BerkeleyGW: A Massively Parallel Excited State Code
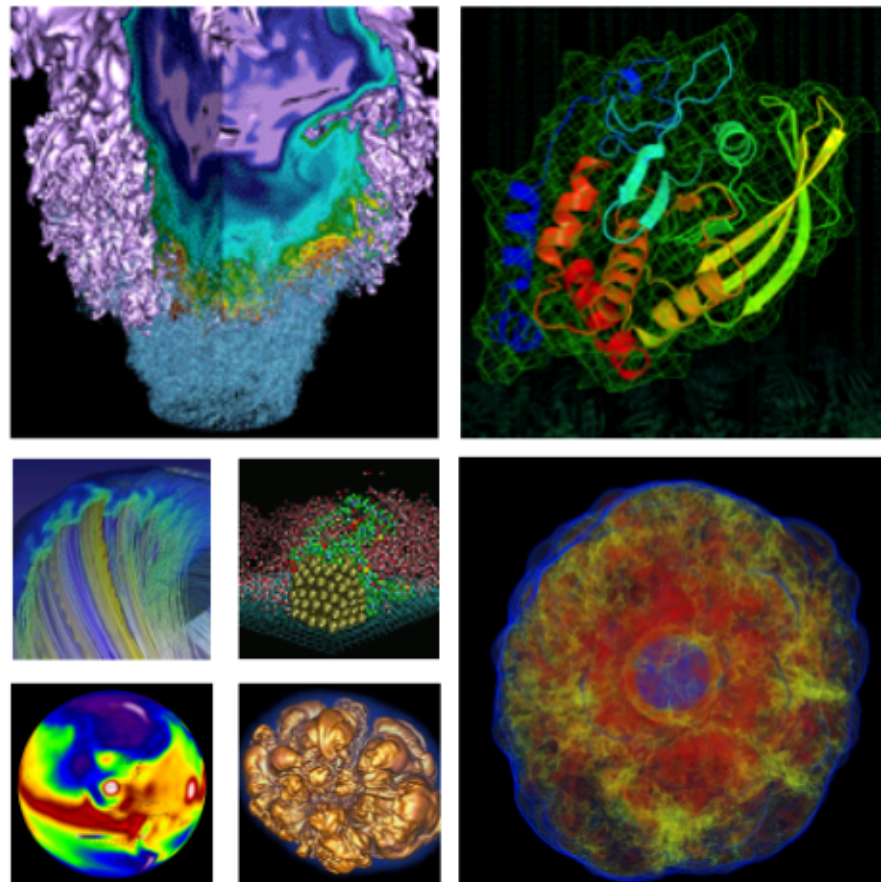

NeRSC

Jack Deslippe

11/22/2013

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

$$\left[E_{n\mathbf{k}} - H_0(\mathbf{r}) - V_H(\mathbf{r}) \right] \psi_{n\mathbf{k}}(\mathbf{r}) - \int \Sigma(\mathbf{r}, \mathbf{r}', E_{n,\mathbf{k}}) \psi_{n\mathbf{k}}(\mathbf{r}') d\mathbf{r}' = 0$$

The Good:

Quantitatively accurate for quasiparticle properties in a wide variety of systems.

Accurately describes dielectric screening important in excited state properties.

The Bad:

Prohibitively slow for large systems. Usually thought to cost orders of magnitude more time that DFT.

Memory intensive and scales badly. Exhausted by storage of the dielectric matrix and wavefunctions. Limited ~50 atoms.

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Materials:

InSb, InAs
Ge
GaSb
Si
InP
GaAs
CdS
AlSb, AlAs
CdSe, CdTe
BP
SiC
C$_{60}$
GaP
AlP
ZnTe, ZnSe
c-GaN, w-GaN
InS
w-BN, c-BN
diamond
w-AlN
LiCl
Fluorite
LiF
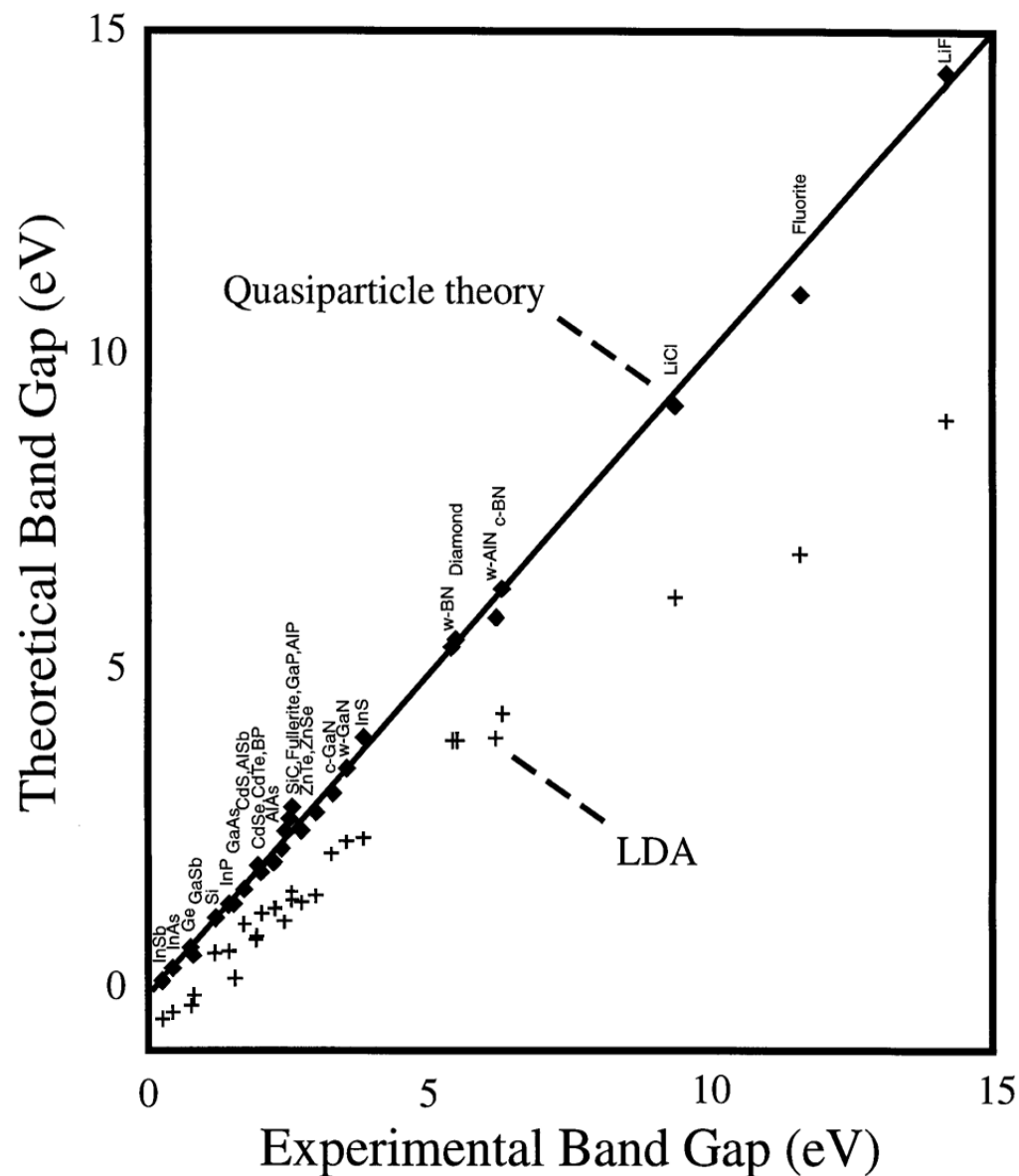
Many-body effects extremely important in Complex Materials.

Dielectric-screened interaction important for quasiparticle properties and electron-hole interaction.

Example – SWCNT: GW-BSE predicts exciton binding energies as large as 1 eV in semiconducting tubes. 100 meV in metallic tubes*
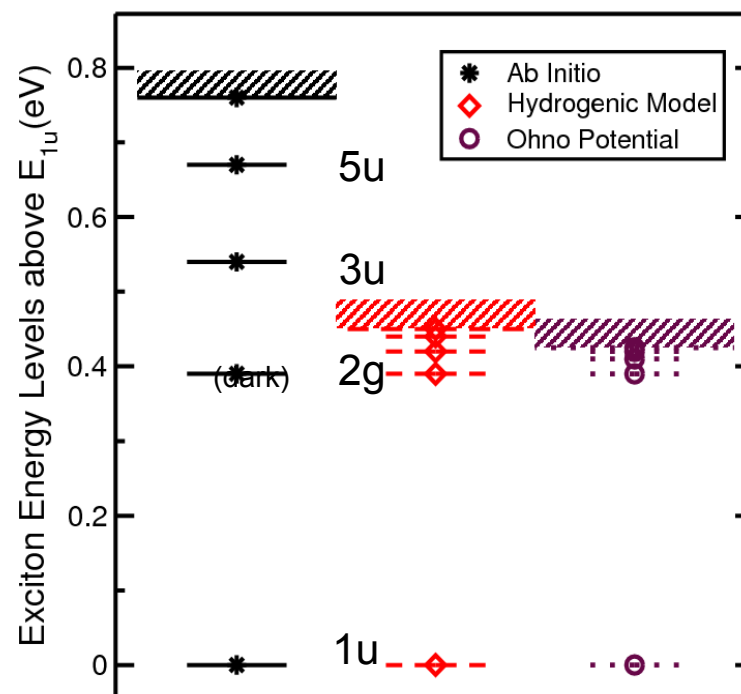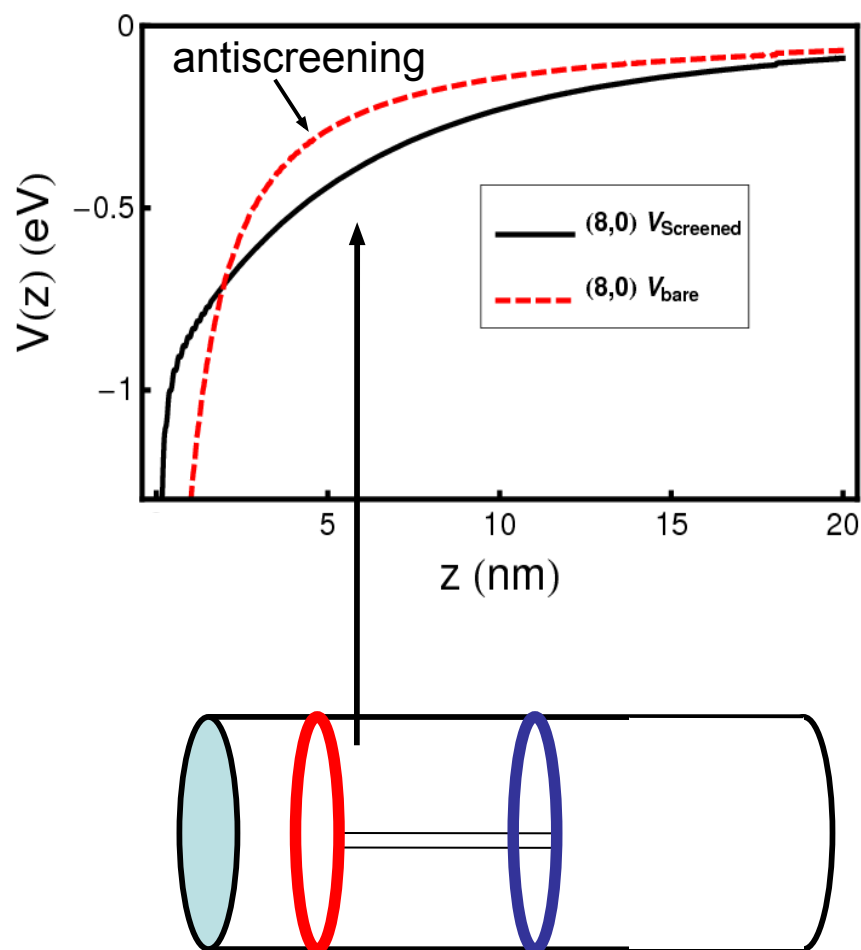
Each interband transition gives rise to exciton complex 1u, 2g, 3u ...

*C.D. Spataru, S. Ismail-Beigi, L.X. Benedict, S.G. Louie. PRL 077402 (2004)

*J. Deslippe, C.D. Spataru, D. Prendergast, S.G Louie. Nano Letters. 7 1626 (2007)

(8,0)

—— with e-h interaction
- - - without e-h interaction

Photon energy (eV)
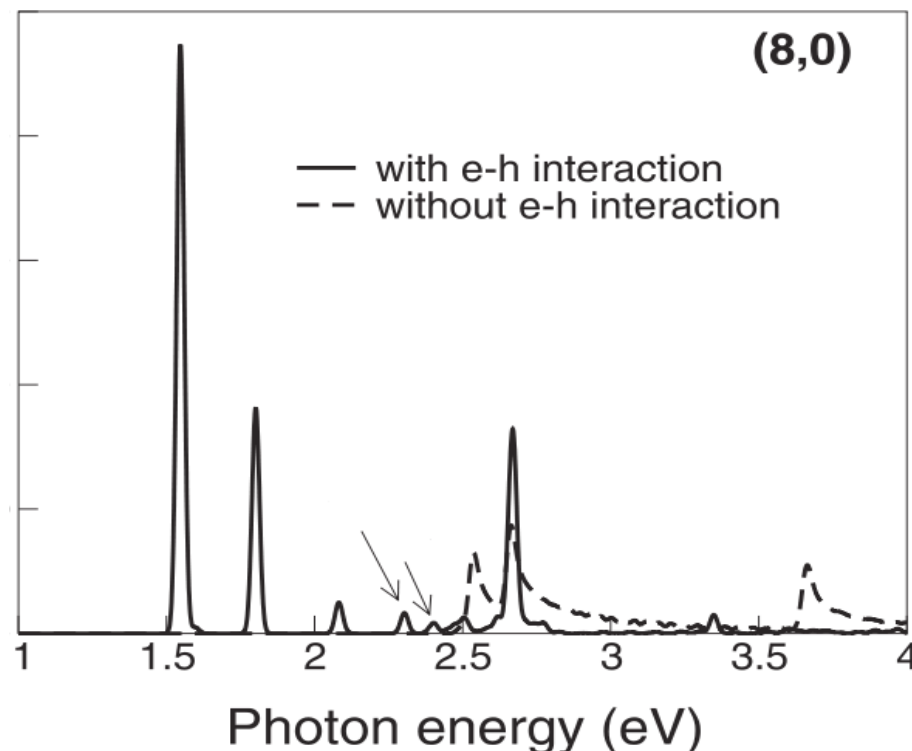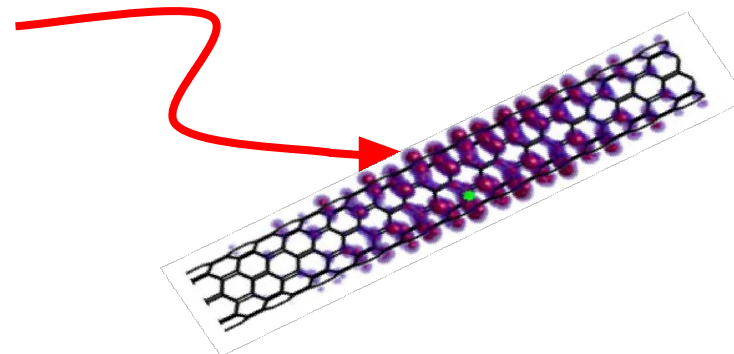
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*J. Deslippe, M. Dipoppa, D. Prendergast, M. Moutinho, R. Capaz, S.G. Louie Nano Letters. (2009) - nl802957t

-Screened electron-hole interaction enhanced for separations greater than tube diameter.

