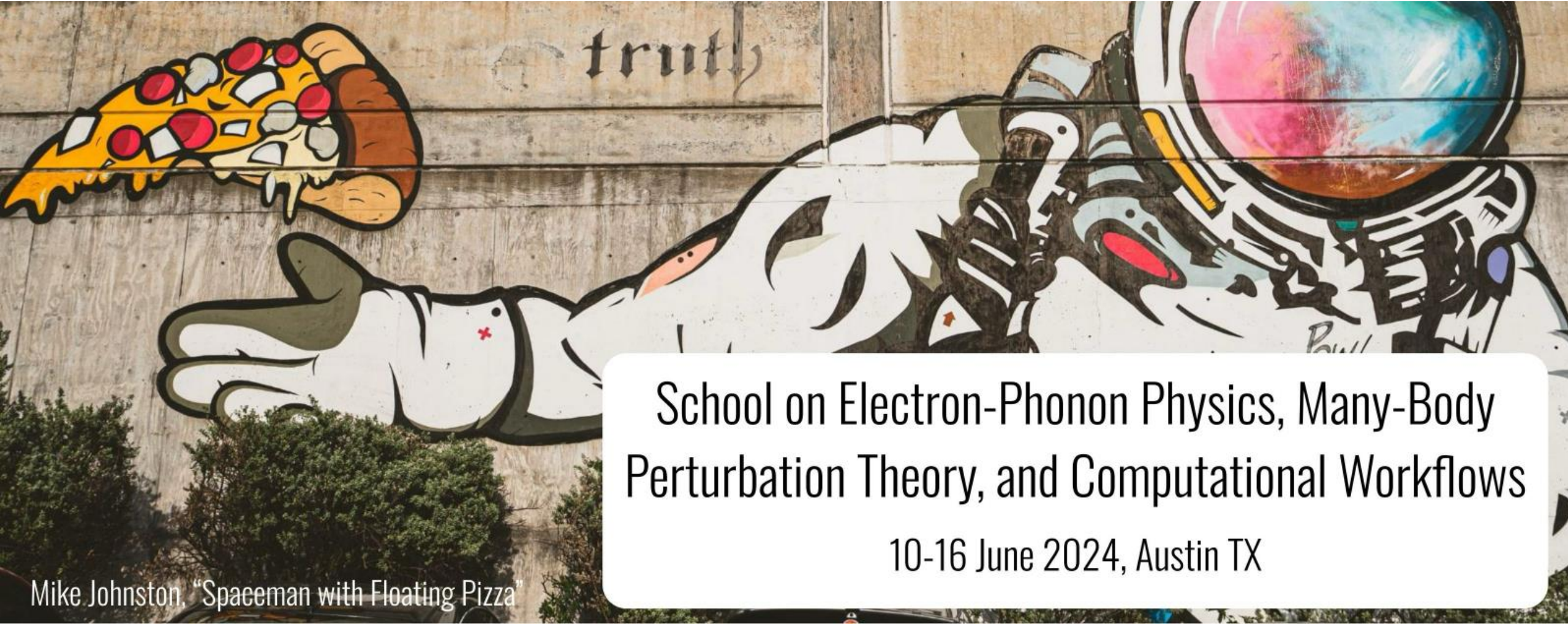

Mike Johnston, "Spaceman with Floating Pizza"

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

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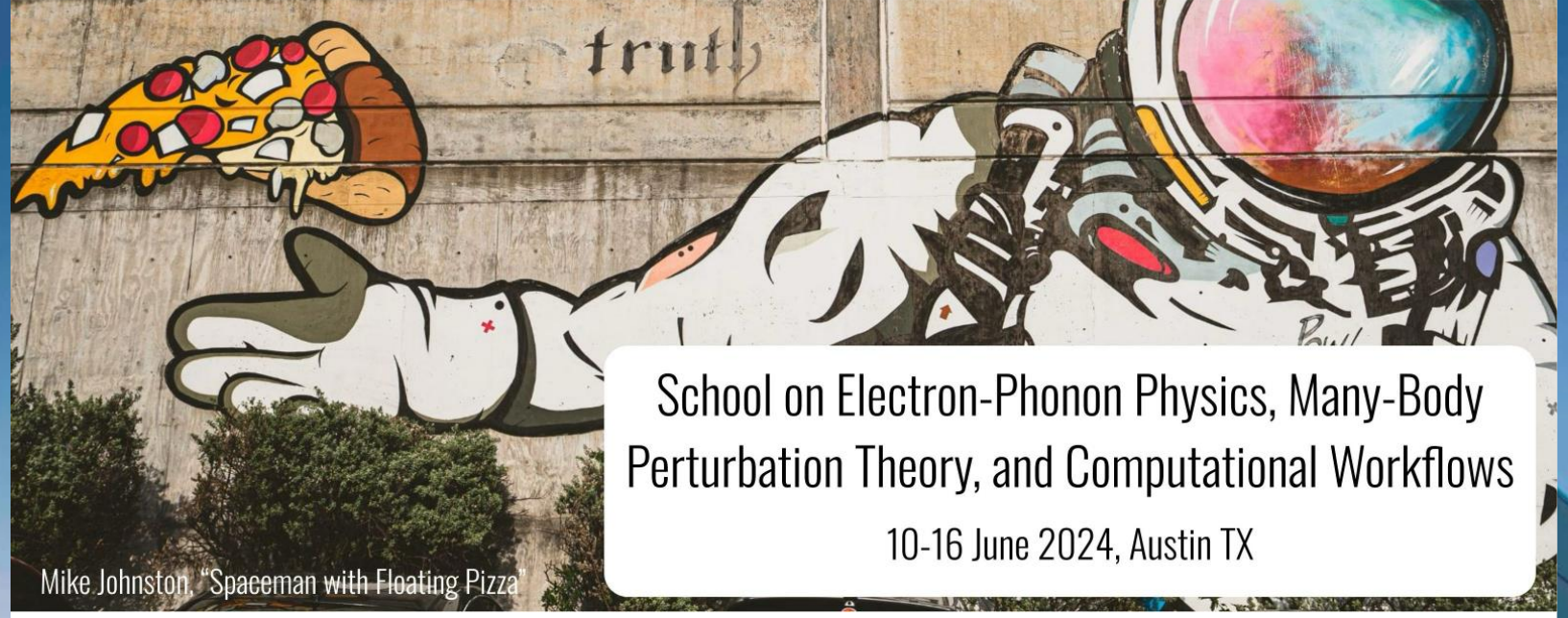

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GW-BSE with BerkeleyGW

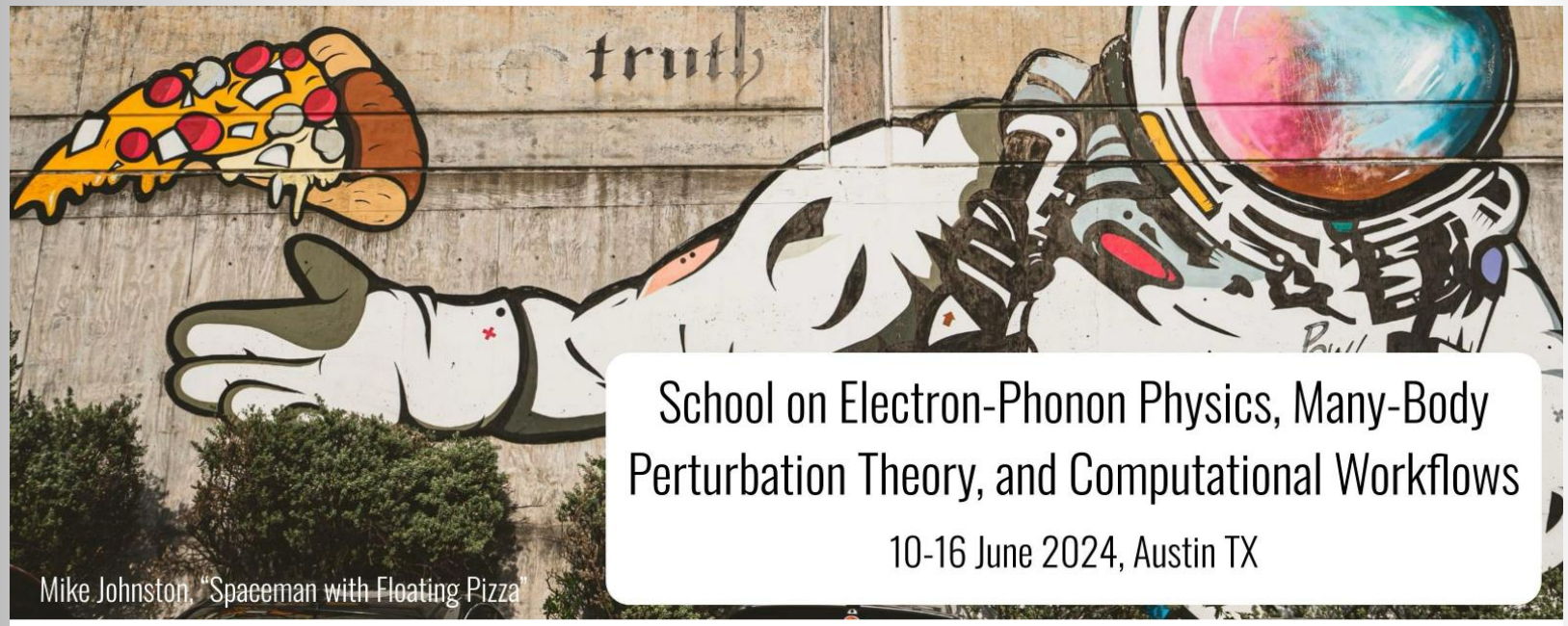
Jack Deslippe (Mauro Del Ben)

