MolSSI Workshop – ELSI Conference:
"Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory"
Richmond, Virginia – 26th August 2018

Recent Advancements in ELPA: Best Practices in Real Applications

Danilo Simoes Brambila and Christian Carbogno

MAX-PLANCK-GESELLSCHAFT

Fritz-Haber-Institut
der Max-Planck-Gesellschaft,
Berlin - Germany

ELPA-AEO is an *Application-Driven* Team-Effort

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Code Testing, Benchmarking, and Validation in *Real Applications*

Fritz Haber

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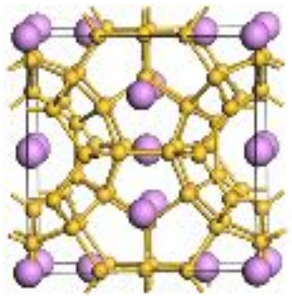
The ab initio molecular simulations package

FHI aims

Electronic Structure Theory
Density Functional Theory

Solid State Physics & Material Science



Thermoelectric Clathrates

A. Bhattacharya, *et al.*,
Phys. Rev. Lett. **118**, 236401 (2017).

Thermoelectric Boron Carbides

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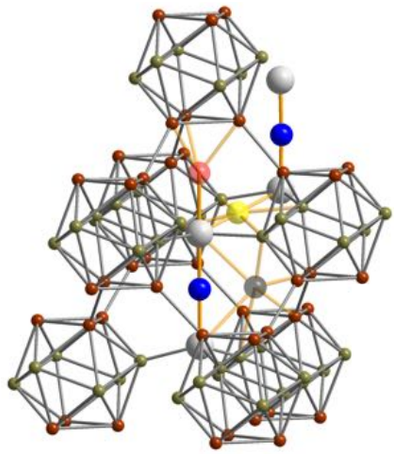

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Solid State Physics & Material Science

Quantum Chemistry

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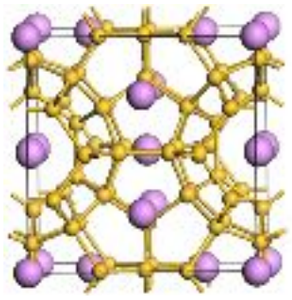

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Free Energy Barriers for H_2O on TiO_2

T. Stecher, *et al.*,
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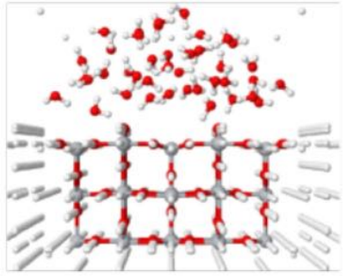

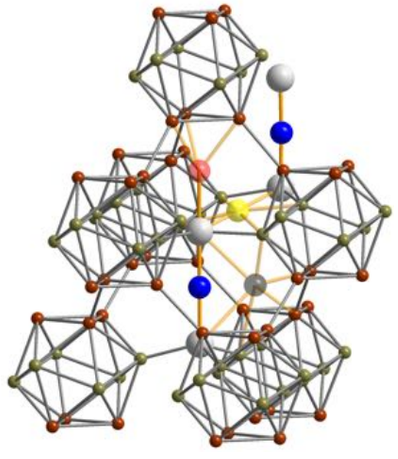

Functional Boron Carbides

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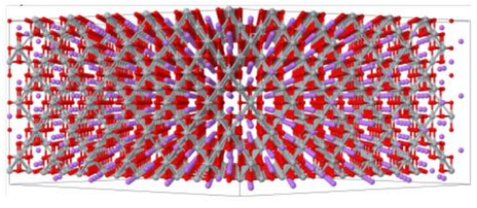

Occupations Disorder in $Li_4Ti_5O_{12}$ Batteries

H. Heenen *et al.*,
Nano Letters **17,** 3884 (2017).

Christoph Scheurer

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Algorithmic Developments & Advancements

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Code Testing, Benchmarking, and Validation in *Real Applications*

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Bruno Lang

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Massive Parallel Numerical Implementation