-Increases binding energies for 2g, 3u, … relative to 1u

-Confirmed by experiment – **J. Lefebvre P. Finnie. Nano Letters 8 1890 (2008).**

- Supports a large set of Mean-Field codes: PARATEC, Quantum ESPRESSO, PARSEC, SIESTA (Coming Soon Abinit)

- Supports 3D, 2D, 1D and Molecular Systems. Coulomb Truncation

- Support for Semiconductor, Metallic and Semi-Metallic Systems

- Efficient Algorithms and Use of Libraries. (BLAS, FFTW, LAPACK, SCALAPACK, FFTW) (OpenMP, FFTW3, HDF5 in BGW 1.1)

- Massively Parallel. Scales to 100,000 CPUs, distributed Memory.

BerkeleyGW Components and Algorithms

DFT Kohn-Sham (SCF and NSCF)
$\{\varphi^{DFT}_{nk}(\mathbf{r}), E^{DFT}_{nk}\}$

Compute Dielectric Function
$\{\ \epsilon_{qGG'}\}$

GW: Quasiparticle Properties
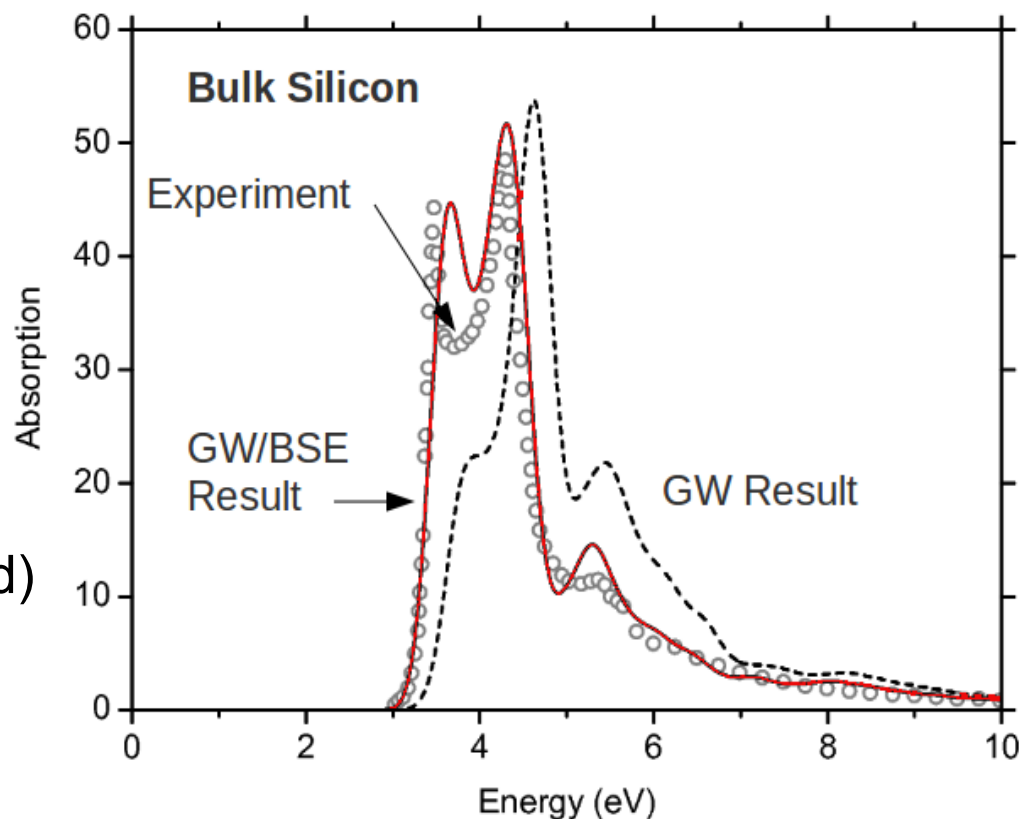$\{\varphi^{QP}_{nk}(\mathbf{r}), E^{QP}_{nk}\}$

BSE: Construct Kernel (coarse grid)
K(k,c,v,k',c',v')

Interpolate Kernel to Fine Grid /
Diagonalize BSE Hamiltonian
$\{A^{s}_{cvk}, E^{s}_{cvk}\}$

Bulk Silicon
Experiment
GW/BSE Result
GW Result

Expt. G.E. Jellison, M.F. Chisholm, S.M. Gorbatkin, Appl. Phys. Lett. 62, 3348 (1993).

DFT Kohn-Sham (SCF and NSCF)
$\{\varphi^{DFT}_{nk}(\mathbf{r}), E^{DFT}_{nk}\}$

Compute Dielectric Function
$\{\ \epsilon_{qGG'}\}$ **epsilon.flavor.x**

GW: Quasiparticle Properties
$\{\varphi^{QP}_{nk}(\mathbf{r}), E^{QP}_{nk}\}$ **sigma.flavor.x**
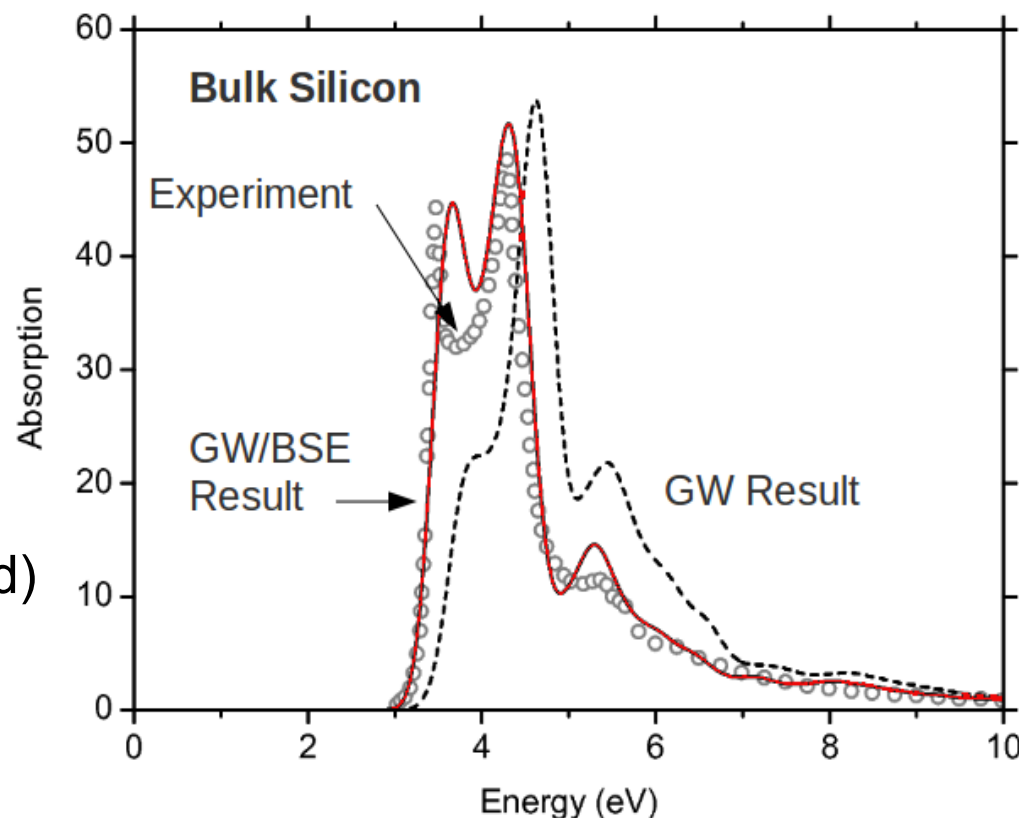
BSE: Construct Kernel (coarse grid)
K(k,c,v,k',c',v')
kernel.flavor.x

Interpolate Kernel to Fine Grid /
Diagonalize BSE Hamiltonian
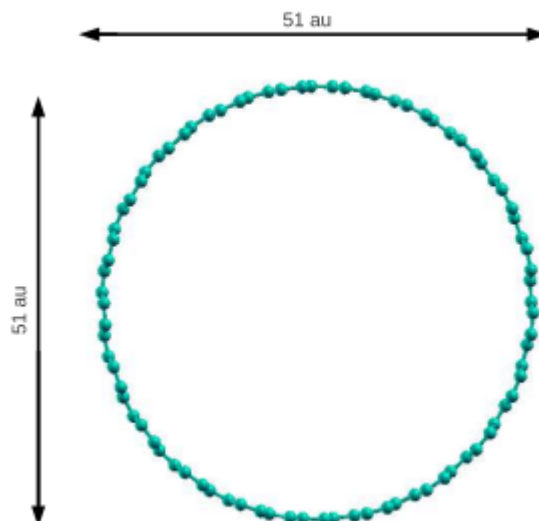$\{A^{s}_{cvk}, E^{s}_{cvk}\}$
absorption.flavor.x

Bulk Silicon

Experiment

GW/BSE Result

GW Result

Absorption — Energy (eV)

Expt. G.E. Jellison, M.F. Chisholm, S.M. Gorbatkin, Appl. Phys. Lett. 62, 3348 (1993).
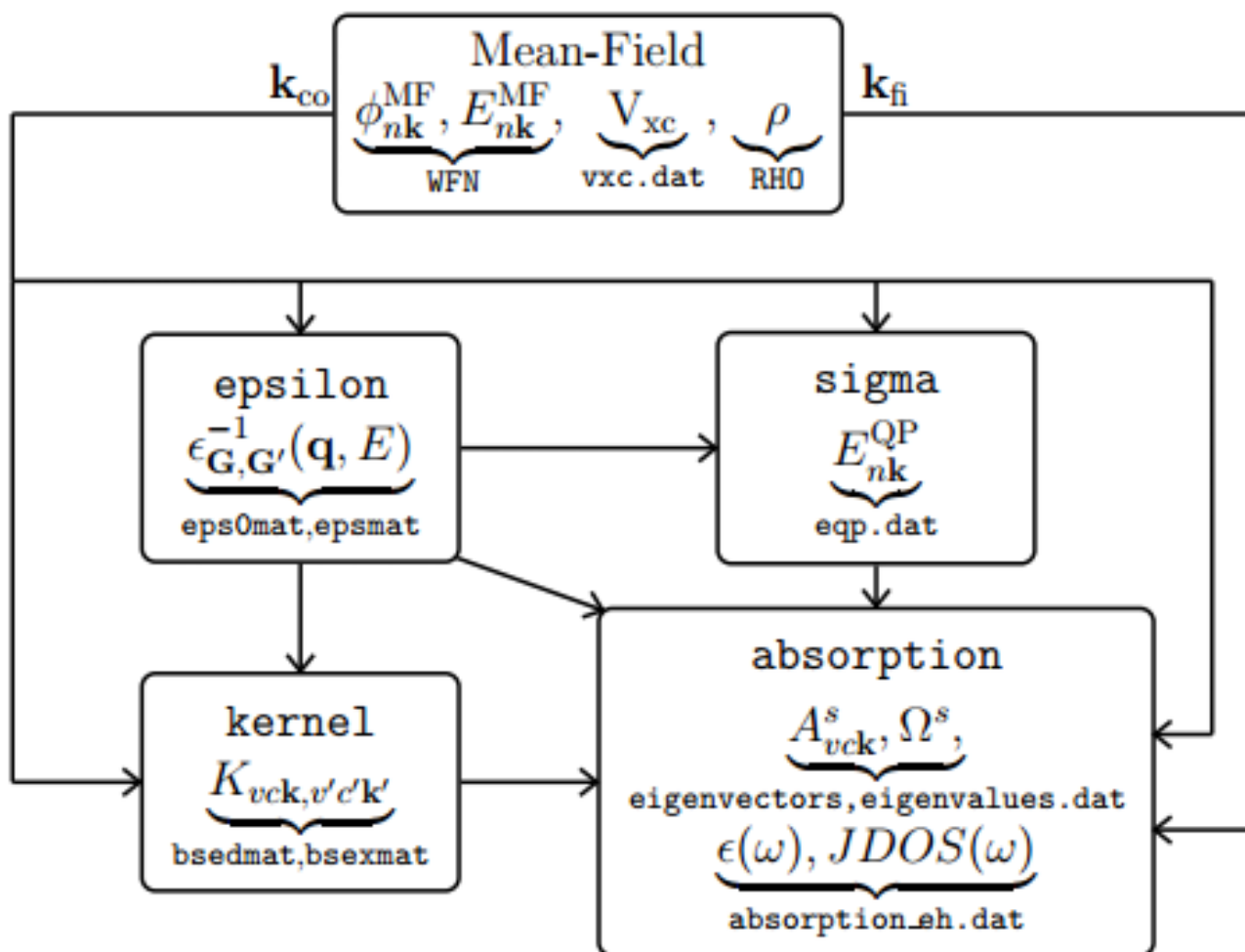
Step	# CPUs	CPU hours	Wall hours
DFT Coarse	64×32	19000	9.1
DFT Fine	64×256	29000	1.8
epsilon	1600×32	61000	1.2
sigma	960×16	46000	3.0
kernel	1024	600	0.6
absorption	256	500	2.0

GW Method

$$[E_{n\mathbf{k}} - H_0(\mathbf{r}) - V_H(\mathbf{r})]\,\psi_{n\mathbf{k}}(\mathbf{r}) - \int \Sigma(\mathbf{r}, \mathbf{r}', E_{n,\mathbf{k}})\psi_{n\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = 0$$

$$\Sigma = iGW \qquad W(\mathbf{q}, \mathbf{G}, \mathbf{G}') = \varepsilon^{-1}(\mathbf{q}, \mathbf{G}, \mathbf{G}') \cdot V(\mathbf{q} + \mathbf{G}')$$

$$\varepsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0) = \delta_{\mathbf{G}\mathbf{G}'} - v(\mathbf{q} + \mathbf{G}')\,\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0)$$

L. Hedin. Phys. Rev. 139, A796 (1965); L. Hedin, S. Lundquist. Solid State Physics 23, 1 (1969); M. S. Hybertsen, S. G. Louie, Phys. Rev. Lett. 55 (1985) 1418.

epsilon.cplx.x

1. Compute via *nxn'* FFTs (N^3 Step. Big Prefactor.):

$$M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \langle n\mathbf{k}{+}\mathbf{q}| \, e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \, |n'\mathbf{k}\rangle$$

$$M_{nn'}(\mathbf{k}, \mathbf{q}, \{\mathbf{G}\}) = FFT^{-1}\left(\phi_{n,\mathbf{k}+\mathbf{q}}(\mathbf{r}) * \phi^*_{n',\mathbf{k}}(\mathbf{r})\right)$$

2. Compute sum via large ZGEMM (N^4 Step. Small Prefactor.):

$$\chi_{\mathbf{GG'}}(\mathbf{q};0) = \mathbf{M}(\mathbf{G}, \mathbf{q}, (n, n', \mathbf{k})) \cdot \mathbf{M}^T(\mathbf{G'}, \mathbf{q}(n, n', \mathbf{k}))$$

Where, $\mathbf{M}(\mathbf{G}, \mathbf{q}, (n, n', \mathbf{k})) = M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) \cdot \dfrac{1}{\sqrt{E_{n\mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}}}$

epsilon.cplx.x

3. Invert matrix via scalapack (N^3 Step):

$$\epsilon_{\mathbf{GG}'}(\mathbf{q};0) = \delta_{\mathbf{GG}'} - v(\mathbf{q}+\mathbf{G})\chi_{\mathbf{GG}'}(\mathbf{q};0)$$

$$W_{\mathbf{GG}'}(\mathbf{q};0) = \epsilon^{-1}_{\mathbf{GG}'}(\mathbf{q};0)v(\mathbf{q}+\mathbf{G}')$$

the W in GW...