Applied Mathematics & Computational Research Division (LBNL)

Outline

1. Introduction
2. Overview of the BerkeleyGW software package
3. The GW+BSE workflow in BerkeleyGW
4. Summary

Introduction



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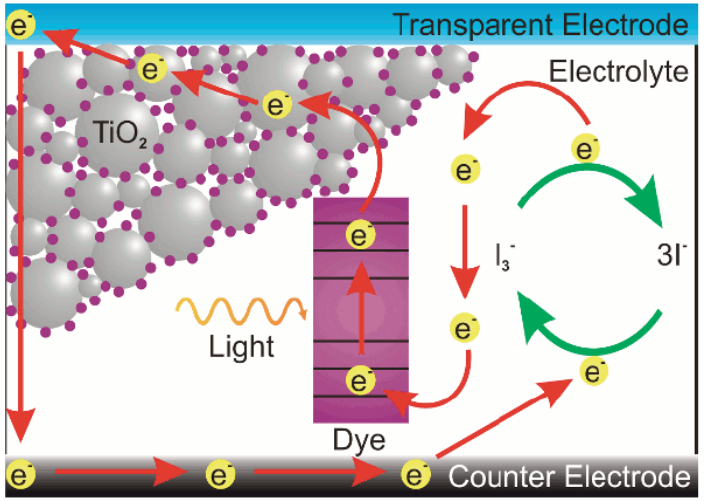
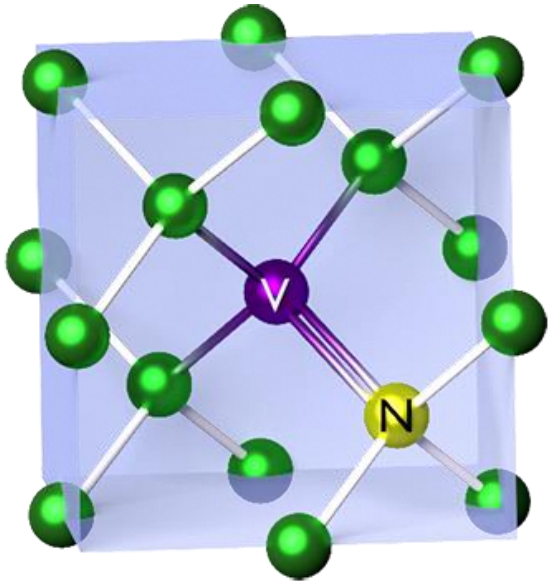
Materials Science/Chemistry and HPC

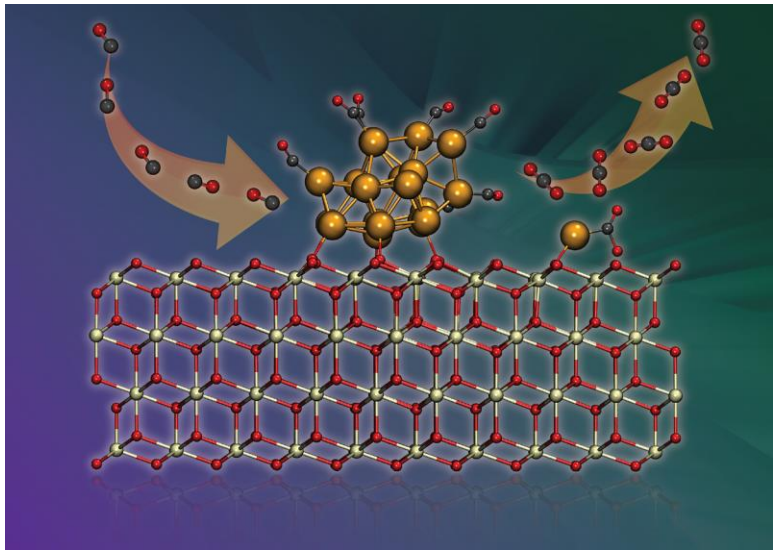
Grätzel cells: Oxide/Organic Interfaces



Cheap, reliable and sustainable **photovoltaics**



Defects in crystals: **qubits/quantum computers**
https://www.nist.gov/programs-projects/diamond-nv-center-magnetometry



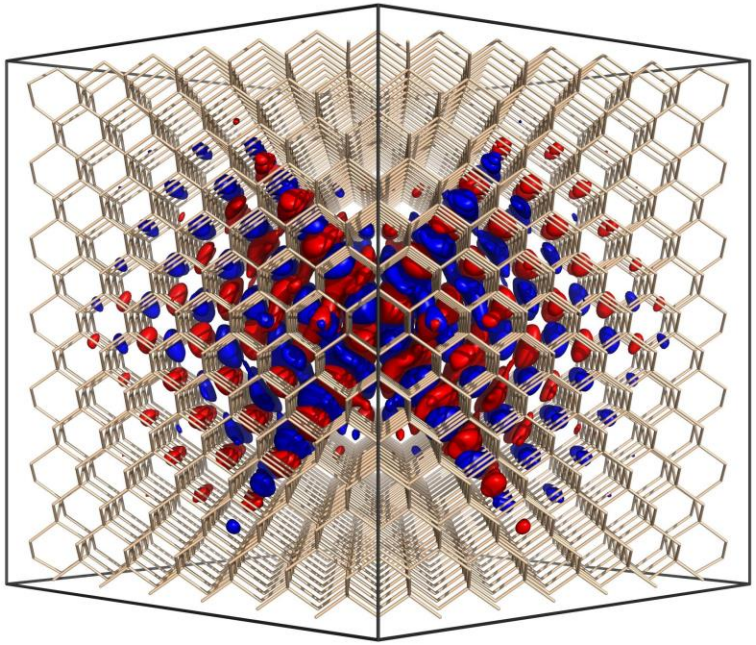
Chemical reaction at interfaces: **Catalysis**

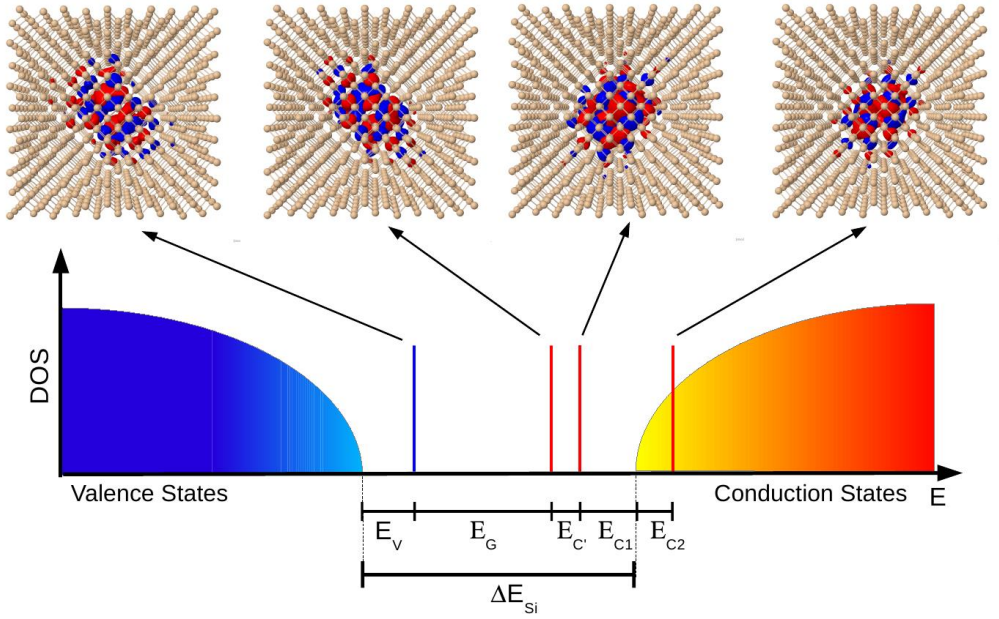
Density Functional Theory (DFT) the workhorse for over three decades

