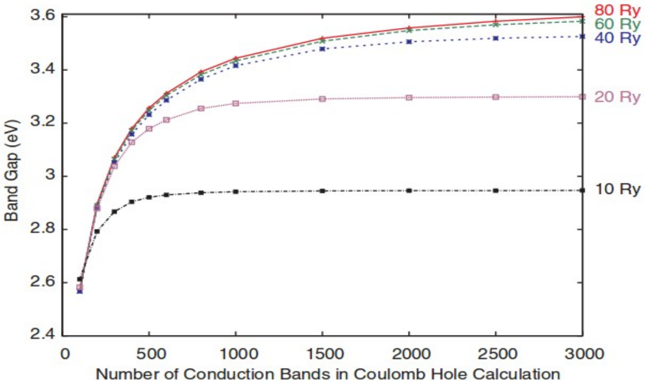

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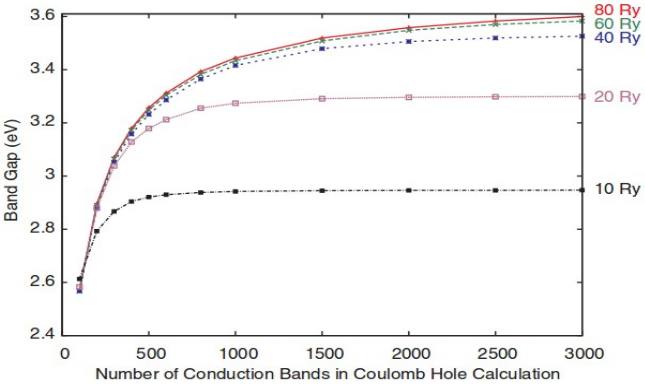

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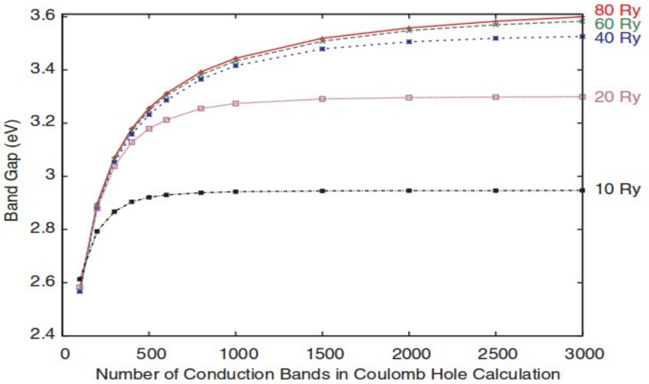

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Since wavefunction and q-grid convergence are independent, do separately later

- After pick desired number of empty states in epsilon, screened cutoff, and number of states in CH summation then use those values to do wavefunction cutoff and k-point convergence tests
  - Should used converged values because gaps change with better convergence, and error in gap will scale with gap

- Pick parameters based on desired total error
  - Rule of thumb : 50% of error from kpoints, wavefunction cutoff

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- Generally don't need screened cutoffs larger than 100 ryd because screening is not present at those short wavelengths/high energies

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- Utility gsphere.py determines number of G-vectors corresponding to screened cutoff