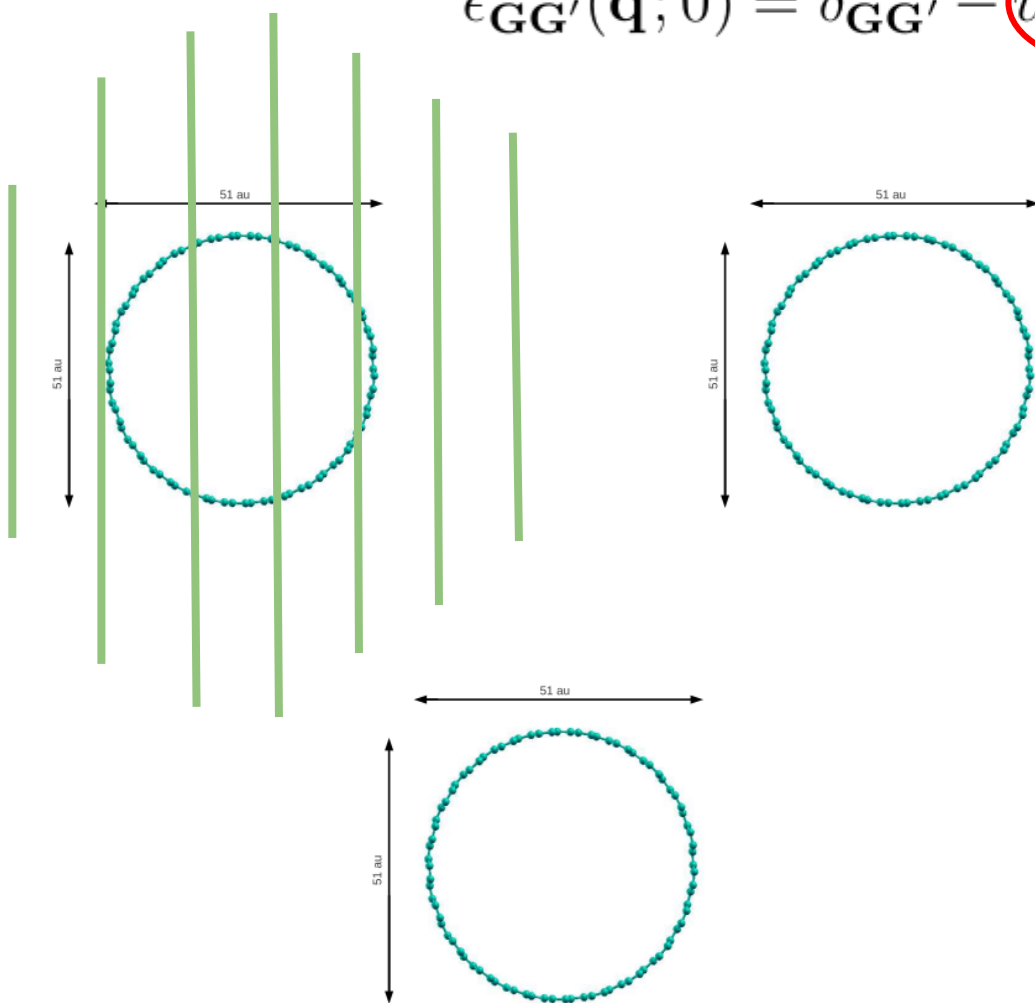$$\epsilon_{\mathbf{GG'}}(\mathbf{q};0) = \delta_{\mathbf{GG'}} - v(\mathbf{q}+\mathbf{G})\chi_{\mathbf{GG'}}(\mathbf{q};0)$$

$$v_{\mathrm{t}}(\mathbf{r}) = \frac{\Theta(f(\mathbf{r}))}{r}$$

Coulomb interaction replaced by truncated interaction in order to prevent interaction with peiodic neighbors. Code supports:

-Sphereical Truncation
-Box Truncation
-Wire Truncation
-Slab Truncation

$$\epsilon_{\mathbf{GG'}}(\mathbf{q};0) = \delta_{\mathbf{GG'}} - v(\mathbf{q+G})\chi_{\mathbf{GG'}}(\mathbf{q};0)$$

at G=0,q -> 0

3D Semiconductors:

$v \sim 1/q^2$
$\chi \sim q^2$
$\epsilon \sim$ constant

To compute values for q->0, we calculate the value at small non-zero q. Requires a wavefunctions on shifted grid.

3D Metals:

$v \sim 1/q^2$
$\chi \sim$ DOS(Ef)
$\epsilon \sim 1/q^2$

To compute values for q->0, we need a very fine k-grid in-order to resolve DOS

sigma.cplx.x

1. Compute matrix elements for desired bands.
   (Scales as N^2 x number of bands interested in)

$$M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \langle n\mathbf{k}+\mathbf{q}| \, e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \, |n'\mathbf{k}\rangle$$

n - bands at which we wish compute sigma
n' - occupied and unoccupied bands over which sum.

... And a few more similar loops.

sigma.cplx.x

2. Manual loop reductions to compute sum for Self-Energy. N^3 x number of bands of interest

$$\langle n\mathbf{k}| \Sigma_{\mathrm{SX}}(E) |n'\mathbf{k}\rangle = -\sum_{n''}^{\mathrm{occ}} \sum_{\mathbf{qGG'}} M^*_{n''n}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G'})$$

$$\times \left[\delta_{\mathbf{GG'}} + \frac{\Omega^2_{\mathbf{GG'}}(\mathbf{q})\left(1 - i\tan\phi_{\mathbf{GG'}}(\mathbf{q})\right)}{(E - E_{n''\mathbf{k}-\mathbf{q}})^2 - \tilde{\omega}^2_{\mathbf{GG'}}(\mathbf{q})} \right] v(\mathbf{q}+\mathbf{G'})$$

$$\langle n\mathbf{k}| \Sigma_{\mathrm{CH}}(E) |n'\mathbf{k}\rangle = \frac{1}{2}\sum_{n''} \sum_{\mathbf{qGG'}} M^*_{n''n}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G'})$$

$$\times \frac{\Omega^2_{\mathbf{GG'}}(\mathbf{q})\left(1 - i\tan\phi_{\mathbf{GG'}}(\mathbf{q})\right)}{\tilde{\omega}_{\mathbf{GG'}}(\mathbf{q})\left(E - E_{n''\mathbf{k}-\mathbf{q}} - \tilde{\omega}_{\mathbf{GG'}}(\mathbf{q})\right)} v(\mathbf{q}+\mathbf{G'})$$

Loops are shown for GPP.

$$\Sigma = \Sigma_{SX} + \Sigma_{CH}; \ \langle n\mathbf{k}| \Sigma_{CH}(E) |n'\mathbf{k}\rangle = \sum_{n'} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M_{n,n'}(\mathbf{k},\mathbf{q},\mathbf{G}) \cdot M^*_{n',n}(\mathbf{k},\mathbf{q},\mathbf{G}') \cdot ...$$

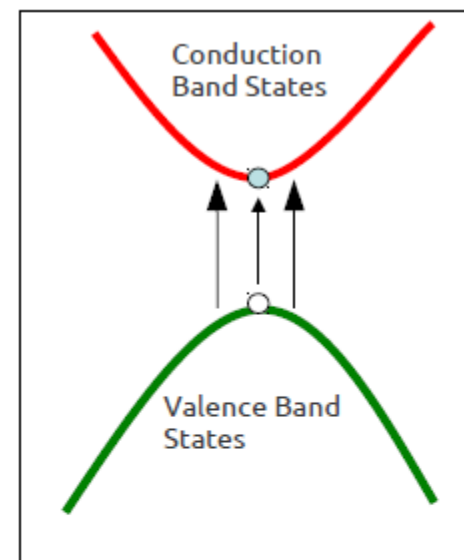Slowly converging with number of conduction bands.

Si

Energy levels converged at ~200 Bands
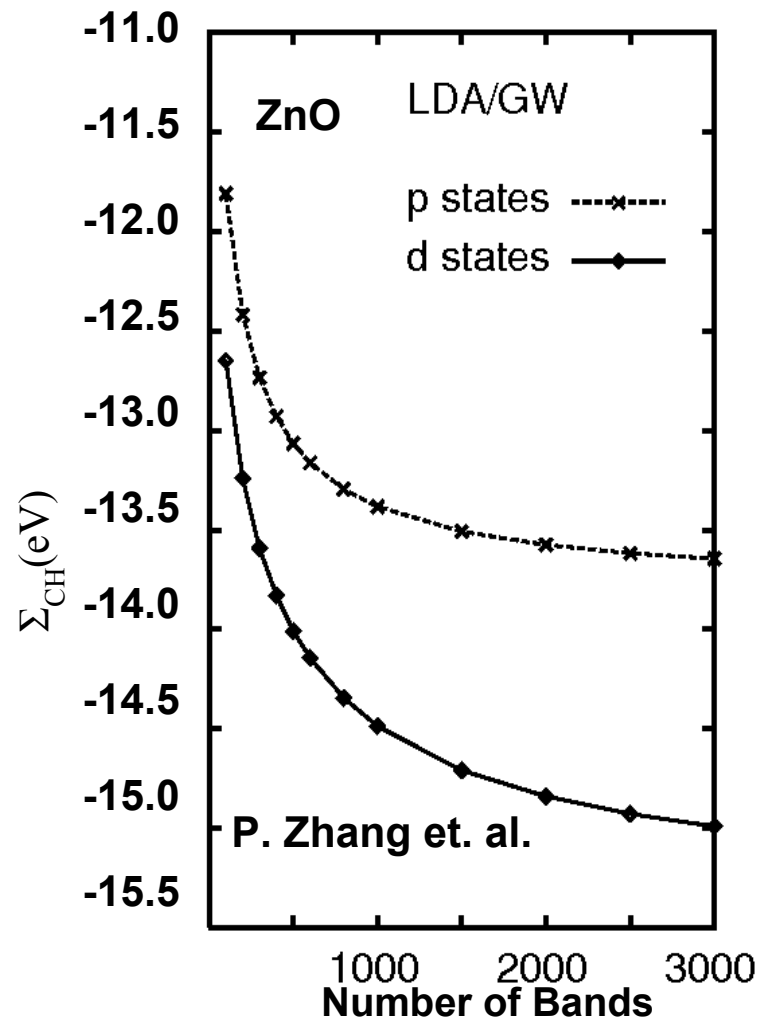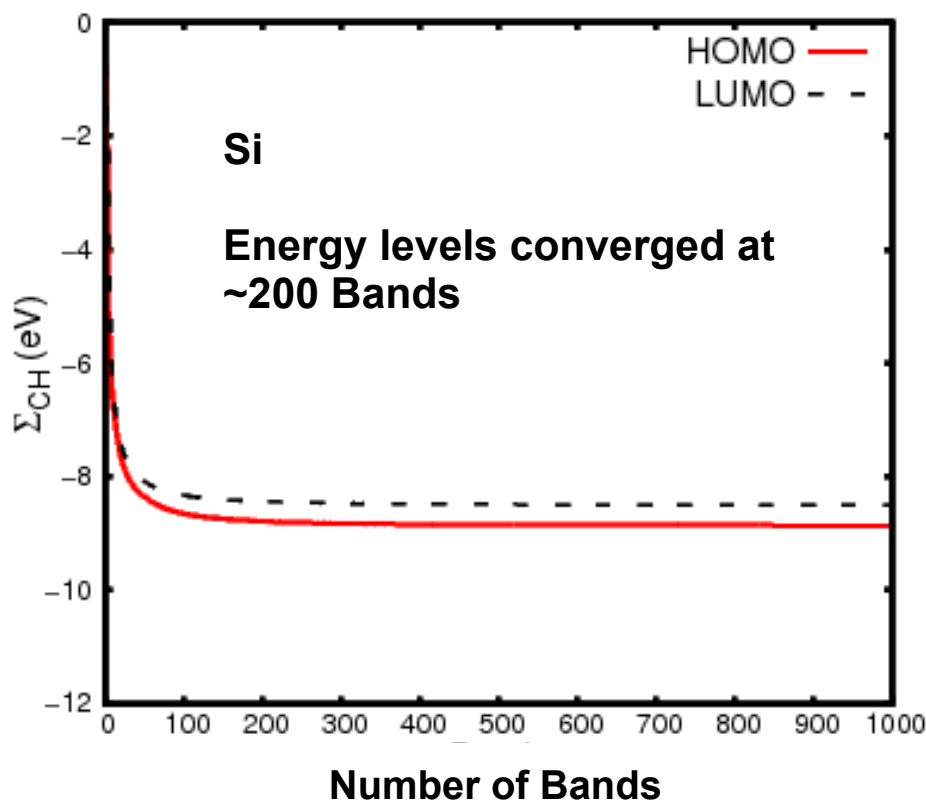
-The relative accuracy of Full-Frequency vs. Generalized Plasmon Pole (GPP) calculations is somewhat contentious.

$$\langle n\mathbf{k}| \Sigma_{\mathrm{CH}}(E) |n'\mathbf{k}\rangle = \frac{i}{2\pi} \sum_{n''} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}) M_{n''n'}(\mathbf{k}, -\mathbf{q}, -\mathbf{G}') \quad (20)$$
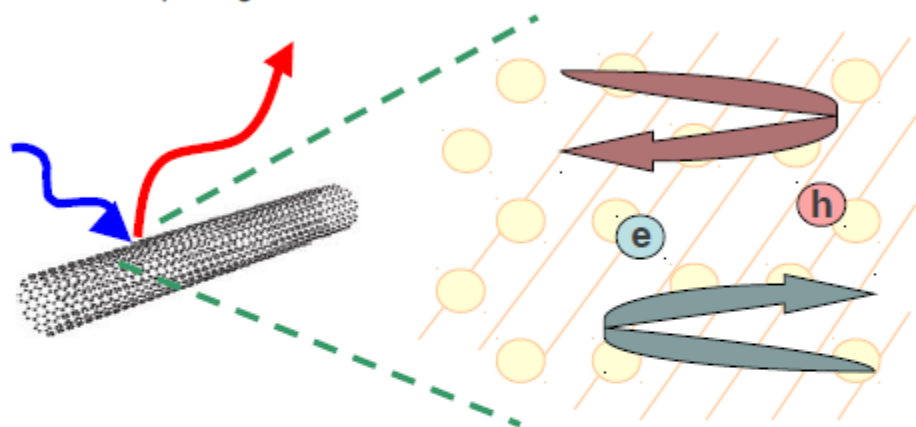
$$\times \int_0^\infty dE' \frac{[\epsilon^{\mathrm{r}}_{\mathbf{G}\mathbf{G}'}]^{-1}(\mathbf{q}; E') - [\epsilon^{\mathrm{a}}_{\mathbf{G}\mathbf{G}'}]^{-1}(\mathbf{q}; E')}{E - E_{n''\mathbf{k}-\mathbf{q}} - E' + i\delta} \; v(\mathbf{q}+\mathbf{G}')$$

GPP is significantly faster, the integral over frequencies can be performed analytically if assume the dielectric response is dominated by a single plasmon pole.