- Excellent compromise between accuracy and computational efficiency
- Ground state theory: often problematic for excited state phenomena

Excited State Properties of Complex Materials

Focus shift from ground to excited state properties





Example: Divacancy point defect in crystalline silicon, prototype of a solid-state Qubit

Accuracy beyond DFT: **GW and GW+BSE**

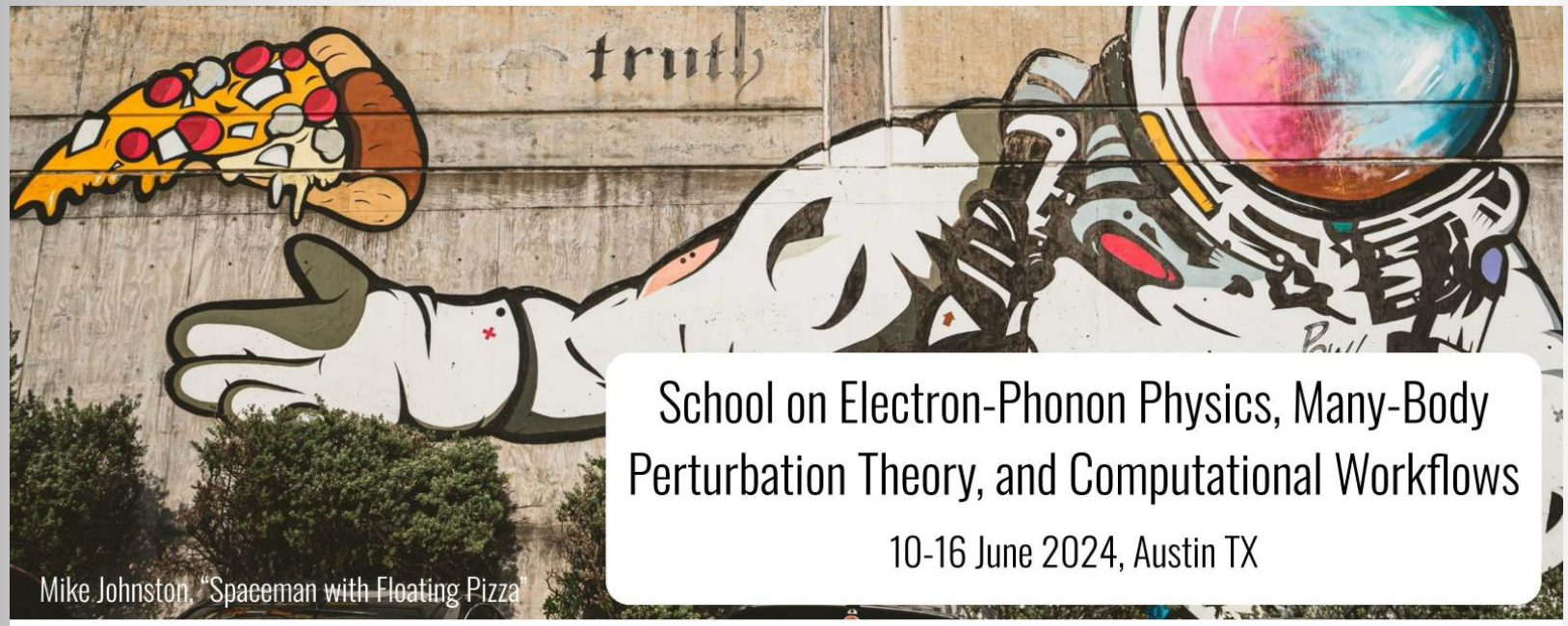
The GW+BSE: State of the Art

The GW+BSE method among the most effective and accurate approaches to predict excited-state properties in a wide range of materials

BerkeleyGW

BerkeleyGW: a massively parallel software package to study the excited state excited state properties of materials using GW-BSE methods and beyond

The BerkeleyGW Software Package



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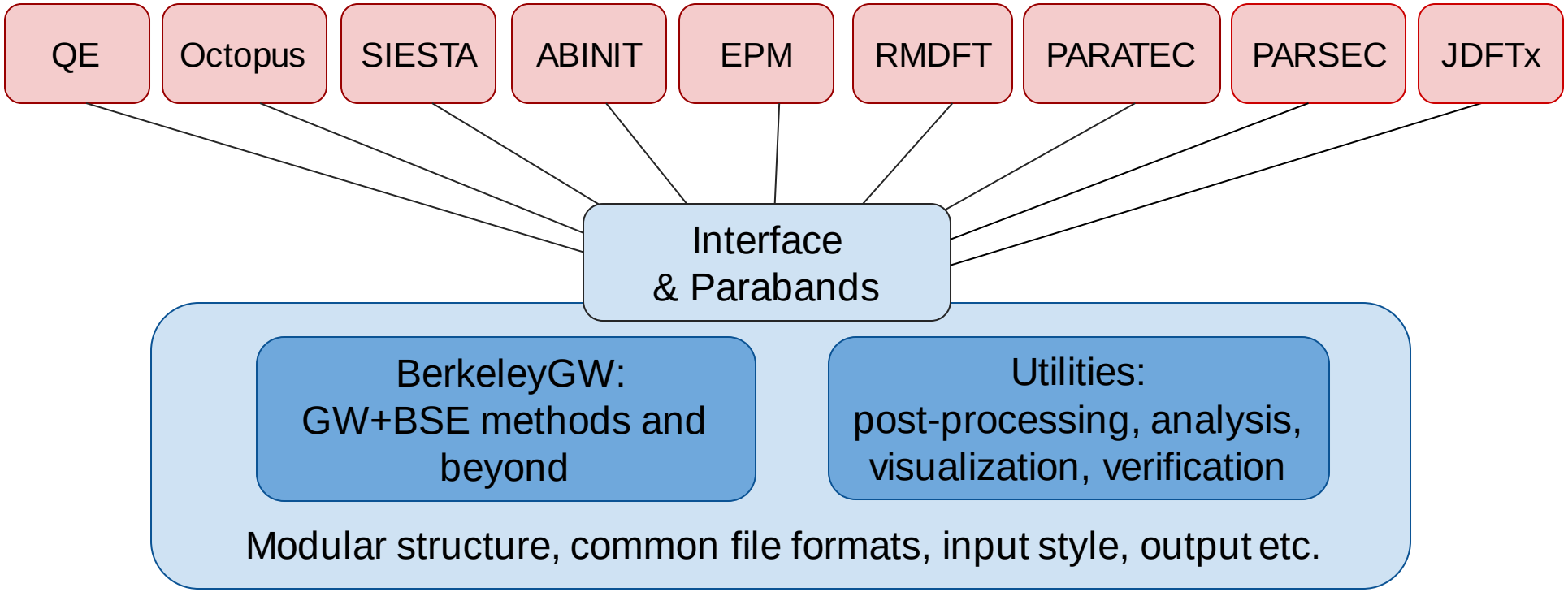
BerkeleyGW Software Design Vision

BerkeleyGW compute the electronic excited-state properties of materials via GW, Bethe-Salpeter equation (BSE) and beyond



https://berkeleygw.org/

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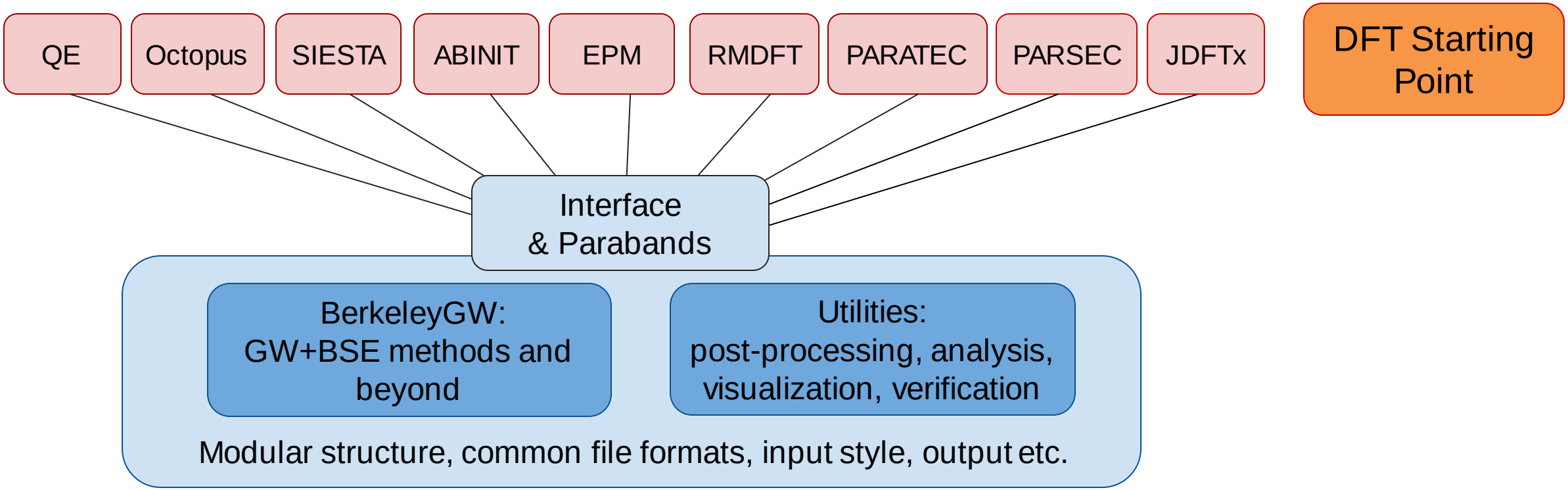