INFORMATICS V

TUM

Architecture-specific Optimization, Adaption, and Code Maintenance

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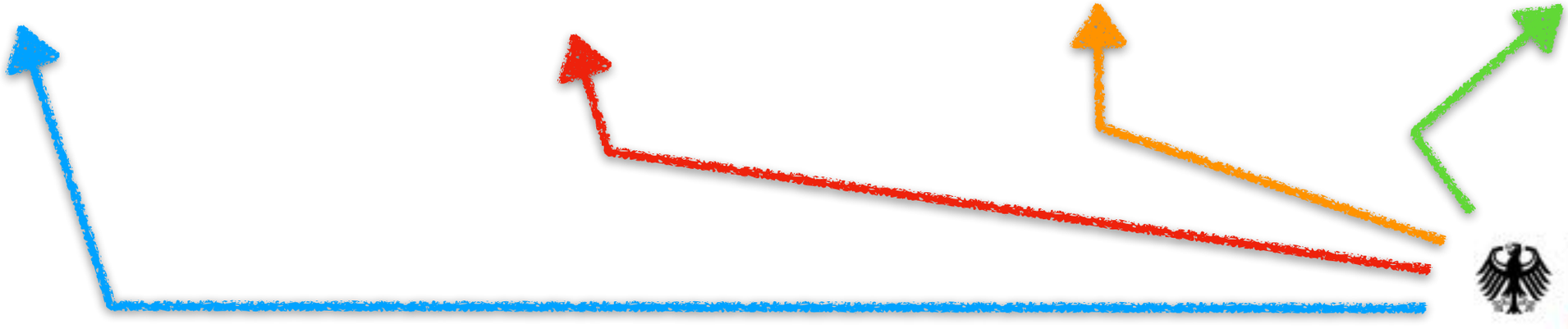

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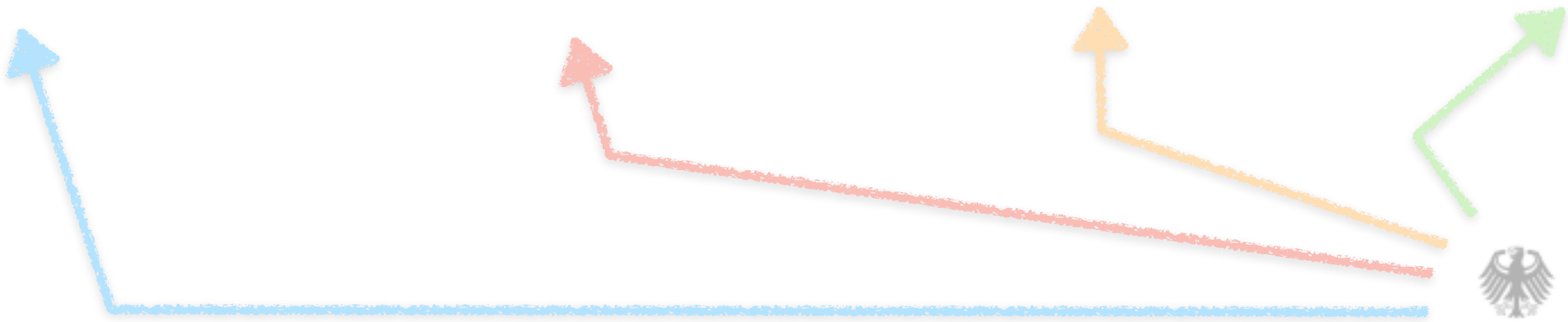

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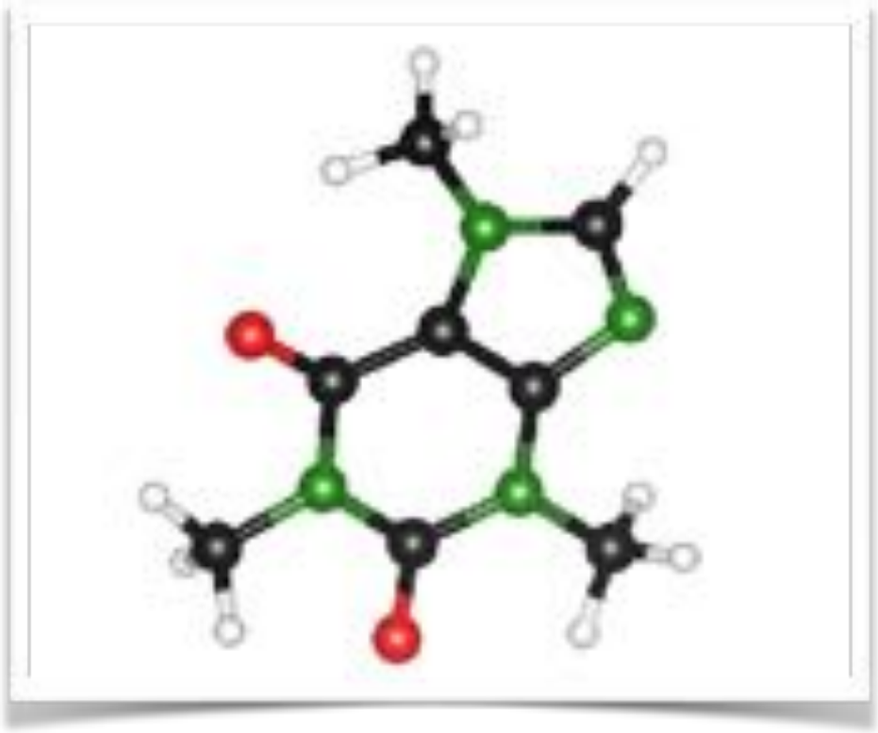
Electronic Structure Theory 101