BerkeleyGW supports both. With full-frequency you can compute spectral functions, lifetimes and weights.
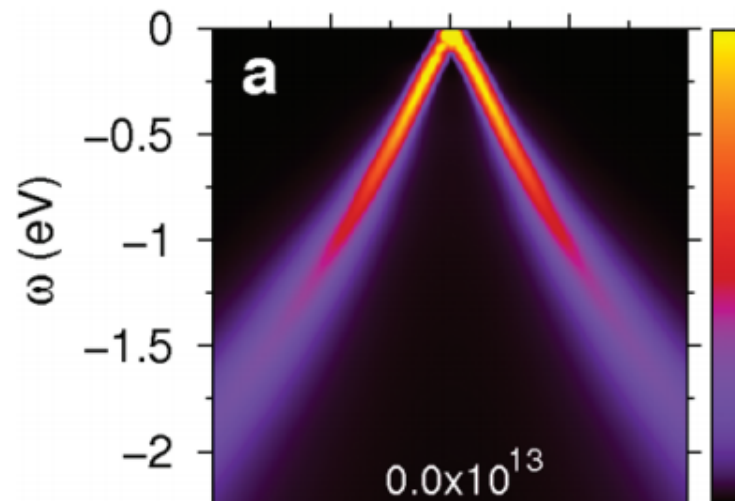
$$|N,S\rangle = \sum_v^{hole} \sum_c^{elec} A_{vc}^S a_v^+ b_c^+ |N,0\rangle + \ldots$$

$$\left(E_{ck}{}^{QP} - E_{vk}{}^{QP}\right) A^S{}_{vck} + \sum_{k'v'c'} \langle vck|K^{eh}|v'c'k'\rangle A^S{}_{v'c'k'} = \Omega^S A^S{}_{vck}$$

$$\varepsilon_2(\omega) = \frac{16\pi^2 e^2}{\omega^2} \sum_S |\langle N,0|e\cdot v|N,S\rangle|^2 \delta(\Omega_S - \hbar\omega)$$

Construct Kernel On Coarse Grid:

$$M_{nn'}(\mathbf{k}, \mathbf{q}, \{\mathbf{G}\}) = FFT^{-1}\left(\phi_{n,\mathbf{k}+\mathbf{q}}(\mathbf{r}) * \phi^*_{n',\mathbf{k}}(\mathbf{r})\right)$$

$$\langle vc\mathbf{k}|K^{\mathrm{d}}|v'c'\mathbf{k}'\rangle =$$

$$\sum_{\mathbf{GG}'} M_{cc'}(\mathbf{k}, \mathbf{q}, \mathbf{G})W_{\mathbf{GG}'}(\mathbf{q}; 0)M^*_{vv'}(\mathbf{k}, \mathbf{q}, \mathbf{G}')$$

Scaling: N^5

$$\langle vc\mathbf{k}|K^{\mathrm{x}}|v'c'\mathbf{k}'\rangle =$$

$$\sum_{\mathbf{GG}'} M_{cv}(\mathbf{k}, \mathbf{q}, \mathbf{G})v(\mathbf{q} + \mathbf{G})\delta_{GG'}M^*_{c'v'}(\mathbf{k}, \mathbf{q}, \mathbf{G}')$$

Excitonic effects Depend critically on k-point sampling. So, we interpolate to finer grid.

1. Compute overlaps between coarse and fine wavefunctions

$$C_{n,n'}^{\mathbf{k}_{co}} = \int d\mathbf{r}\, u_{n\mathbf{k}_{fi}}(\mathbf{r}) u_{n'\mathbf{k}_{co}}^{*}(\mathbf{r}).$$

2. Use overlaps to interpolate Kernel to Fine Grid

$$\langle vc\mathbf{k}_{fi}|K|v'c'\mathbf{k}_{fi}'\rangle =$$

$$\sum_{n_1,n_2,n_3,n_4} C_{c,n_1}^{\mathbf{k}_{co}} C_{v,n_2}^{*\mathbf{k}_{co}} C_{c',n_3}^{*\mathbf{k}_{co}'} C_{v',n_4}^{\mathbf{k}_{co}'} \langle n_2 n_1 \mathbf{k}_{co}|K|n_4 n_3 \mathbf{k}_{co}'$$

3. Use overlaps to interpolate QP energies without missing band crossings etc..

$$E_n^{QP}(\mathbf{k}_{fi}) =$$

$$E_n^{MF}(\mathbf{k}_{fi}) + \left\langle \sum_{n'} \left|C_{n,n'}^{\mathbf{k}_{co}}\right|^2 \left(E_{n'}^{QP}(\mathbf{k}_{co}) - E_{n'}^{MF}(\mathbf{k}_{co})\right)\right\rangle_{\mathbf{k}_{co}}$$
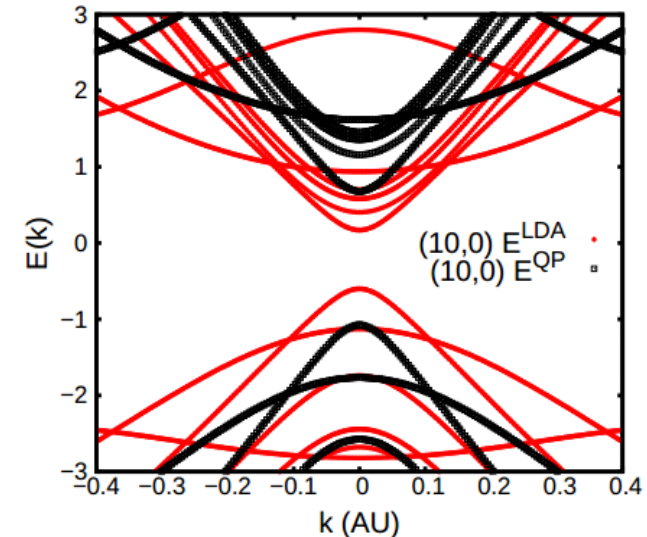
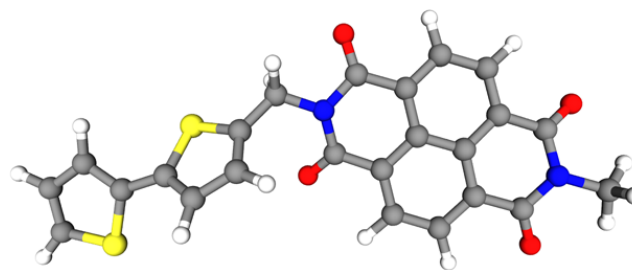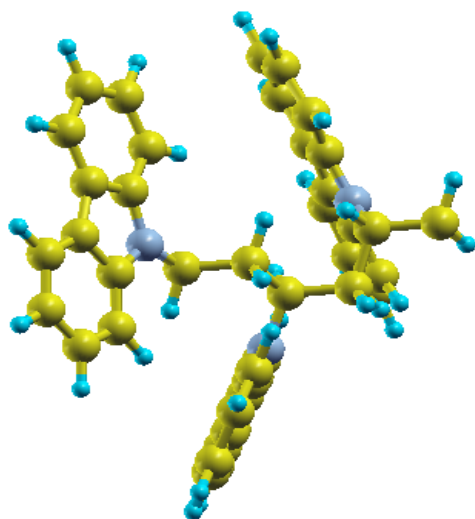(example interpolated QP band-structure for (10,0) SWCNT)

absorption.cplx.x :

-Exact Diagonalization. Scaling N^6
-Computes exciton states and energies

haydock.cplx.x:

-Uses Haydock-Recursion Method. Scaling N^4 (Mat-Vec Products only)
-Computes only the absorption spectra

BerkeleyGW Scaling and Performance

-Size (Atoms, Basis, Bands)

-Interfaces/Vacuum

-Very scalable on next-generation HPCs

$$\chi_{\mathbf{GG'}}(\mathbf{q};0) = \sum_n^{\mathrm{occ}} \sum_{n'}^{\mathrm{emp}} \sum_{\mathbf{k}} M_{n,n'}(\mathbf{k},\mathbf{q},\mathbf{G}) \cdot M^*_{n',n}(\mathbf{k},\mathbf{q},\mathbf{G'}) \cdot \ldots$$

1. $M_{n,n'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \langle n\mathbf{k}+\mathbf{q}| \, e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \, |n'\mathbf{k}\rangle$

Naïve scaling – N^4
Actual scaling – $N^3 \ln(N)$
MPI Parallel scaling – $N \times \ln(N)$ (parallel over n,n')
Additional OpenMP Threading over G coming in BGW 1.1

2. Sum: $\chi_{\mathbf{GG'}} = \mathbf{M}(\mathbf{G},(n,n',\mathbf{k})) * \mathbf{M}^T((n,n',\mathbf{k}),\mathbf{G'})$

MPI Distributed over $\mathbf{G},\mathbf{G'}$
Use of threaded Level 3 Blas (Threaded)

Ideal number of MPI tasks: a divisor of Nc x Nv
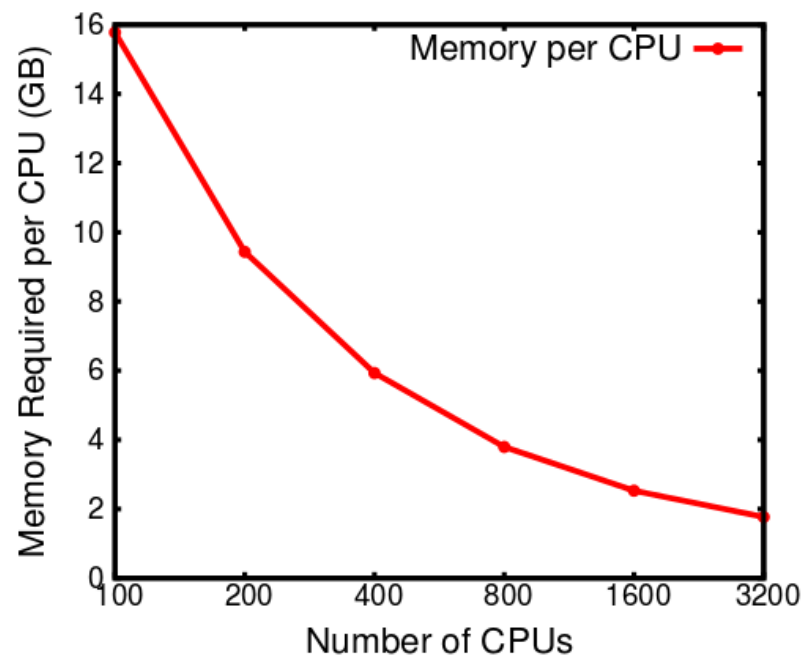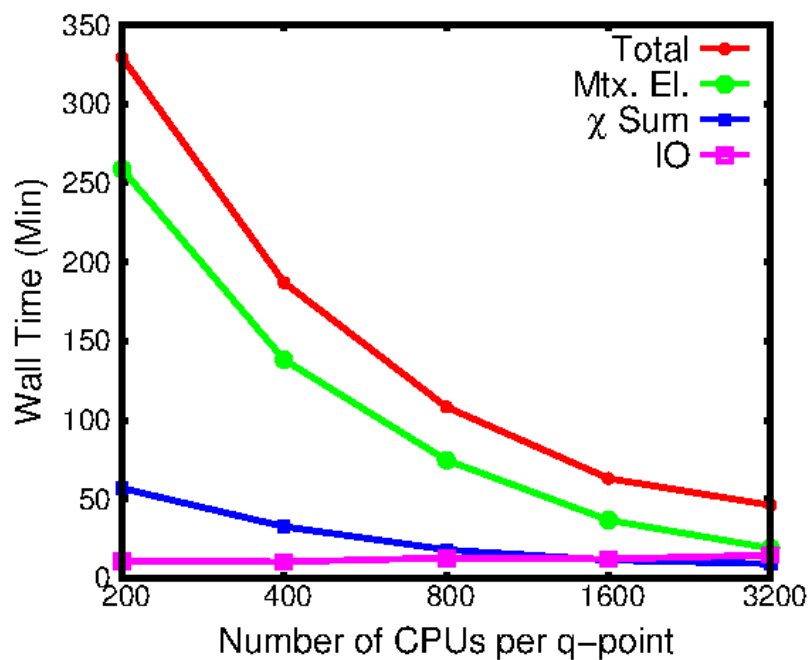
Hyrbrid MPI/OpenMP (BGW 1.1)

Utilize:

Threaded FFTW3
Threaded BLAS
Threaded ScaLAPACK

A handful of threaded loops.