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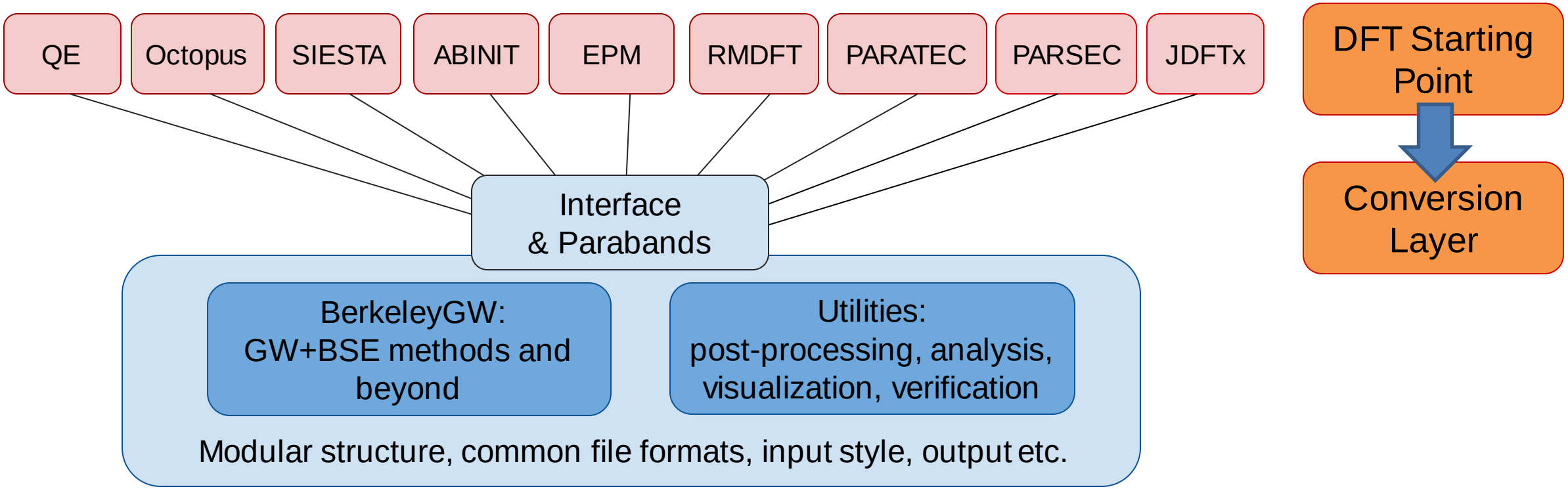

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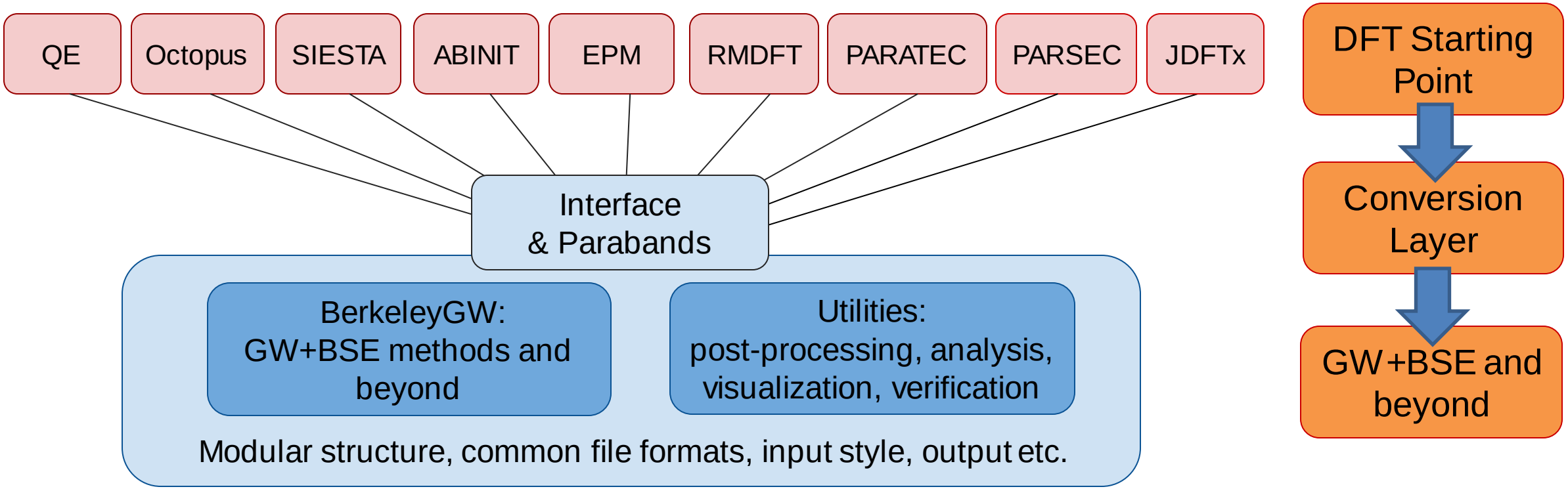