INPUT

M three-dimensional vectors $\boldsymbol{R_I}$ defining
the **position** of the individual nuclei *I* in space

M values Z_I for the charge defining
the **chemical species** of the nuclei *I*

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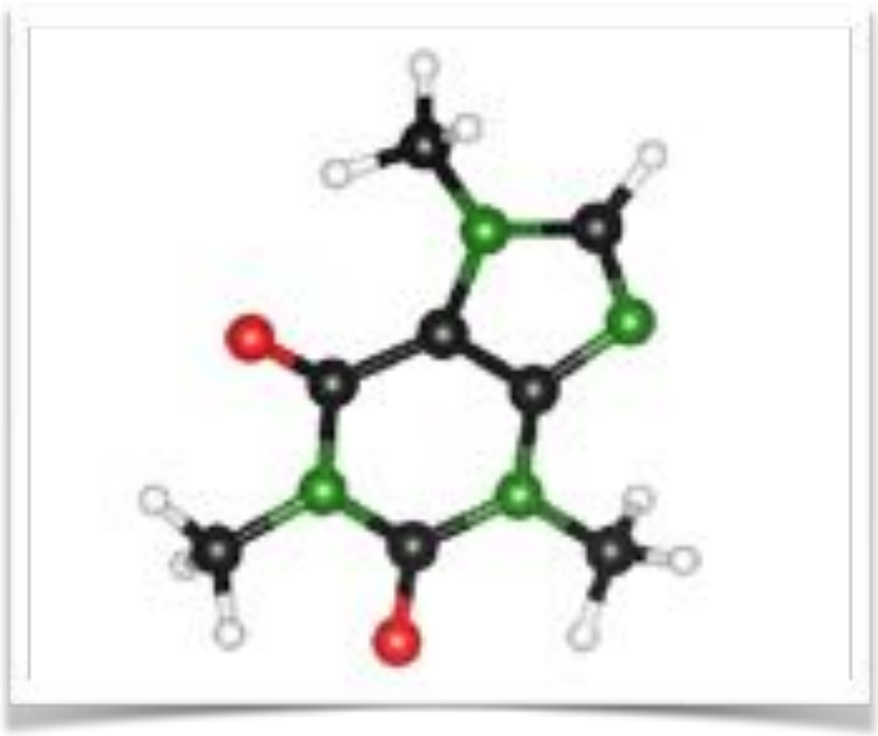