BGW: Intel + MKL

Legend:
- 1 Thread/Task
- 2 Threads/Task
- 4 Threads/Task
- 8 Thread/Task

Y-axis: Wall Time (Sec)
X-axis: Number of Cores (16, 32, 64, 128, 256)
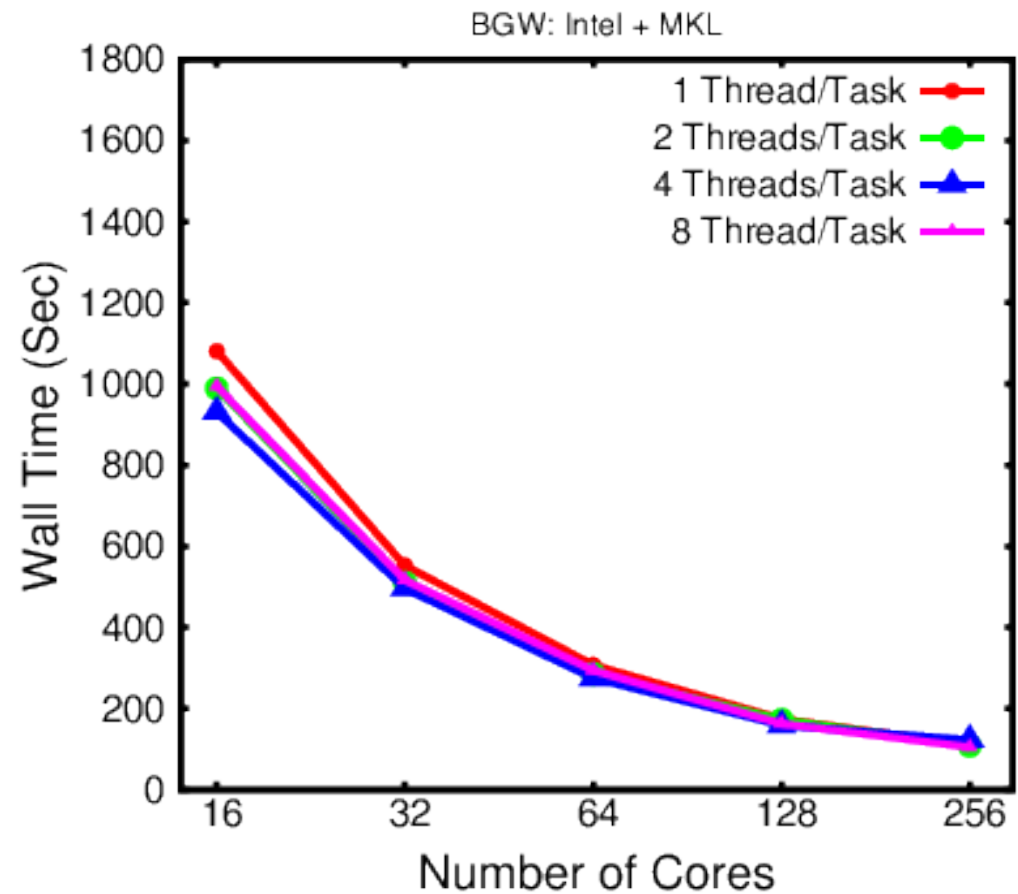
$$\langle n\mathbf{k}|\,\Sigma_{\mathrm{CH}}(E)\,|n'\mathbf{k}\rangle = \sum_{n'}\sum_{\mathbf{qGG'}} M_{n,n'}(\mathbf{k},\mathbf{q},\mathbf{G})\cdot M^{*}_{n',n}(\mathbf{k},\mathbf{q},\mathbf{G}')\cdot\ldots$$

1. $M(n,n',\mathbf{k},\mathbf{q},\mathbf{G}) = \langle n\mathbf{k}{+}\mathbf{q}|\,e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\,|n'\mathbf{k}\rangle$

Naïve scaling – N_sig*N^3
Actual scaling – N_sig*N^2 ln(N)
MPI Parallel scaling – N x ln (N) (parallel over n,n')
Threaded over G

2. Summation:

Naïve scaling – N_sig x N^3
MPI Parallel scaling – N^2 x ln (N) (parallel over N_sig, G')
Threaded over G,G'

Ideal number of MPI tasks: a divisor of N_sig x Nb
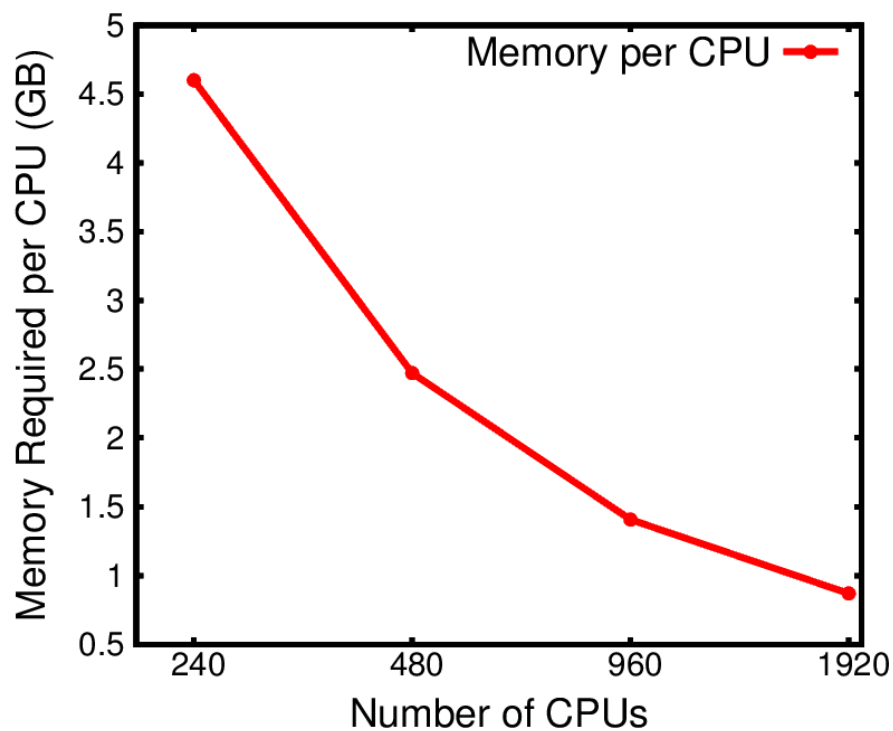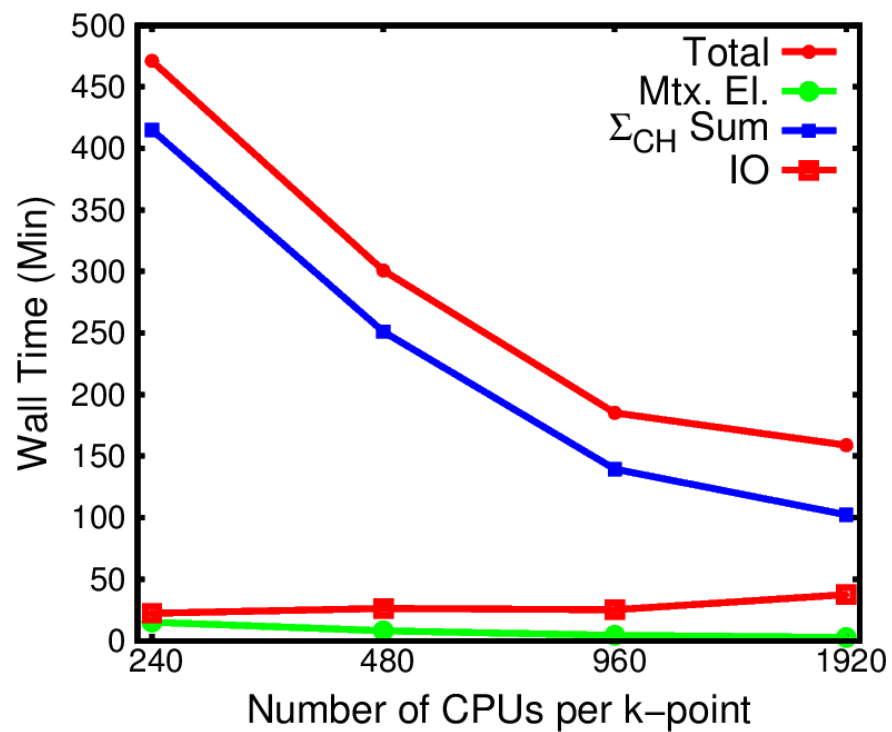
$$\left\langle v, c, \mathbf{k} \middle| K^{eh} \middle| v', c', \mathbf{k}' \right\rangle$$
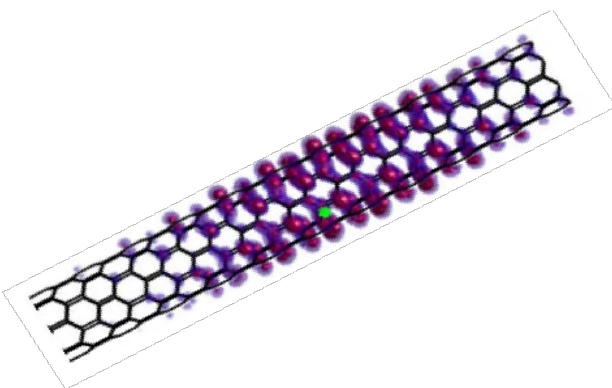
1. Kernel Construction:

MPI over nk^2, $(nk \times nv)^2$ or $(nk \times nv \times nc)^2$
OpenMP over G (BGW 1.1)

Naïve Scaling – $(N_v \times N_c \times N_{\mathbf{k}})^2 \times N_G \ln(N_G)$
MPI Parallel Scaling – $N_G \ln(N_G)$
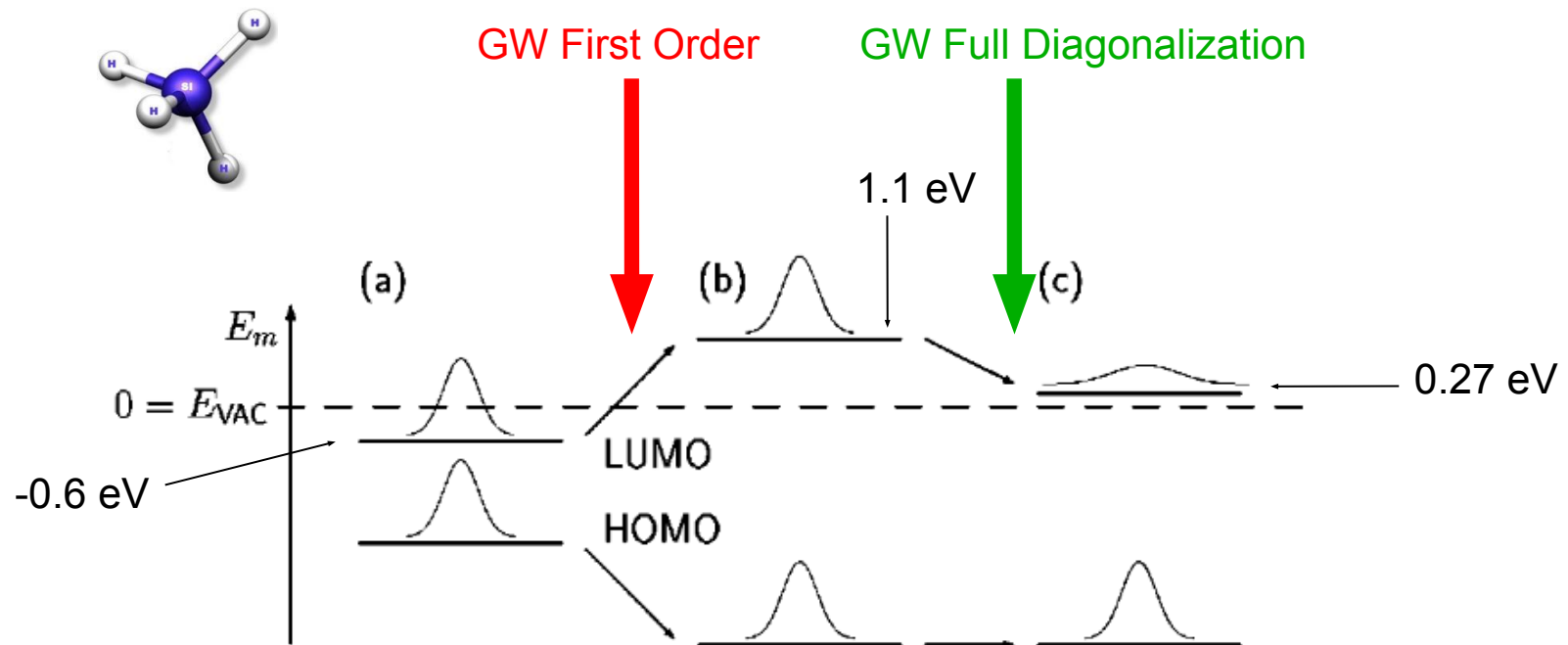
2. Diagonalization
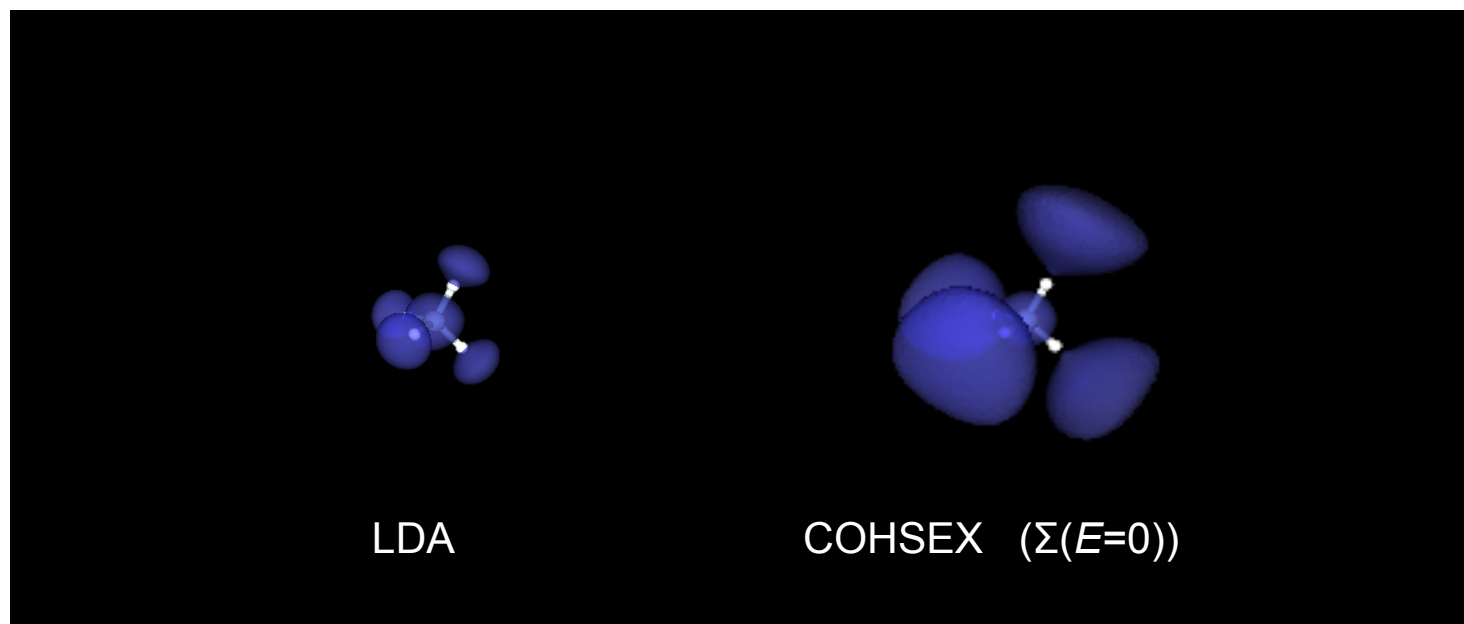
Using threaded scaLAPACK.