BerkeleyGW: developments are focuses on GW+BSE methodologies

https://berkeleygw.org/

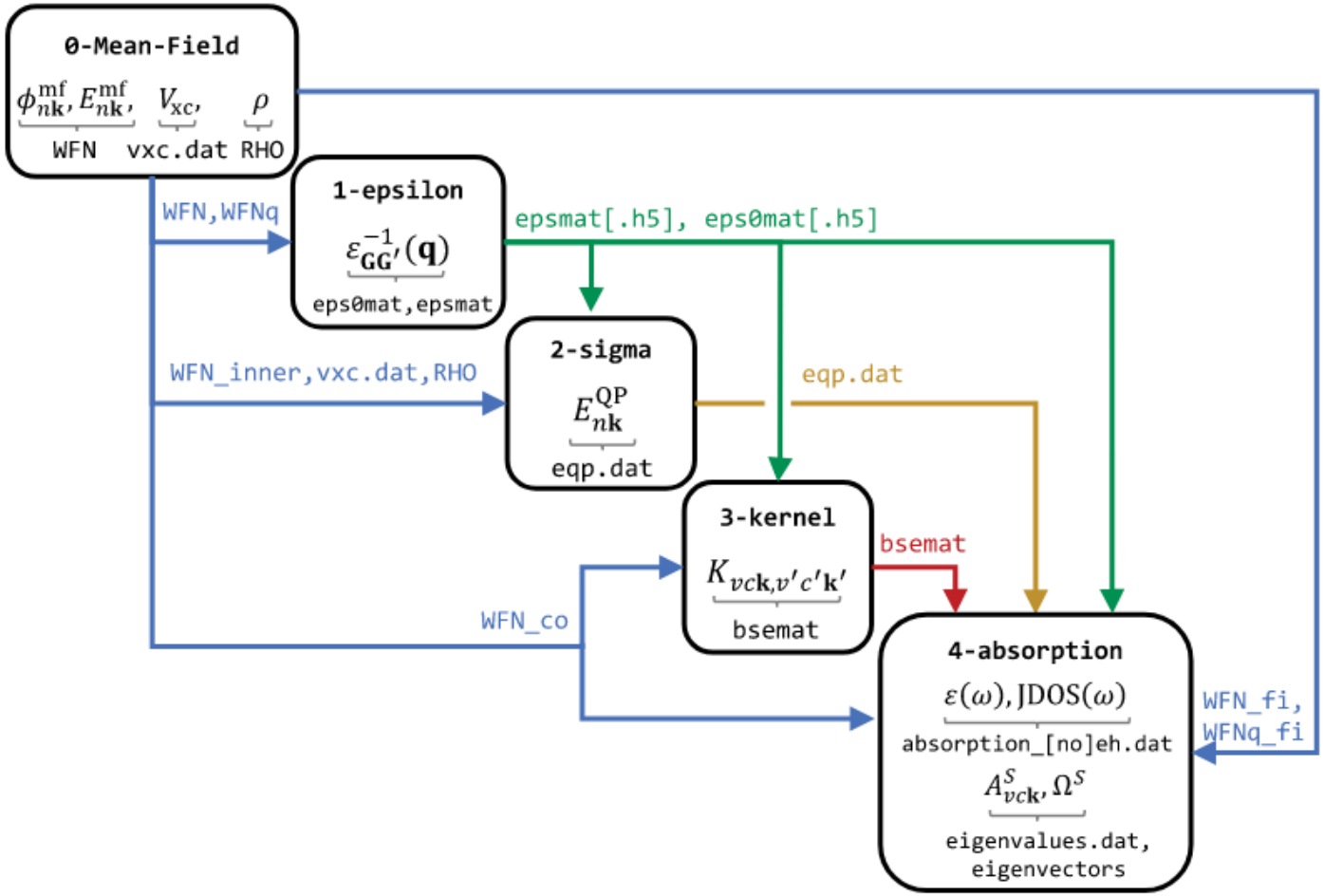
BerkeleyGW Highlights

- Supports a large set of Mean-Field codes: PARATEC, Quantum ESPRESSO, PARSEC, SIESTA, Octopus, ABINIT, RMGDFT
- Supports 3D, 2D, 1D and Molecular Systems. Coulomb Truncation
- Support for Semiconductor, Metallic and Semi-Metallic Systems
- Efficient Algorithms and Use of Libraries for (Pre-) Exascale HPC systems.
- Massively Parallel. Scales to 100,000 CPUs, and recently up to 10,000 of GPUs.

BerkeleyGW New Features (v4.0)

- Full GPU acceleration for the entire GW and GW-BSE (NVIDIA, AMD, Intel GPUs).
- Stochastic pseudoband: accelerate convergence with respect to empty states
- Portable GPU accelerated full-frequency static subspace approximation
- NV-block algorithm: overcome epsilon cubic scaling memory bottleneck
- Partial occupations for metallic systems
- Patched sampling method: accelerate **k**-point sampling convergence
- External screening (such as from a substrate or liquid environment)
- Iterative diagonalization including GPU offload of the BSE's matvec driver
- New tools: interface to Wannier90, analyzing circularly polarized optical properties, exciton-phonon coupling, and performing wavefunction self-consistent calculations

BerkeleyGW Workflow



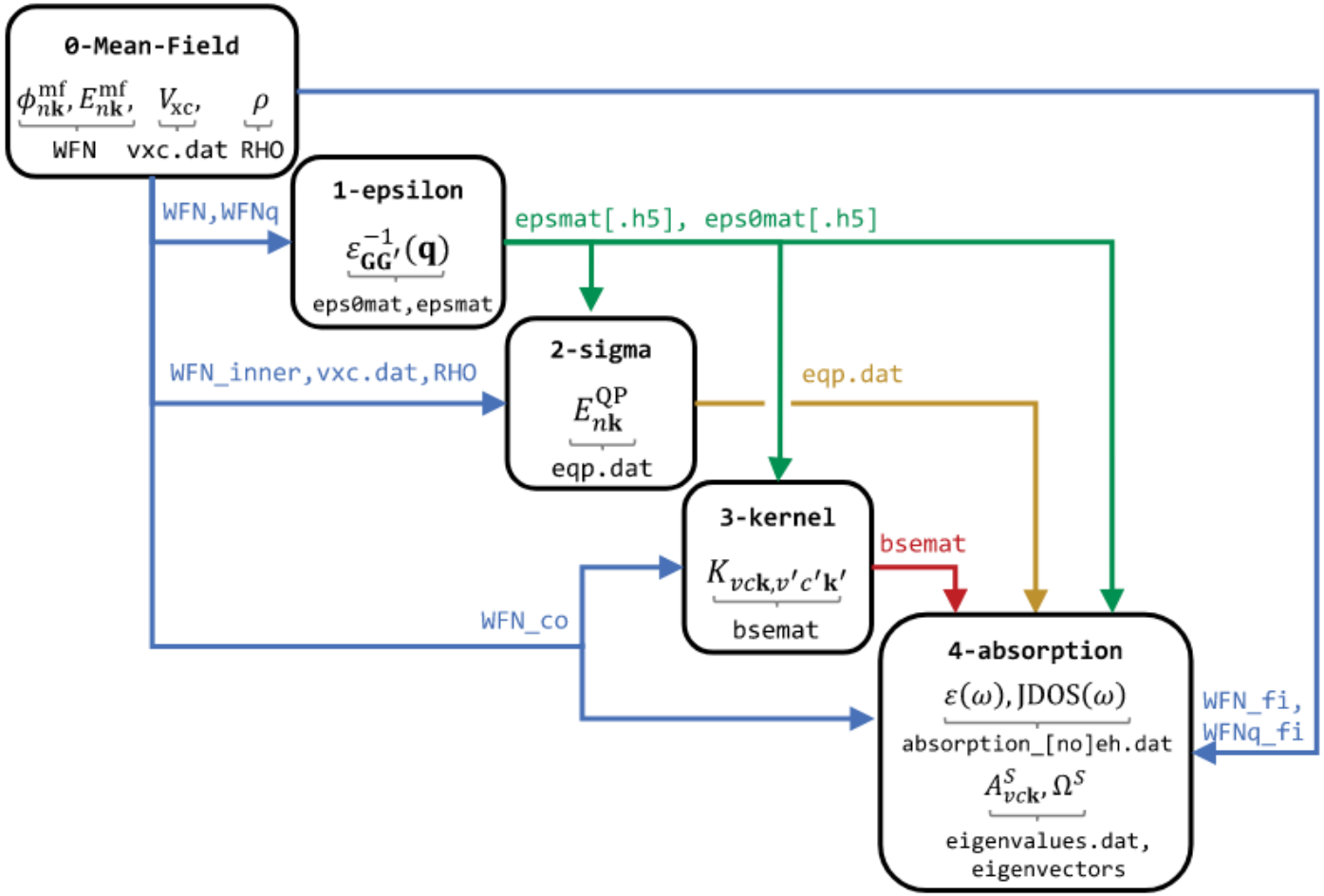
Four major modules: epsilon, sigma, kernel and absorption; *why?*