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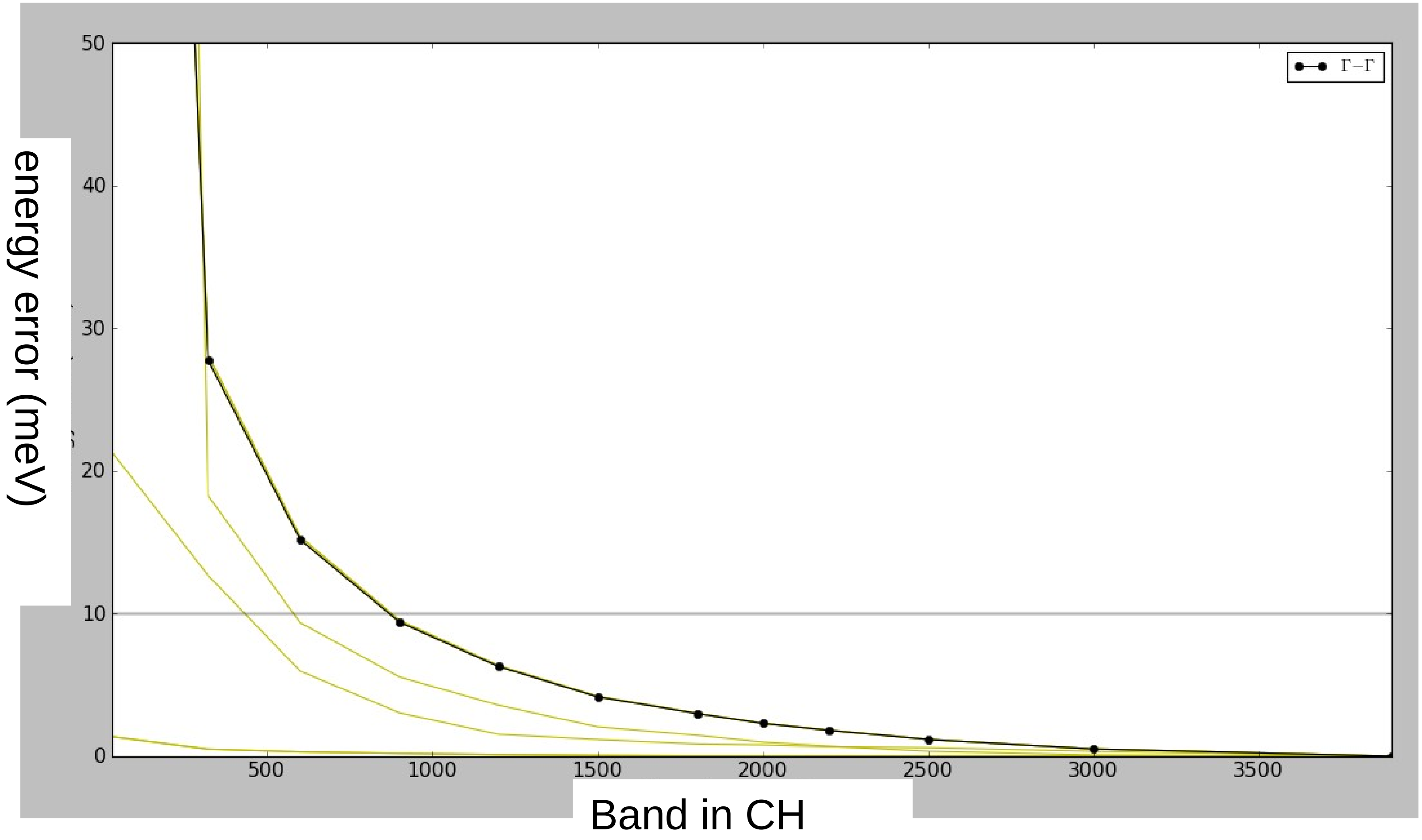