MPI Parallel Scaling - N^2

BerkeleyGW Common Issues

For a typical GW calculation, the LDA starting point is sufficient:

$$E_n^{QP} \approx \langle \psi_n^{MF} | H_{Hartree} | \psi_n^{MF} \rangle + \langle \psi_n^{MF} | \Sigma | \psi_n^{MF} \rangle$$
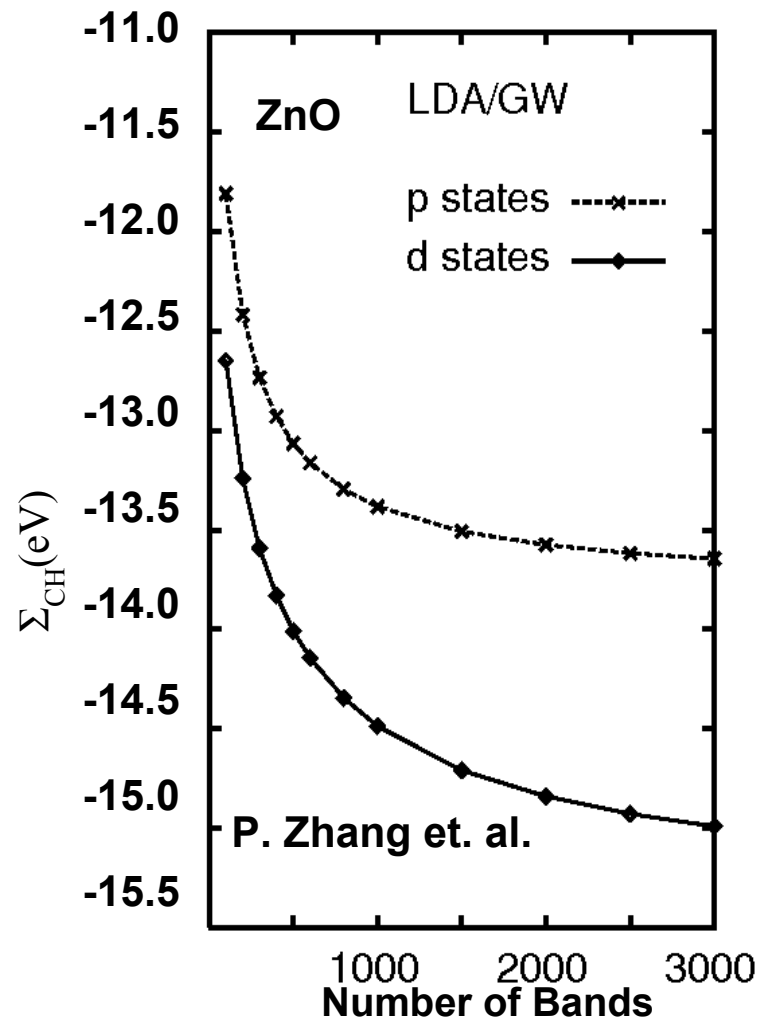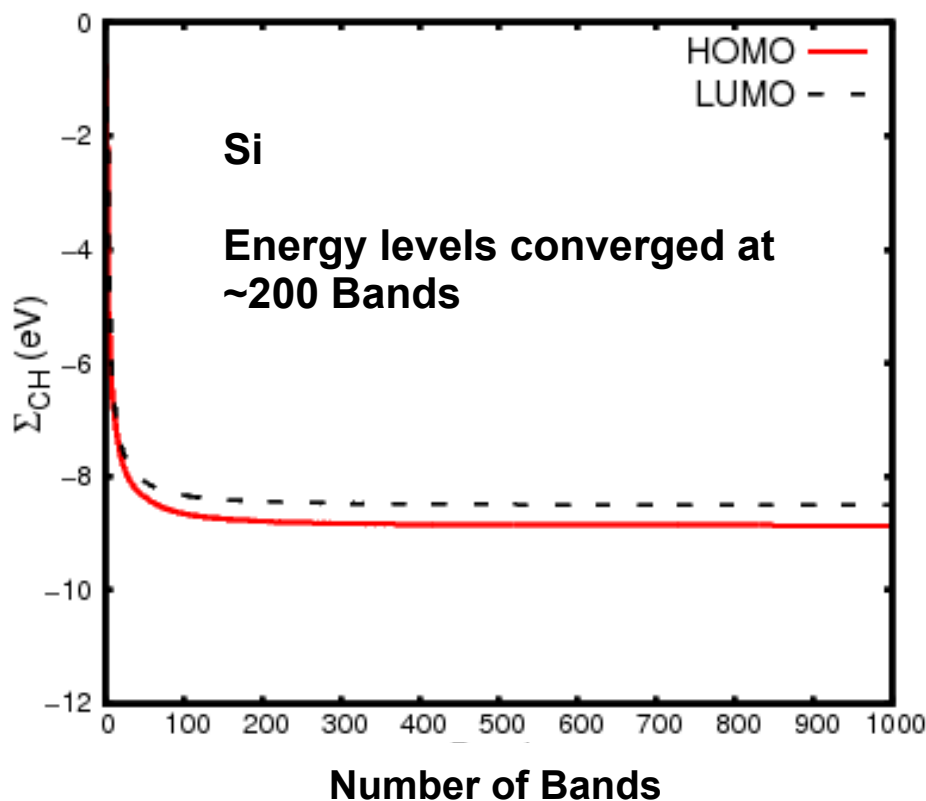
Notable exceptions - Silane:

GW First Order   GW Full Diagonalization

1.1 eV

0.27 eV

(a) (b) (c)

E_m

$0 = E_{VAC}$

-0.6 eV

LUMO

HOMO

M. Rohlfing and S.G. Louie Phys. Rev. B 62 4927 (2000).

LDA   COHSEX   ($\Sigma(E=0)$)

	LDA	LDA+GW	CSX	CSX+GW	
HOMO	-8.52	-12.80	- 13.2	-12.80	
LUMO	-0.465	1.02	.1	.29	
QP gap	8.06	13.82	13.3	13.10	

$$\langle n\mathbf{k} | \Sigma_{CH}(E) | n'\mathbf{k} \rangle = \sum_{n'} \sum_{\mathbf{qGG'}} M_{n,n'}(\mathbf{k},\mathbf{q},\mathbf{G}) \cdot M^*_{n',n}(\mathbf{k},\mathbf{q},\mathbf{G'}) \cdot \ldots$$
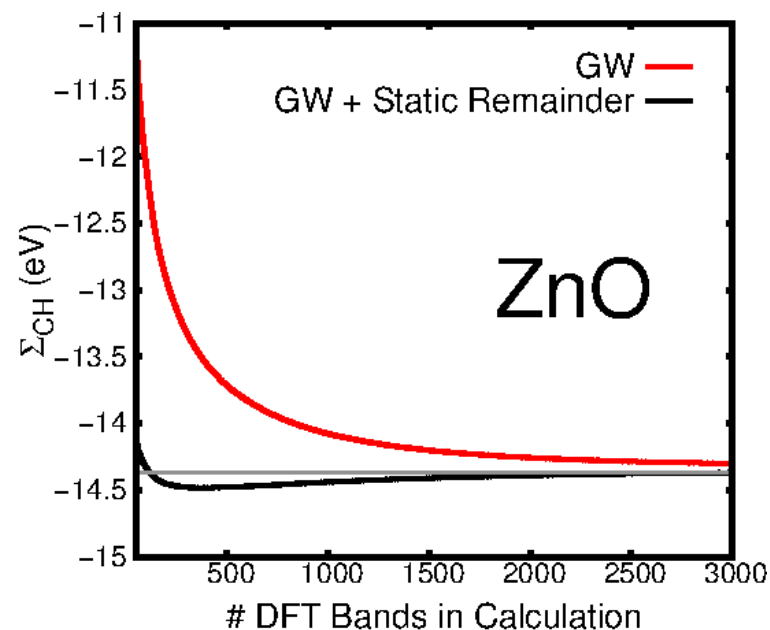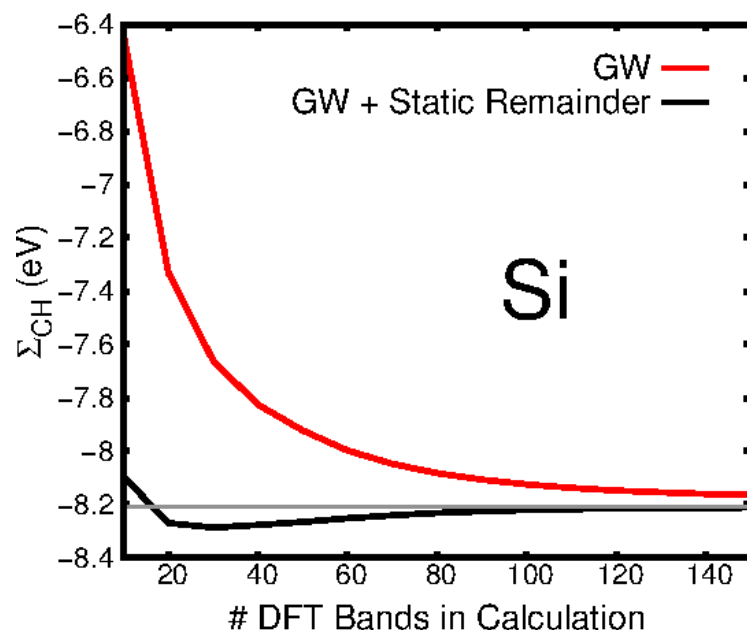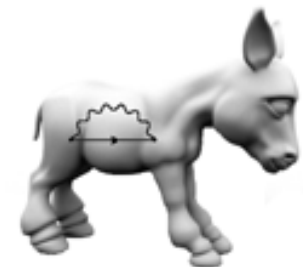
Slowly converging with number of conduction bands.

Si

Energy levels converged at ~200 Bands

HOMO ——
LUMO – –

Σ_{CH} (eV)

Number of Bands

ZnO LDA/GW

p states ····×····
d states ——◆——

Σ_{CH}(eV)

P. Zhang et. al.

Number of Bands

Static remainder:

$$\langle n\mathbf{k}|\Sigma_{\mathrm{CH}}^{\infty}(\mathbf{r},\mathbf{r}';E)|n'\mathbf{k}\rangle =$$

$$\langle n\mathbf{k}|\Sigma_{\mathrm{CH}}^{N}(\mathbf{r},\mathbf{r}';E)|n'\mathbf{k}\rangle + \frac{1}{2}\left(\langle n\mathbf{k}|\Sigma_{\mathrm{CH}}^{Coh/\infty}(\mathbf{r},\mathbf{r}')|n'\mathbf{k}\rangle - \langle n\mathbf{k}|\Sigma_{\mathrm{CH}}^{Coh/N}(\mathbf{r},\mathbf{r}')|n'\mathbf{k}\rangle\right).$$

http://www.berkeleygw.org

Support for ESPRESSO/PARSEC/PARATEC/EPM/SIESTA

Support for LDA/GGA/Hybrid/HF/COHSEX starting points as well as off-diagonal Σ calculations

Support for Metals/Semiconductors/Insulators and a variety of Coulomb truncation schemes*

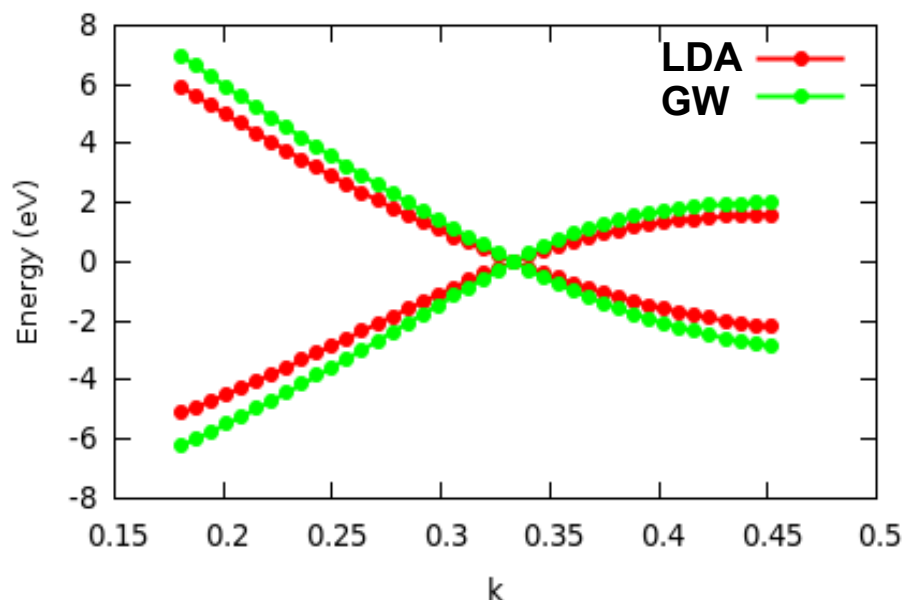Compute self-energies, lifetimes, photo-emission spectra, optical spectra etc...