(1) Each have different data layout, computational cost and memory requirements

(2) Intermediates from each modules reused by others in multiple runs

http://manual.berkeleygw.org/4.0/overview-workflow/

BerkeleyGW Workflow

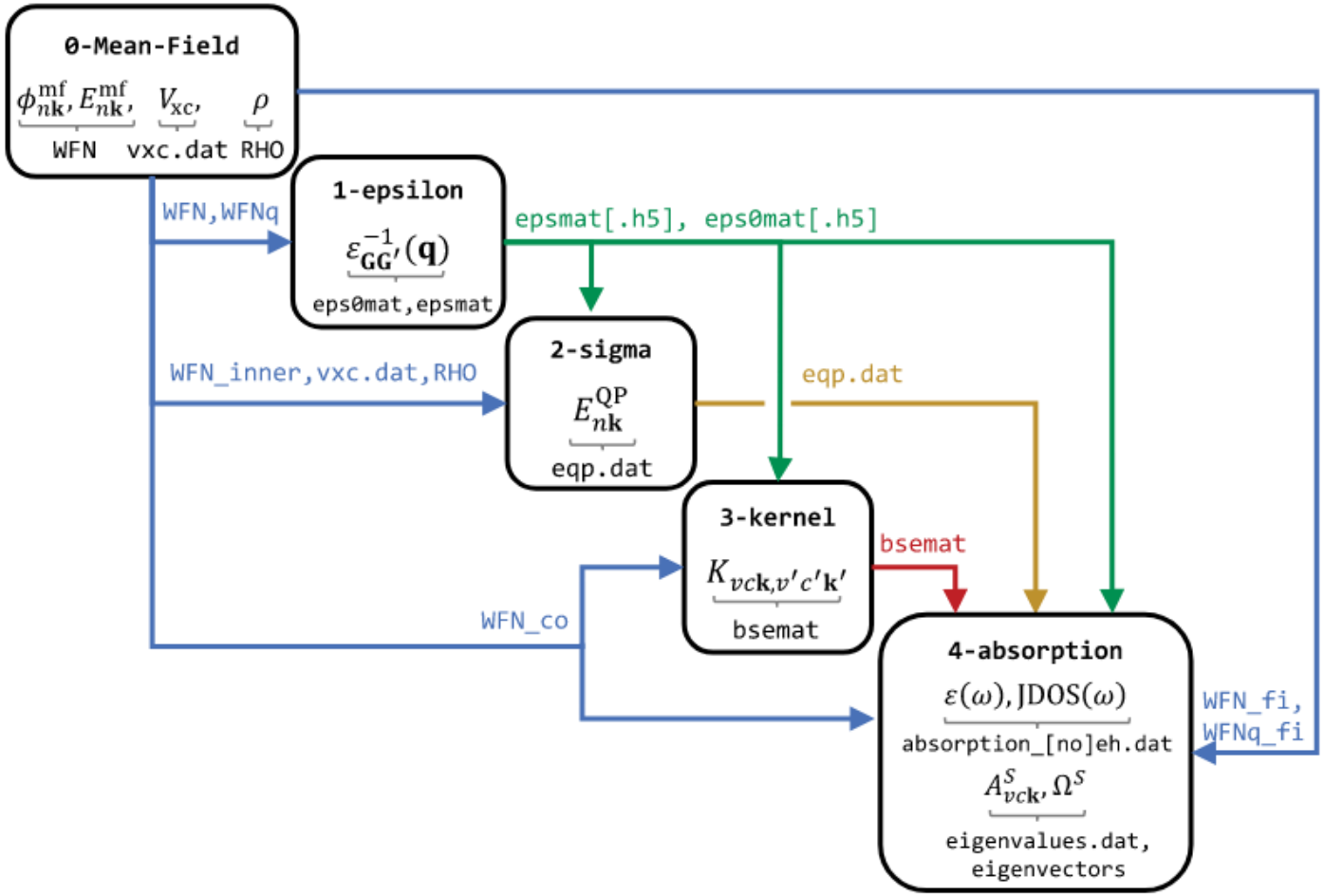


GW Workflow
epsilon + sigma

BSE Workflow
kernel + absorption

http://manual.berkeleygw.org/4.0/overview-workflow/

BerkeleyGW Workflow



http://manual.berkeleygw.org/3.0/overview-workflow/

Synopsis

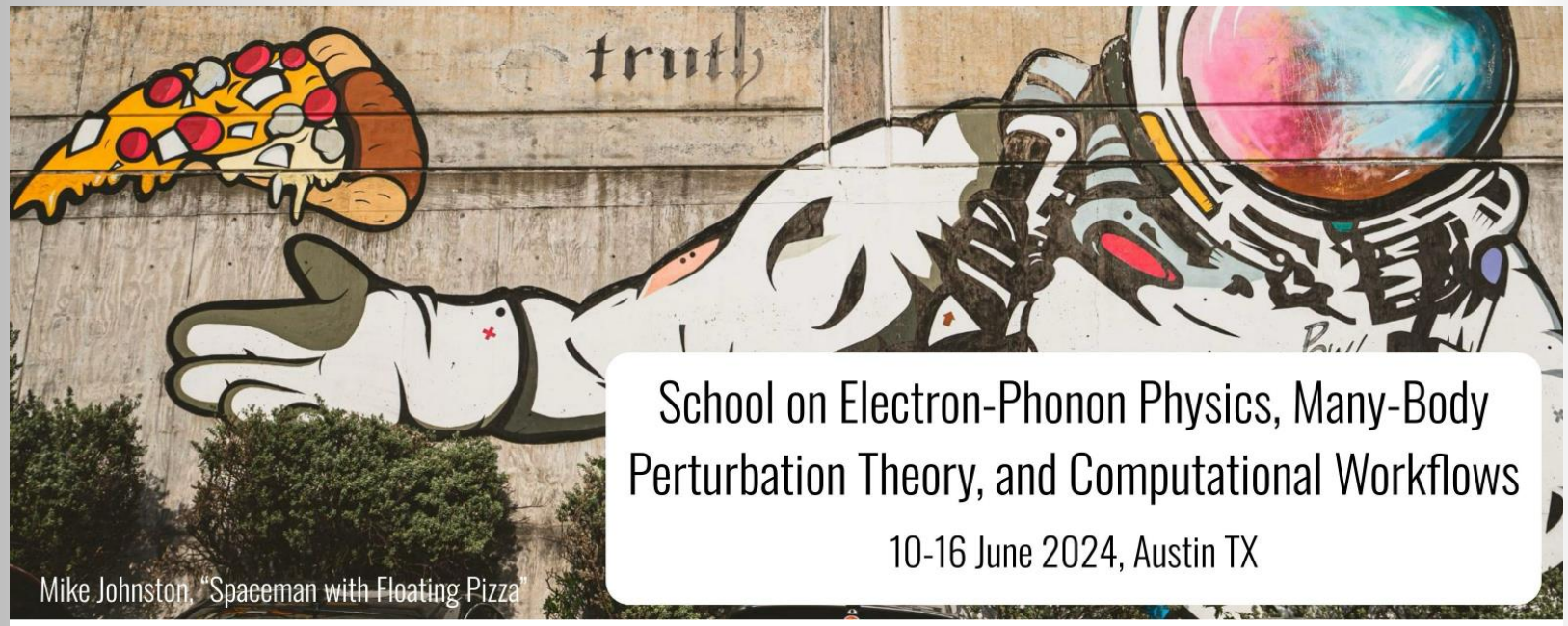
Epsilon: Generate the dielectric function and its frequency dependence

Sigma: Solve Dyson's equation for quasiparticle energies

Kernel: Compute BSE kernel matrix elements on a coarse k-point grid

Absorption: Interpolate BSE kernel matrix elements onto a fine k-point grid, diagonalize the BSE Hamiltonian, and compute optical absorption spectrum

The BerkeleyGW Modules



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The GW Workflow: Epsilon + Sigma

Dynamical properties of electrons as solution of Dyson's equation:

$$h_0(\mathbf{r})\phi_n(\mathbf{r}) + \int \Sigma(\mathbf{r}, \mathbf{r}'; E_n)\phi_n(\mathbf{r}')\mathrm{d}\mathbf{r}' = E_n\phi_n(\mathbf{r})$$

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GW Self-Energy Operator Σ : non-Hermitian, non-local, frequency dependent

(Note: In DFT, the role of self-energy is replaced by static and local $V_{\mathrm{xc}}(\mathbf{r})$)

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High GW Computational Cost in Two Major Bottlenecks:

The GW Workflow: Epsilon + Sigma

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- **Epsilon**: Inverse Dielectric Matrix **O(N^4)**

The GW Workflow: Epsilon + Sigma

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High GW Computational Cost in Two Major Bottlenecks:

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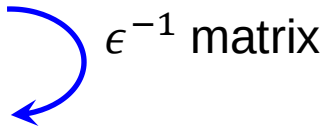
- **Sigma**: Self-Energy Matrix Elements **O(N^4)**



Epsilon: Inverse Dielectric Function (Matrix)

Three major computational steps: input $\psi_{m\mathbf{k}}$, $\epsilon_{m\mathbf{k}}$, $\{\mathbf{q}\text{-points}\}$, $\{\omega_i\}$

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1. Calculate plane-waves matrix elements (FFT's) O(N^3)

$$M^G_{ja\mathbf{k}}(\mathbf{q}) = \langle \psi_{j\mathbf{k}+\mathbf{q}} | \, e^{i(\mathbf{G}+\mathbf{q})\cdot\mathbf{r}} \, | \psi_{a\mathbf{k}} \rangle$$

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2. Calculate RPA polarizability (Matrix-Multiplication/ZGEMM) O(N^4)

$$\chi(\mathbf{q},\omega_i) = \mathbf{M}(\mathbf{q})^\dagger \mathbf{\Delta}_{ja\mathbf{k}}(\epsilon_{j\mathbf{k}}, \epsilon_{a\mathbf{k}}, \mathbf{q}, \omega)\mathbf{M}(\mathbf{q})$$

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3. Compute dielectric matrix and its inverse (ScalaPACK) O(N^3)

$$\epsilon^{-1}(\mathbf{q},\omega_i) = (I - v\chi(\mathbf{q},\omega_i))^{-1}$$

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For large scale applications the evaluation of the polarizability (CHI-0) is by far the most computationally intensive part of the calculation:
large distributed matrix-multiplication over fat and short matrices

Sigma: Quasiparticle Properties

Compute a set (100-1000) of Self-Energy matrix elements to solve the Dyson equation

$$h_0(\mathbf{r})\phi_n(\mathbf{r}) + \int \Sigma(\mathbf{r}, \mathbf{r}'; E_n)\phi_n(\mathbf{r}')\mathrm{d}\mathbf{r}' = E_n\phi_n(\mathbf{r})$$

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Each Self-Energy matrix element:

$$\Sigma_{lm}(E) = \frac{i}{2\pi}\int_0^\infty d\omega \sum_n \sum_{GG'} M_{nl}^{-G} \frac{\epsilon^{-1}_{GG'}(\omega)\cdot v(G')}{E - E_n - \omega} M_{nm}^{-G'}$$