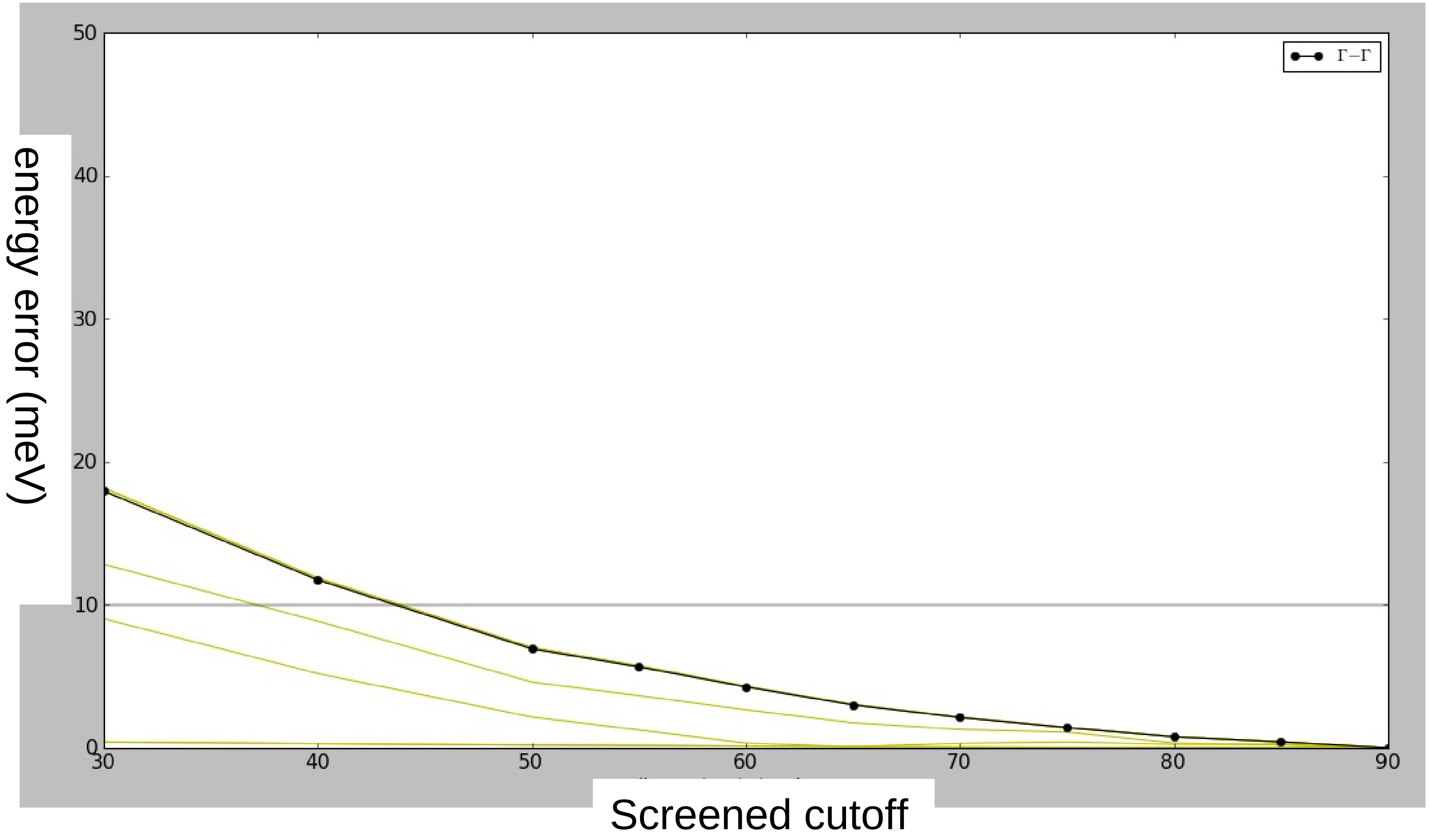
- Wanted 20 meV error total