Extra Slides

Graphene GW Quasiparticle Band Dispersion

.Quasiparticle energy corrections are large in Graphene and increase with increasing diameter in Metallic Nanotubes.
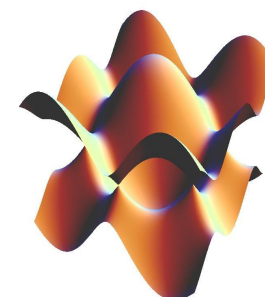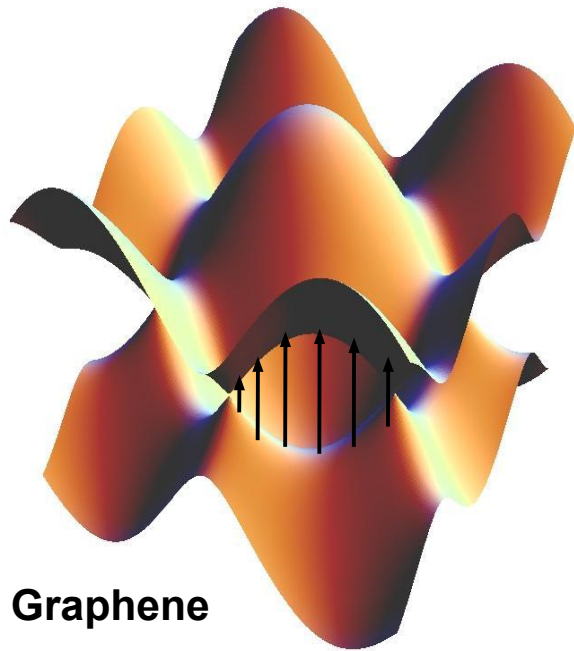
Convergence requires 64x64 k-grid

Quasiparticle Fermi Velocities (10^6 m/s)

	LDA	QP	% Diff
(5,5)	0.72	0.85	19.%
(10,10)		0.81	1.00	25%
(21,21)	0.82	1.03	28%
Graphene		0.85	1.15	33%
Experiment*	1.1		

*Y. Zhang, YW Tan, HL Stormer; P. Kim. Nature 438 201 (2005)
*KS Novoselov et. al Nature 438 197 (2005)
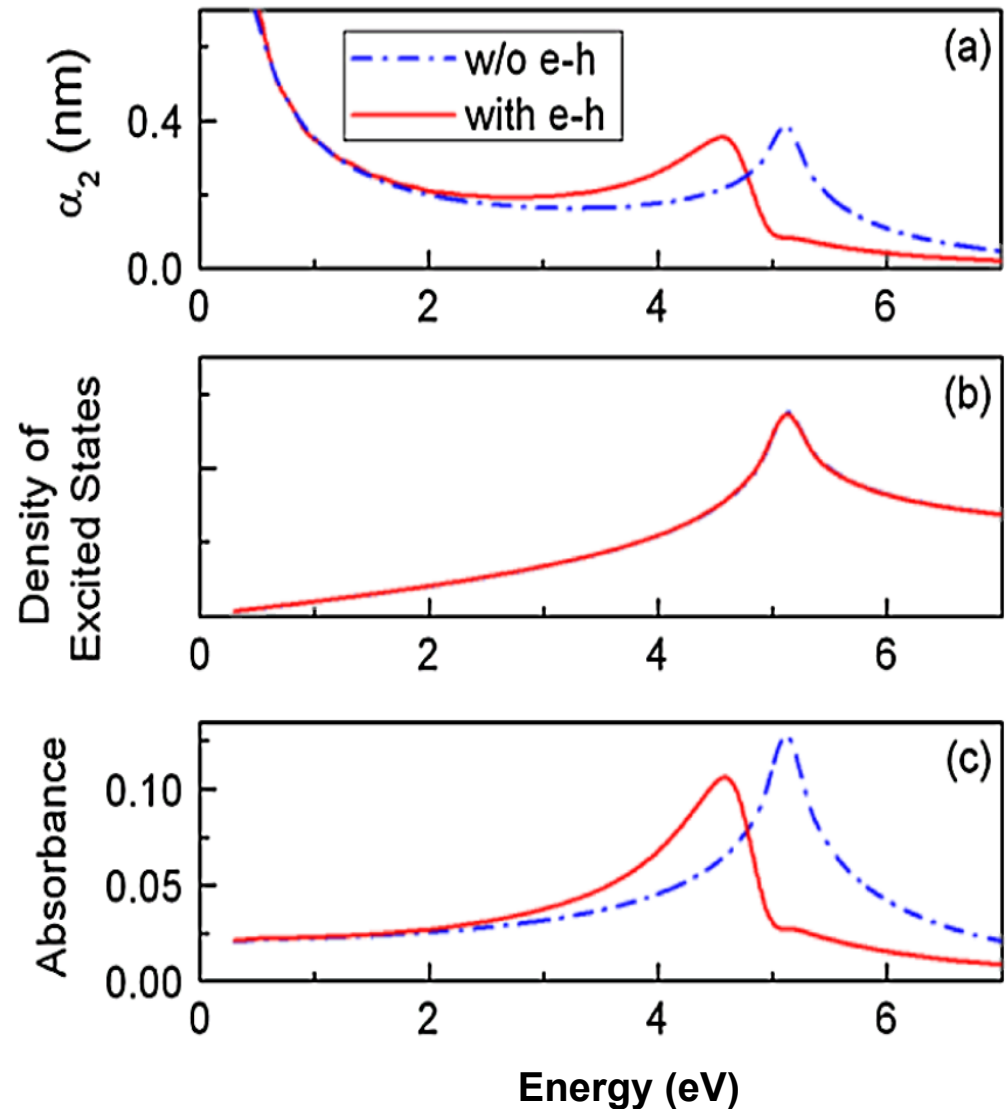
Many K-Points in BSE

Graphene

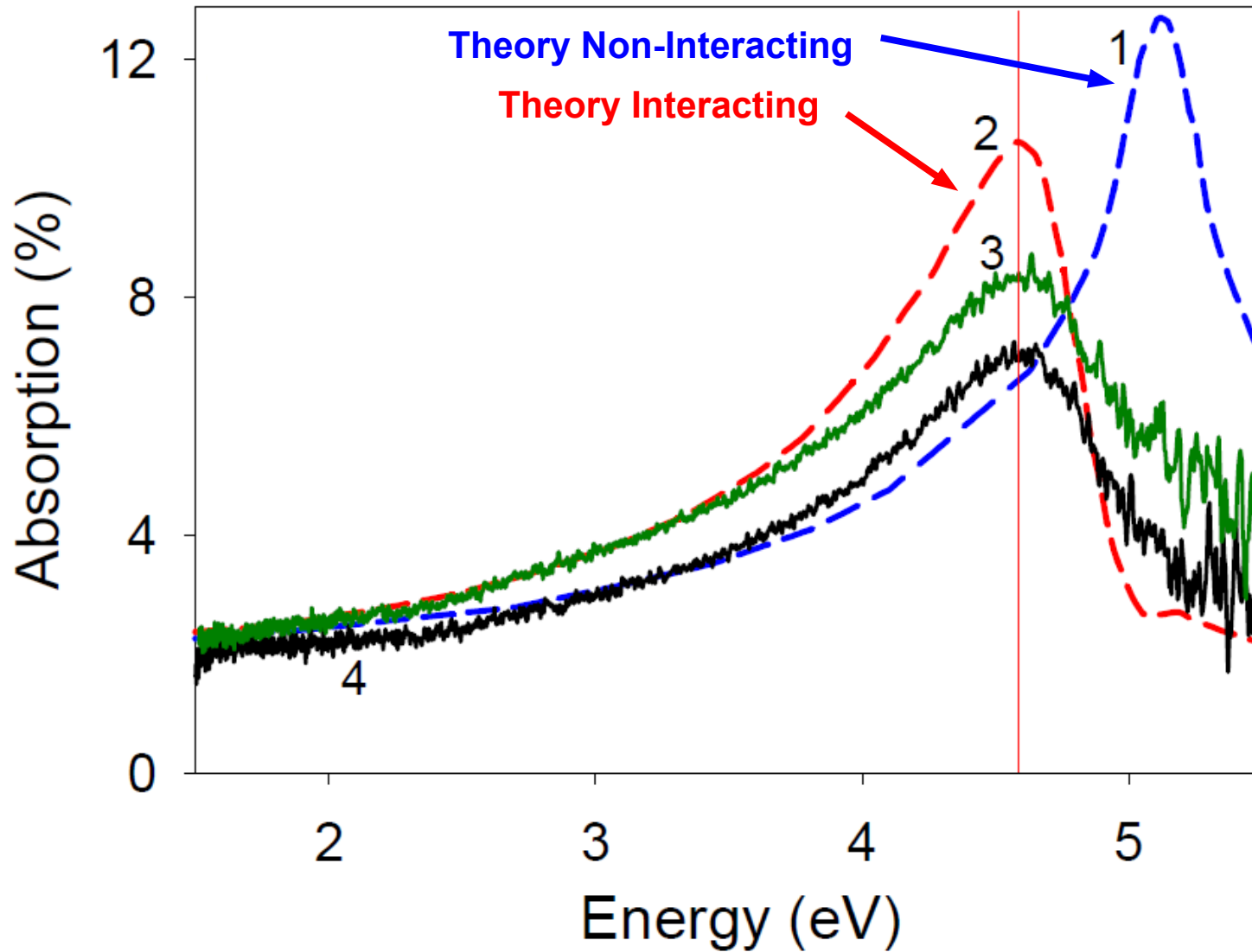. Smooth/Accurate absorption spectra requires a tremendous amount of kpoints. **256X256 k-point sampling.**

.Requires excellent parallelization and memory distribution.

Energy (eV)

**Yang. L, Deslippe, J. et. al. Phys. Rev. Lett. 103, 186802 (2009)**

Agreement with Experiment

VG Kravets, AN Grigorenko, RR Nair, P Blake, S Anissimova, KS Novoselov, AK Geim. Phys. Rev. B 81 155413 (2010).
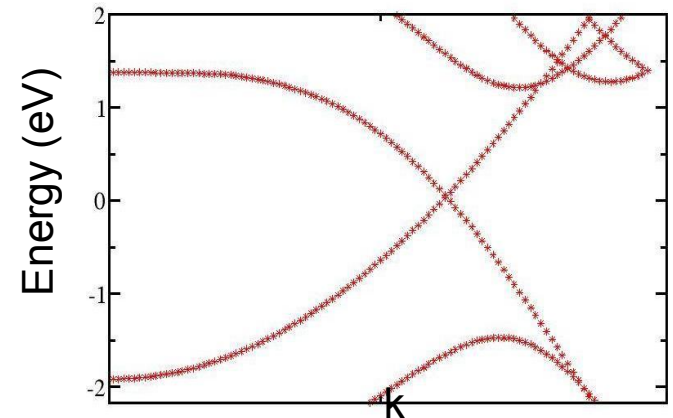
Examples: Armchair SWCNT

Armchair tube (n,n) bands pass through K-point of Graphene. Metallic with Fermi velocities near that of graphene
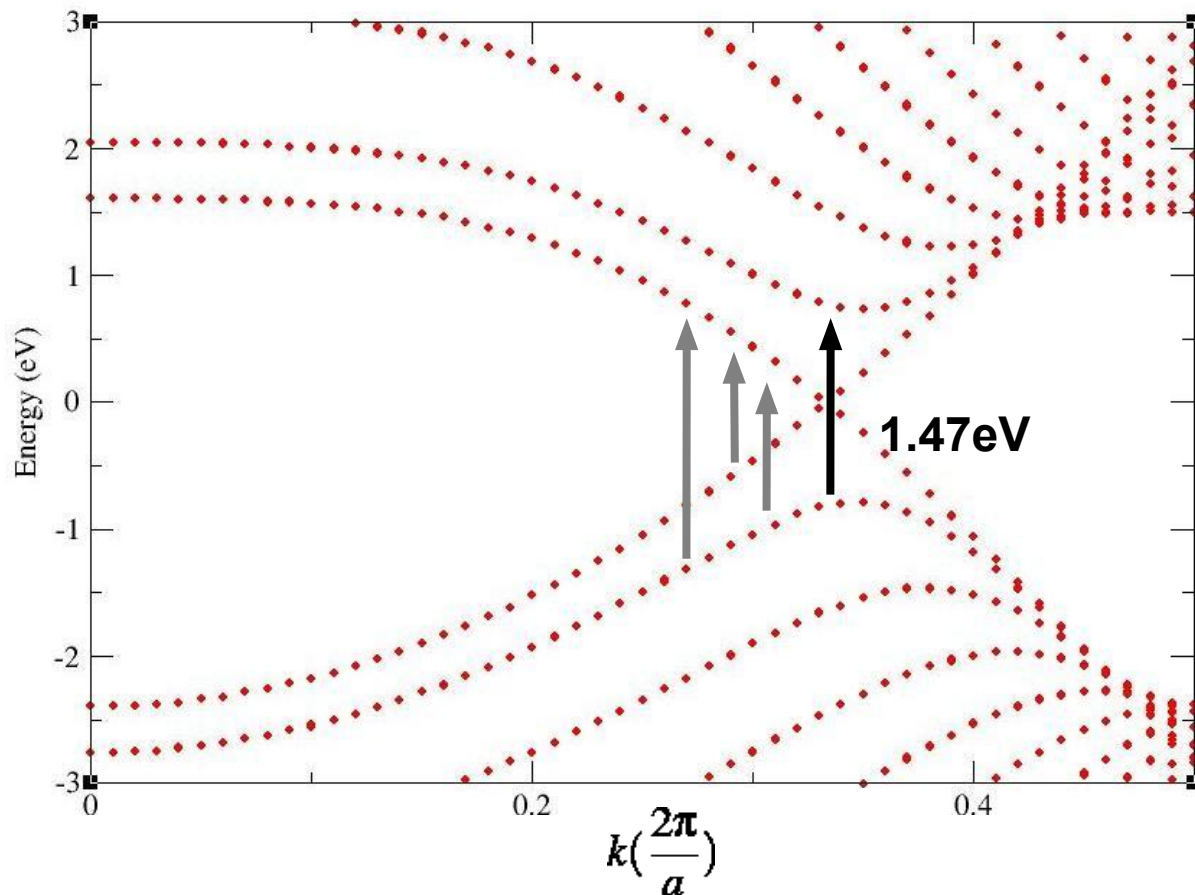
Pure axial rotation symmetry commutes with the k-point Hamiltonian across entire bands. Leading to an **angular momentum quantum number**
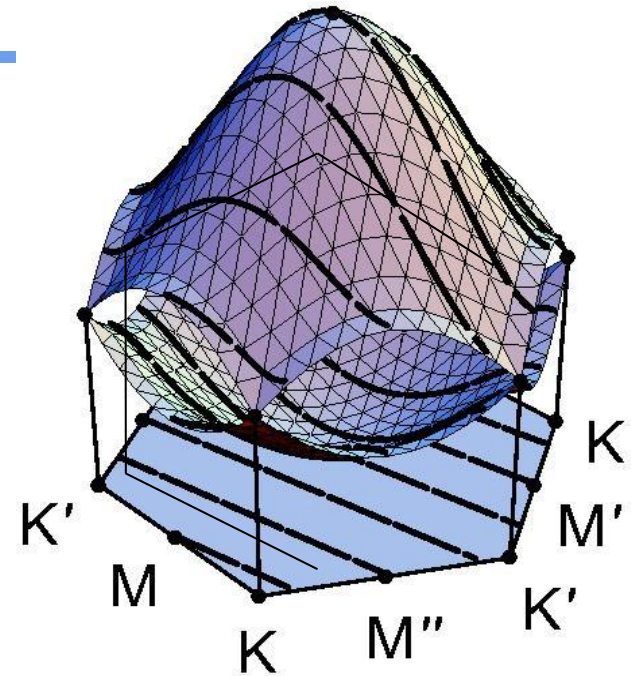
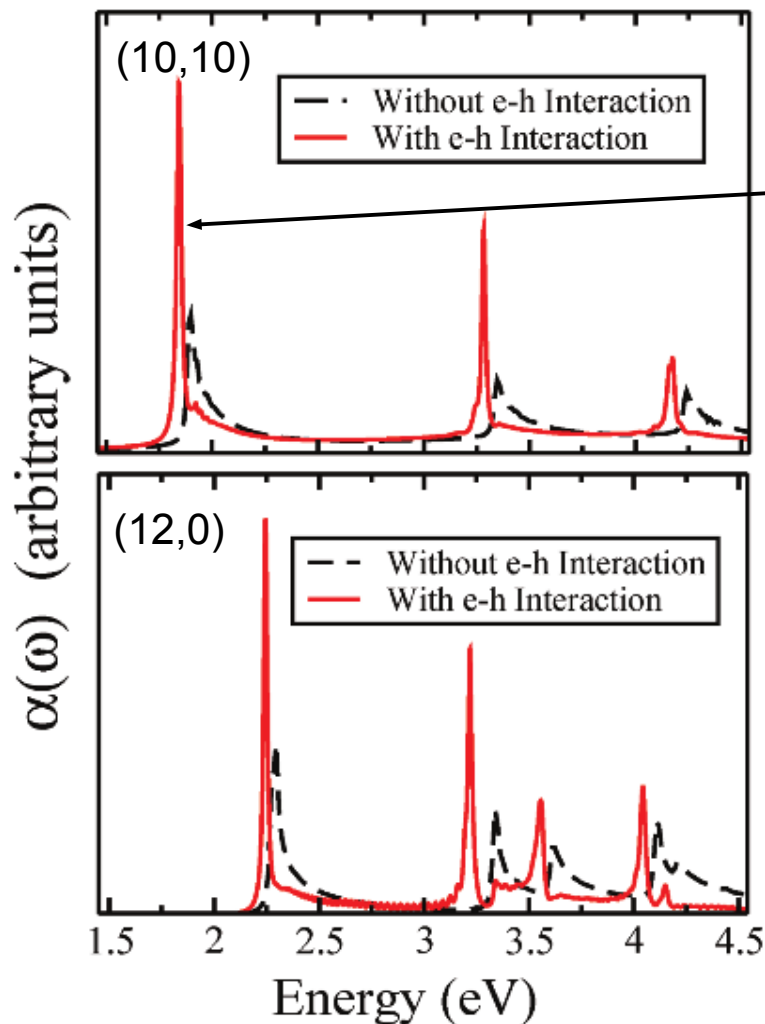(5,5) Band Structure