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Frequency treatment

- Generalized Plasmon Pole (GPP) model
  - Analytical approximation to the frequency dependence
  - Require only the static dielectric matrix
- Full-Frequency (FF) model
  - Analytical integration over frequency (Contor-Deformation)
  - Require frequency dependent dielectric matrix

The BSE Workflow: Kernel + Absorption

Calculate the electron-hole excitation states for each exciton state S:

$$\left(E^{\mathsf{QP}}_{c\mathbf{k}} - E^{\mathsf{QP}}_{v\mathbf{k}}\right) A^{S}_{vc\mathbf{k}} + \sum_{v'c'\mathbf{k}'} \langle vc\mathbf{k}| \, K^{\mathsf{eh}} \, |v'c'\mathbf{k}'\rangle \, A^{S}_{v'c'\mathbf{k}'} = \Omega^{S} A^{S}_{vc\mathbf{k}}$$

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Eigenvalue Problem

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Eigenvalue Problem

GW quasiparticle energies (diagonal matrix)

Electron-Hole interaction kernel (dense matrix)

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→ Eigenvalue Problem

GW quasiparticle energies (diagonal matrix)

Electron-Hole interaction kernel (dense matrix)

The solution gives eigenvalues and eigenvectors:

- Excitation energy Ω^{S}
- Exciton wavefunction $A^{S}_{vc\mathbf{k}}$

} Calculate: exciton WFN in real space, optical response etc...

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High BSE Computational Cost in Two Major Bottlenecks:

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- **Kernel**: calculate kernel matrix elements on a coarse grid **O(N^5)**

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- Excitation energy Ω^{S}
- Exciton wavefunction $A^{S}_{vc\mathbf{k}}$

Calculate: exciton WFN in real space, optical response etc...

High BSE Computational Cost in Two Major Bottlenecks:

- **Kernel**: calculate kernel matrix elements on a coarse grid **O(N^5)**
- **Absorption**: interpolate E^{QP} and kernel matrix elements onto a fine grid and diagonalize the BSE Hamiltonian **O(N^6)**

Kernel: Kernel Matrix Elements

The electron hole interaction kernel is composed of the **screened direct** interaction and a **bare exchange** interaction $K^{\mathrm{eh}} = K^{\mathrm{d}} + K^{\mathrm{x}}$

Kernel: Kernel Matrix Elements

The electron hole interaction kernel is composed of the **screened direct** interaction and a **bare exchange** interaction $K^{\mathrm{eh}} = K^{\mathrm{d}} + K^{\mathrm{x}}$

1) Compute intermediates plane-wave matrix elements (cv, cc, vv blocks)

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

Kernel: Kernel Matrix Elements

The electron hole interaction kernel is composed of the **screened direct** interaction and a **bare exchange** interaction $K^{\mathrm{eh}} = K^{\mathrm{d}} + K^{\mathrm{x}}$

1) Compute intermediates plane-wave matrix elements (cv, cc, vv blocks)

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

2) Compute screen direct terms (ZGEMM + DotProducts) O(N^5)

$$\langle vc\mathbf{k}|K^{\mathrm{d}}|v'c'\mathbf{k}'\rangle = \sum_{\mathbf{G}\mathbf{G}'} M_{cc'}(\mathbf{k},\mathbf{q},\mathbf{G}) W_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0) M^*_{vv'}(\mathbf{k},\mathbf{q},\mathbf{G}')$$

Screen Coulom interaction W computed from the inverse dielectric function (epsilon)

3) Compute bare exchange terms (DotProducts) O(N^5)

$$\langle vc\mathbf{k}|K^{\mathrm{x}}|v'c'\mathbf{k}'\rangle = \sum_{\mathbf{G}\mathbf{G}'} M_{cv}(\mathbf{k},\mathbf{q},\mathbf{G}) v(\mathbf{q}+\mathbf{G}) \delta_{GG'} M^*_{c'v'}(\mathbf{k},\mathbf{q},\mathbf{G}')$$

Bare coulomb interaction v (diagonal)

Absorption: Interpolation

- Excitonic effects depend critically on k-point sampling -> **Fine k-grid required**
- Compute E^{QP} and kernel matrix elements on a fine grid -> **Expensive**

Interpolate E^{QP} and kernel matrix elements from a coarse onto a fine grid

Absorption: Interpolation

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Interpolate E^{QP} and kernel matrix elements from a coarse onto a fine grid

1) Compute overlaps between coarse and fine wavefunctions

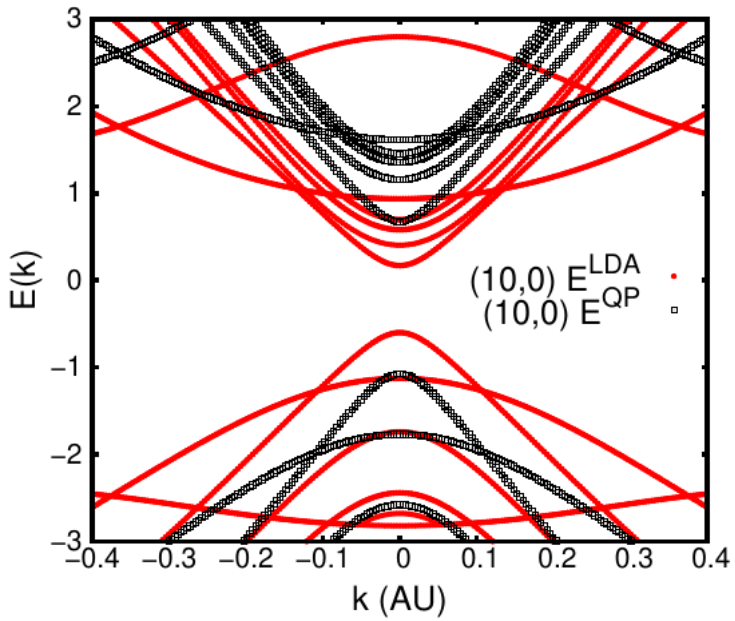
$$C^{\mathbf{k}_{\rm co}}_{n,n'} = \int d\mathbf{r}\, u_{n\mathbf{k}_{\rm fi}}(\mathbf{r}) u^*_{n'\mathbf{k}_{\rm co}}(\mathbf{r})$$

2) Use overlaps to interpolate Kernel to Fine Grid

$$\langle vc\mathbf{k}_{\rm fi}|K|v'c'\mathbf{k}'_{\rm fi}\rangle = \sum_{n_1,n_2,n_3,n_4} C^{\mathbf{k}_{\rm co}}_{c,n_1} C^{*\mathbf{k}_{\rm co}}_{v,n_2} C^{*\mathbf{k}'_{\rm co}}_{c',n_3} C^{\mathbf{k}'_{\rm co}}_{v',n_4} \langle n_2 n_1 \mathbf{k}_{\rm co}|K|n_4 n_3 \mathbf{k}'_{\rm co}\rangle$$

3) Use overlaps to interpolate E^{QP} energies without missing band crossings etc..

$$E^{\rm QP}_n(\mathbf{k}_{\rm fi}) = E^{\rm MF}_n(\mathbf{k}_{\rm fi}) + \langle \sum_{n'} |C^{\mathbf{k}_{\rm co}}_{n,n'}|^2 (E^{\rm QP}_{n'}(\mathbf{k}_{\rm co}) - E^{\rm MF}_{n'}(\mathbf{k}_{\rm co}))\rangle_{\mathbf{k}_{\rm co}}$$



Example: interpolated E^{QP} band-structure for (10,0) SWCNT

Absorption: Diagonalization

Excitation energy, exiton wavefunctions and absorption spectrum are obtained as solution of the eigenvalue problem associated to the BSE Hamiltonian