- Wavefunction cutoff = 800 ryd, qgrid = 2x2x2

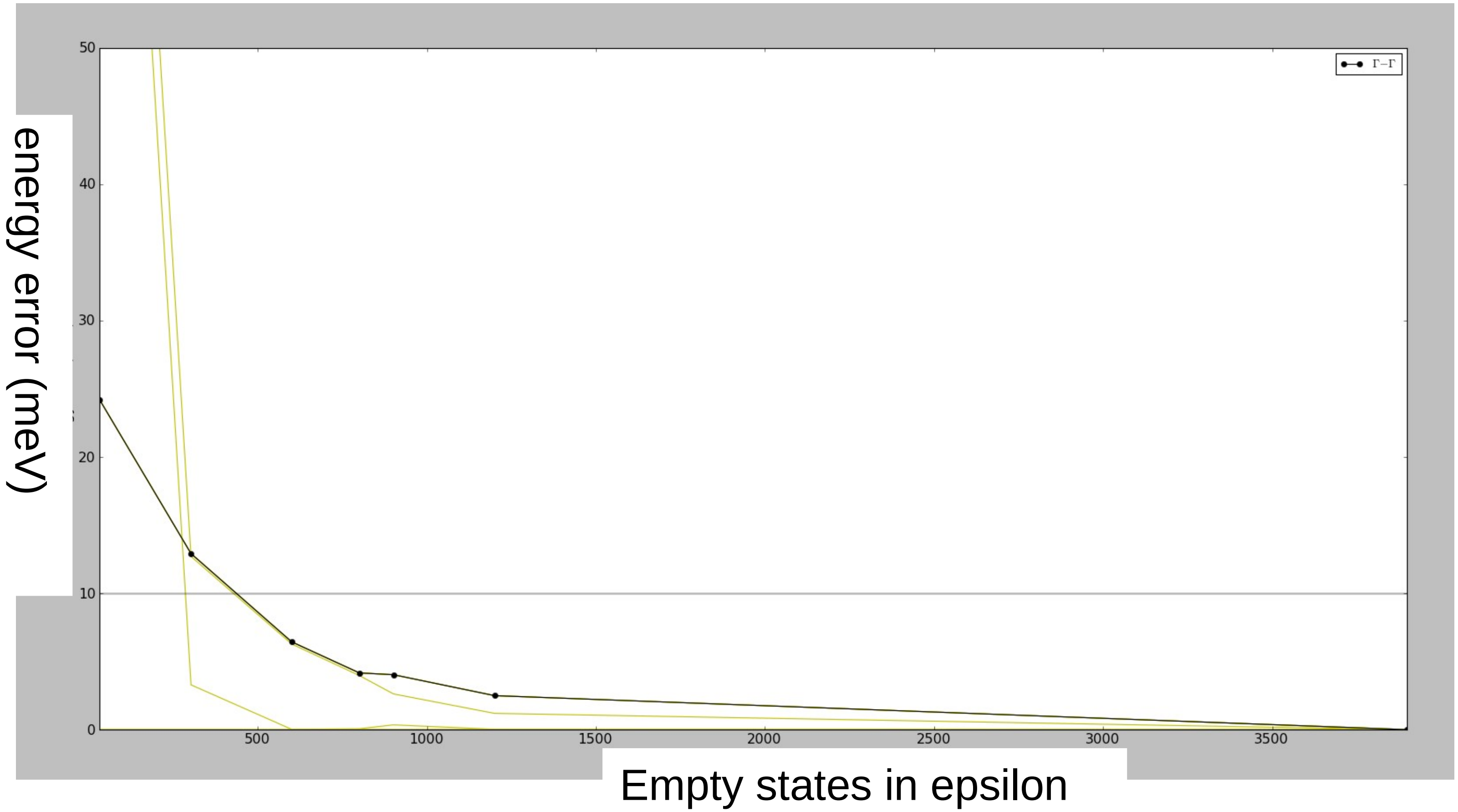
Bands in CH summation



Screened cutoff



Empty bands in dielectric matrix



Chose 1500 bands in epsilon, sigma and 60 ryd screened cutoff for 10 meV error

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- Wavefunction cutoff = 700 ry
- qgrid = 8x8x8
  - Total of 10 meV error from these two sources
    - Grand total of 20 meV error

Systematic, physically motivated scheme to get well-converged GW calculations

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  - Wavefunction cutoff from hartree-fock
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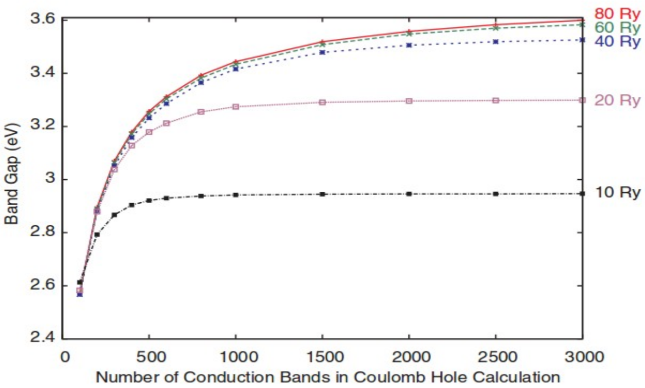

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- More examples of why important later