1.47eV

Optically Forbidden

Optically Allowed

Due to symmetry have optical gap.

Metallic screening usually prohibits bound excitonic states.

- Peak from a single eigenvalue.
- Exciton binding energy - 0.06 eV.
- The onset is calculated to be 1.84 eV.

Experimental value*: 1.89 eV

(Experiment) Fantini, C.; Jorio, A.; Souza, M.; Strano, M. S.; Dresselhaus, M. S.; Pimenta, M. A. Phys. Rev. Lett. 93, 147406. (2004)

(Theory) J. Deslippe, D. Prendergast, CD Spataru, S.G. Louie, Nano Lett. 7 (6) 1626-1630, (2007)

$(70 \times 70 \times 5)$ a.u.^{3}

60 Rydberg Wavefunction Cutoff
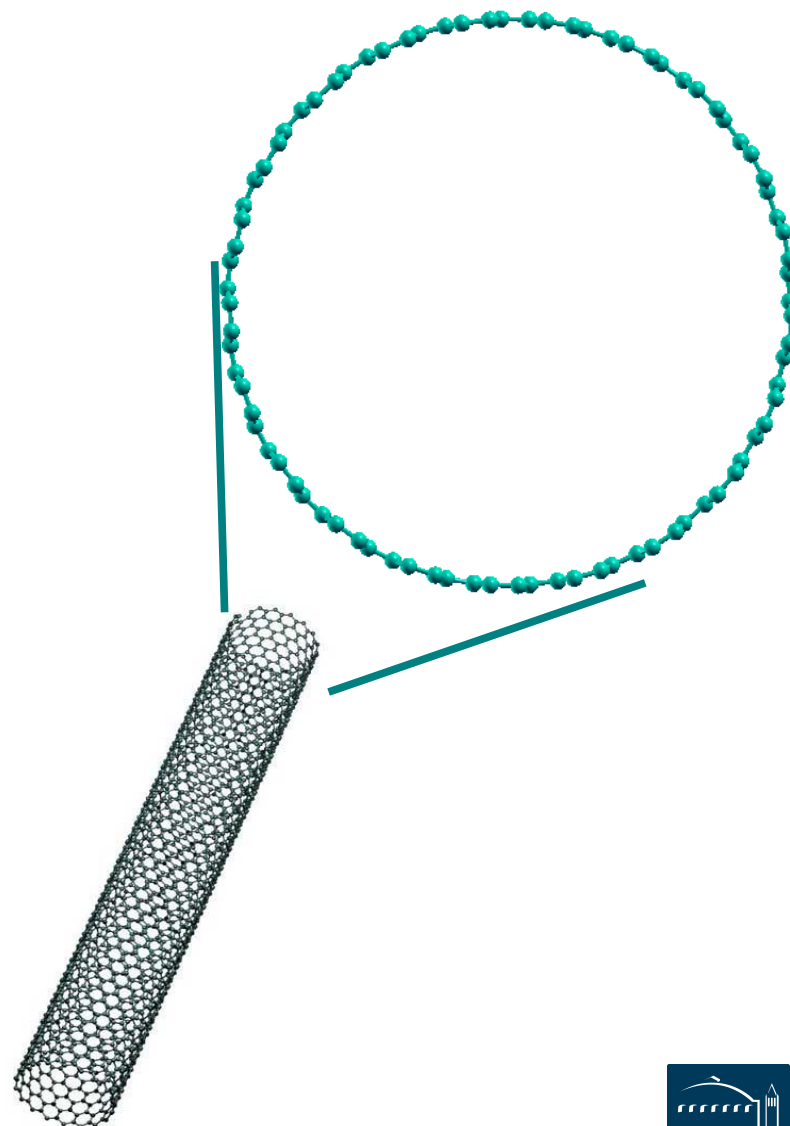6 Rydberg Dielectric Cutoff

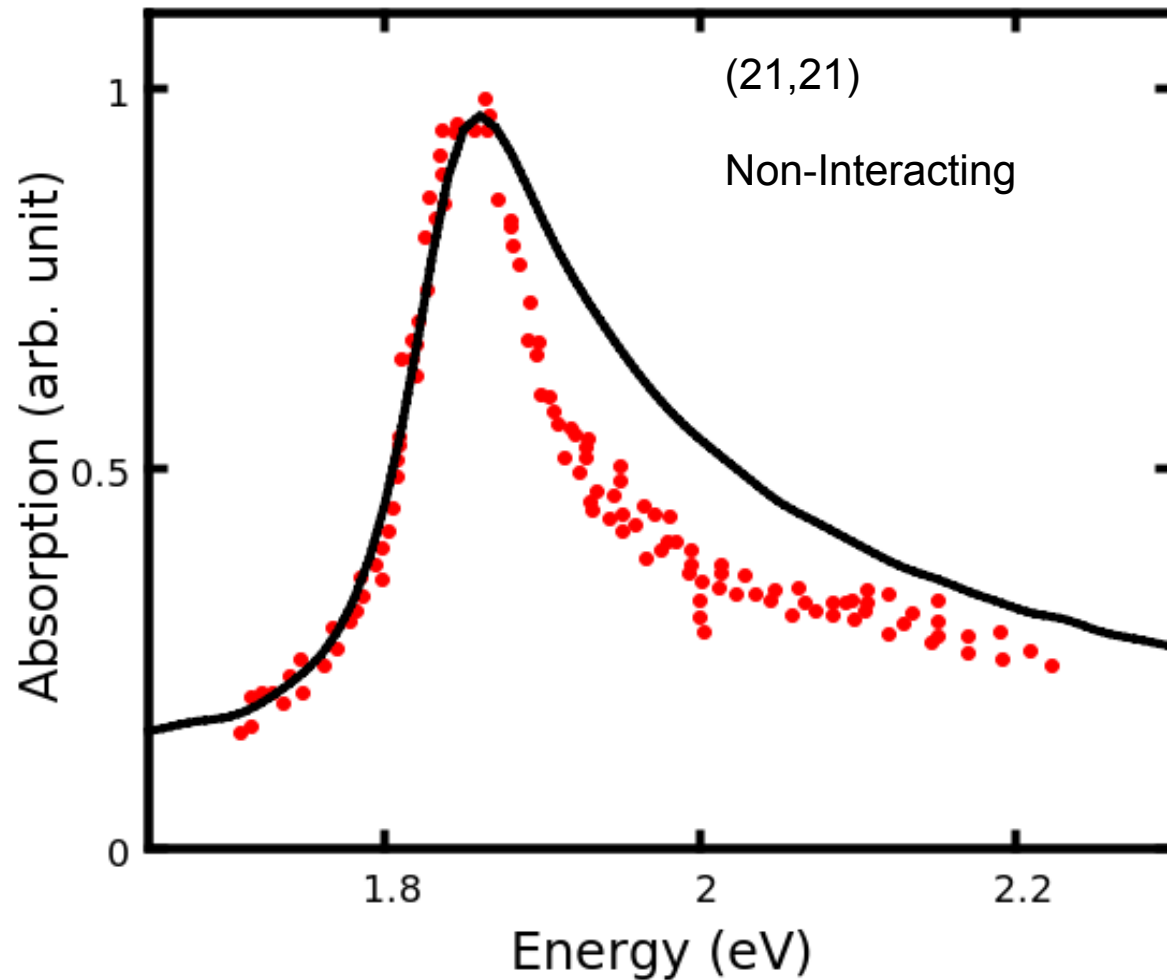6000 G-vectors $\varepsilon^{-1}(\mathbf{q}, \mathbf{G}, \mathbf{G}')$
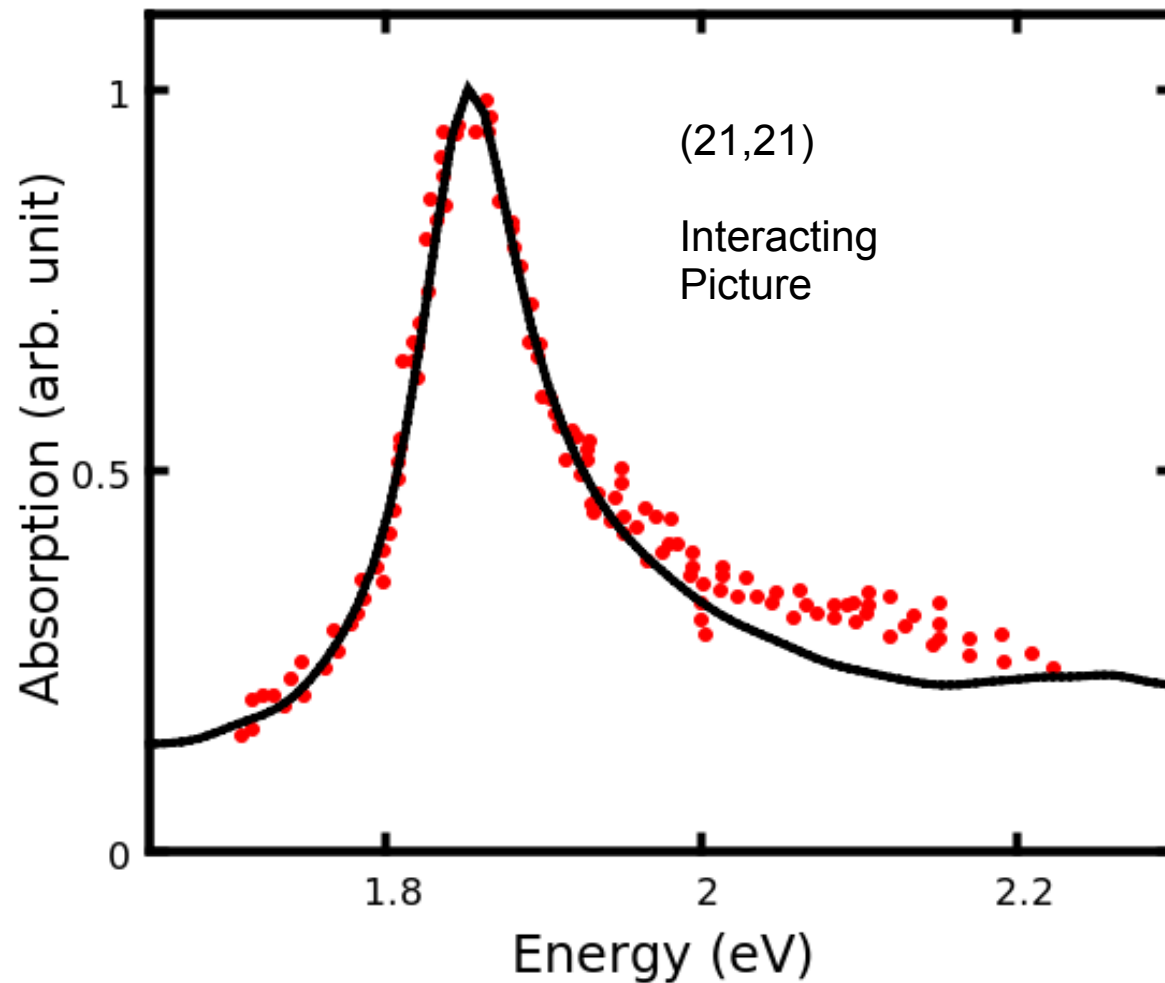
5000 Bands

CPUS – 2000-5000

Total Parallel Wall Time ~ 48 hours
Human Time < 1 Week

(21,21)

Non-Interacting

(Experiment) F. Wang, D. Cho,1 B. Kessler, J. Deslippe. P.J. Schuck, S. G. Louie, A. Zettl, T. Heinz, R. Shen. Phys. Rev. Lett. 99, 227401 (2007)

(21,21)

Interacting
Picture

(Experiment) F. Wang, D. Cho,1 B. Kessler, J. Deslippe. P.J. Schuck, S. G. Louie, A. Zettl, T. Heinz, R. Shen. Phys. Rev. Lett. 99, 227401 (2007)