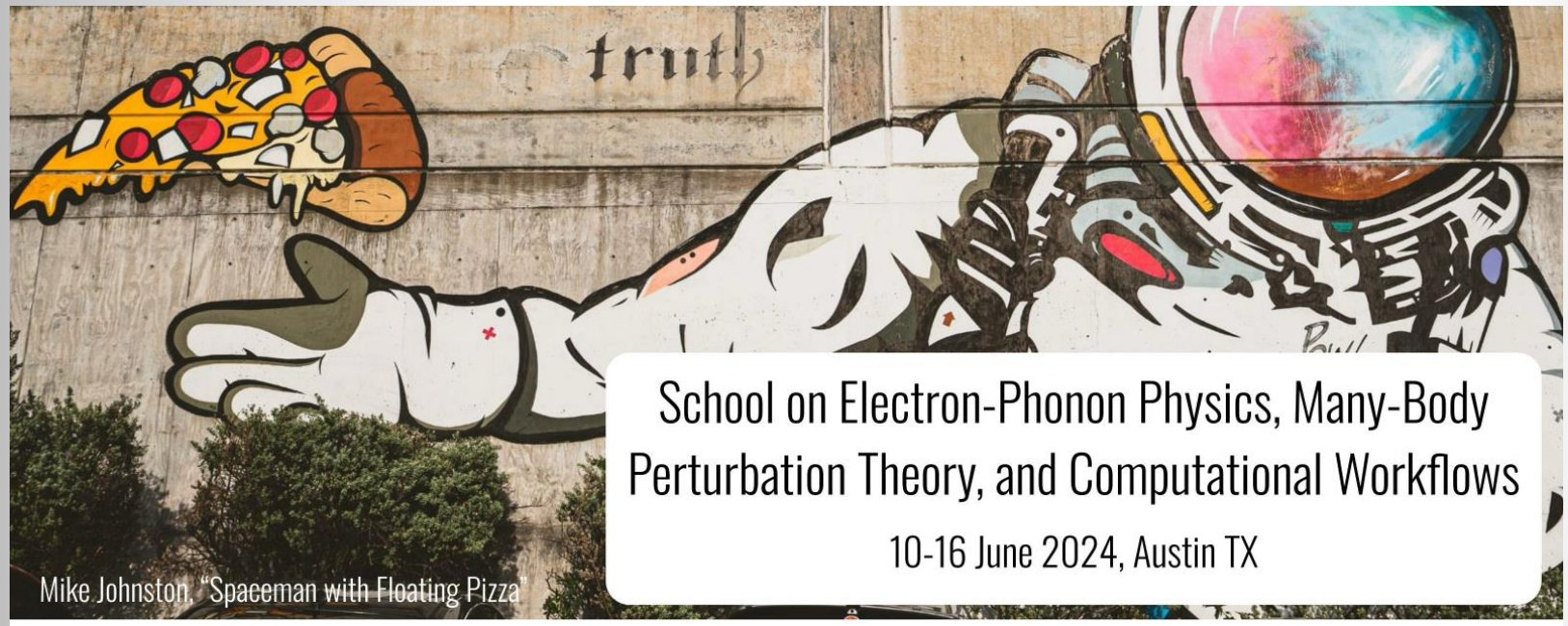
Fine **k**-grid: $$\left(E^{\mathrm{QP}}_{c\mathbf{k}} - E^{\mathrm{QP}}_{v\mathbf{k}}\right) A^S_{vc\mathbf{k}} + \sum_{v'c'\mathbf{k}'} \langle vc\mathbf{k}| K^{\mathrm{eh}} |v'c'\mathbf{k}'\rangle A^S_{v'c'\mathbf{k}'} = \Omega^S A^S_{vc\mathbf{k}}$$

Interpolated E^{QP}

Interpolated kernel matrix elements

- Direct Solver (ScalaPACK, ELPA) $O(N^6)$
  Exact diagonalization, compute all exciton states
- Iterative Solvers (PRIMME)
  Exact diagonalization, compute selected lowest exciton states
- Haydock-Recursion Method (haydock.cplx.x) $O(N^4)$
  Computes only the absorption spectra

Summary


truth
School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows
10-16 June 2024, Austin TX
Mike Johnston, "Spaceman with Floating Pizza"
U.S. DEPARTMENT OF ENERGY
NSF
TACC
TEXAS ADVANCED COMPUTING CENTER
ODEN

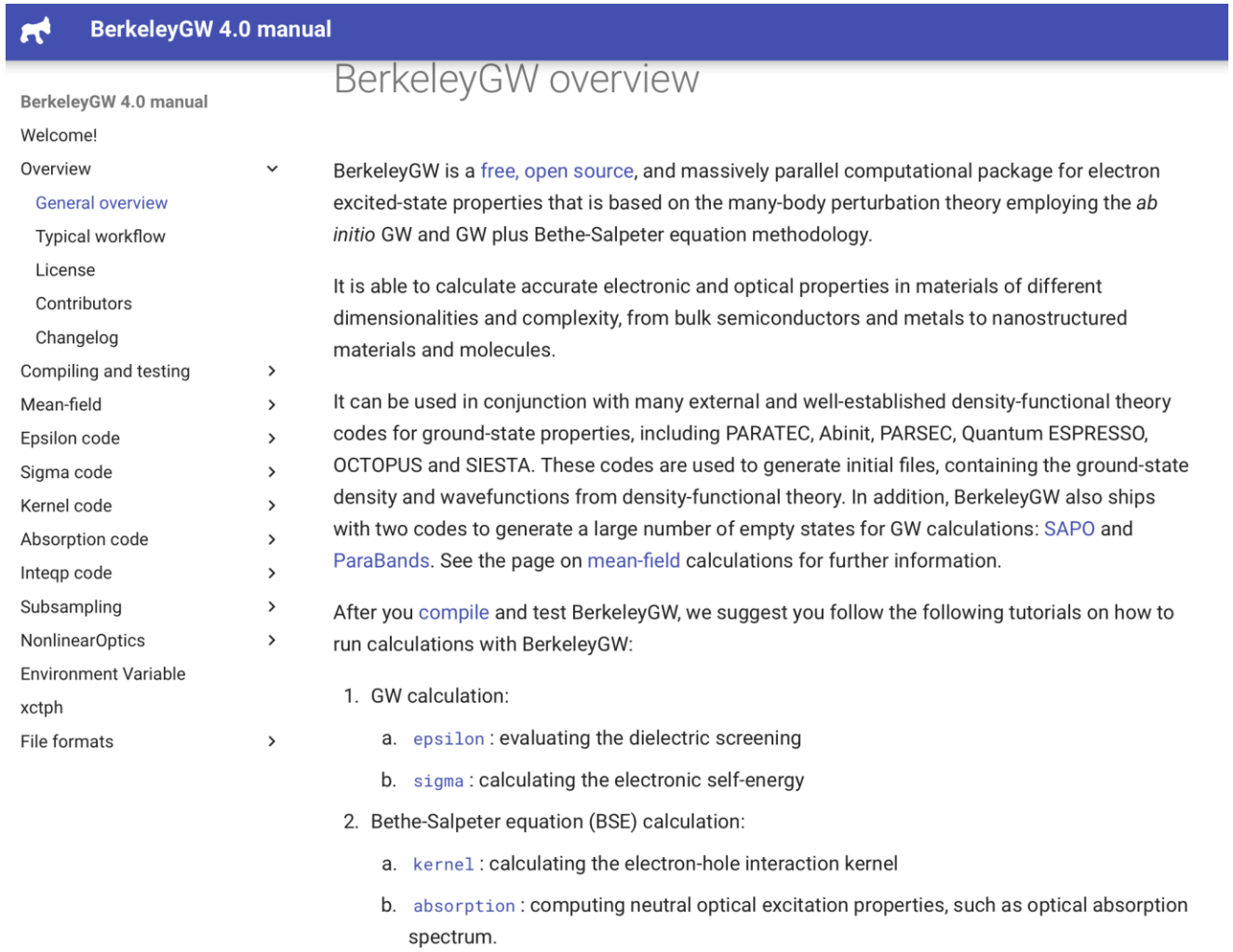
BerkeleyGW Summary

- Overview of the BerkeleyGW software package, software vision design, structure and main workflow

- General algorithms, parallelization strategies and computational motifs

- More specific details about the structures of the four major modules
  - Epsilon: Generate the dielectric function and its frequency dependence
  - Sigma: Solve Dyson's equation for quasiparticle energies
  - Kernel: Compute BSE kernel matrix elements on a coarse k-point grid
  - Absorption: Interpolate BSE kernel matrix elements on a fine k-point grid, diagonalize the BSE Hamiltonian, and compute optical absorption spectrum

BerkeleyGW Useful Resources



- The BerkeleyGW online manual http://manual.berkeleygw.org/4.0/
- BerkeleyGW-Help mailing list: help@berkeleygw.org

Papers about implementation:

- **MPI and overview**: J Deslippe et al, *Computer Physics Communications* 183 (6), 1269-1289
- **Multi-core/OpenMP**: M Del Ben et al, *Computer Physics Communications* 235, 187-195
- **GPU**: M Del Ben et al, *International Conference for High Performance Computing, Networking, Storage and Analysis*, 2020, pp. 1-11

Follow instructions in: `Thur.6.DelBen.pdf`

Setup Instructions

To run this tutorial we will use an interactive session on Stampede3. First copy and extract the tutorial folder:

```
$ cd $SCRATCH
$ mkdir EP-SCHOOL_BGW ; cd EP-SCHOOL_BGW
$ cp /work2/06868/giustino/EP-SCHOOL/Thur.6.DelBen.tar .
$ tar -xvf Thur.6.DelBen.tar
```

To start the **interactive session** use the following command:

```
$ /work2/05193/sabyadk/stampede3/EPWSchool2024/BGW/bgw_interactive
```