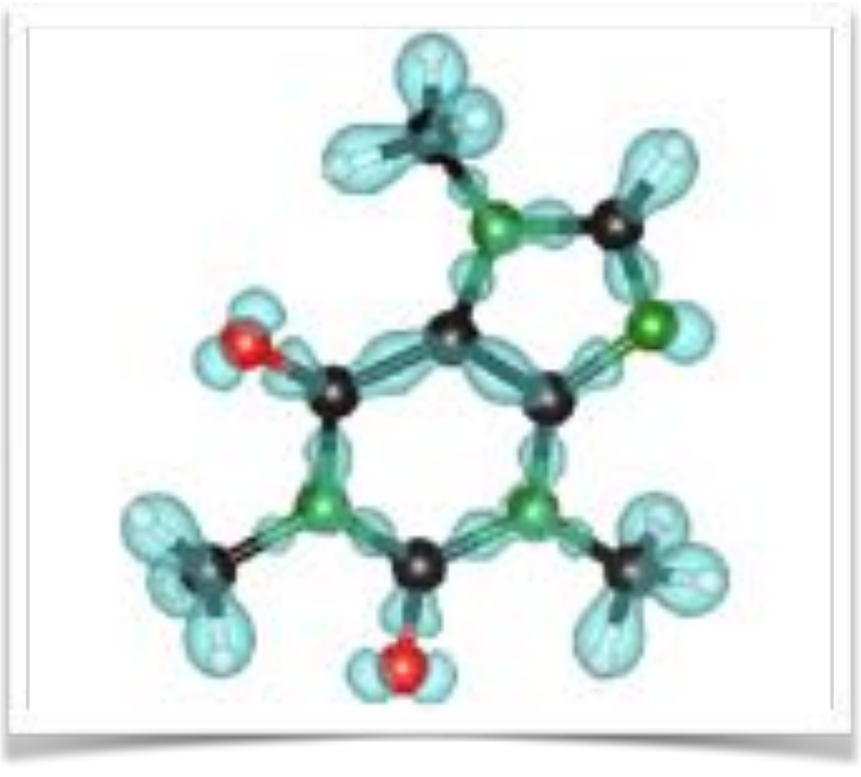

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Electronic Structure Theory

OUTPUT

Spatial distribution of *N* **electrons**, e.g.,
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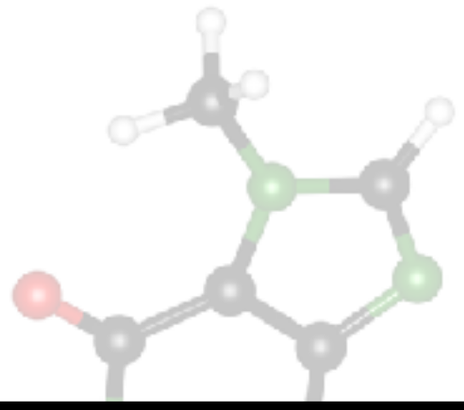
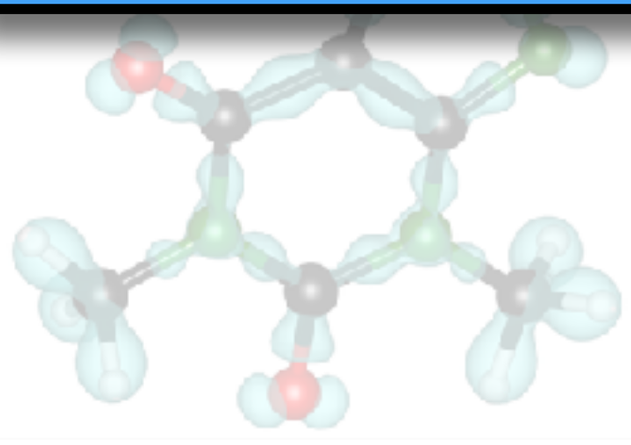
$$N = \int n(\mathbf{r}) d\mathbf{r}$$

in ***density-functional theory*** (1998 Nobel Prize).

Electronic Structure Theory 101



Eigenvalue Problem Computationally Dominant!



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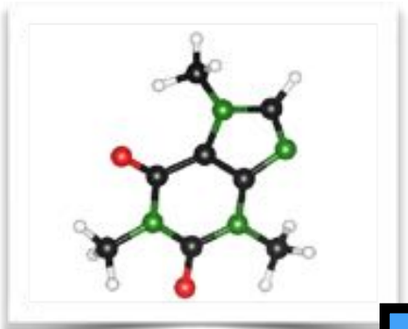
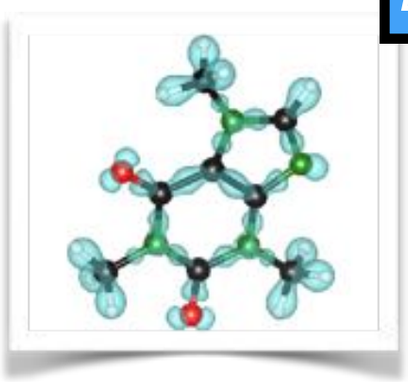


Geometry & **Species**

Electronic Structure Theory



Electronic Structure

The Self-Concistency Cycle

Construct Matrix $\underline{\boldsymbol{A}}[n_i(\boldsymbol{r})]$ & $\underline{\boldsymbol{B}}$

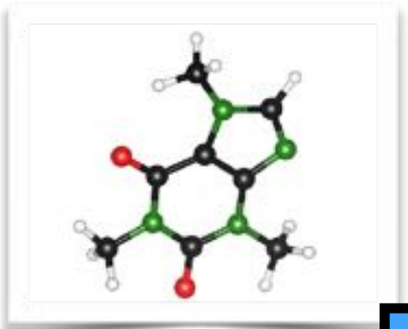
Solve **Eigenvalue Problem**
$\underline{\boldsymbol{A}}[n_i(\boldsymbol{r})]\ \boldsymbol{x} = \lambda\ \underline{\boldsymbol{B}}\ \boldsymbol{x}$
to obtain $n_{i+1}(\boldsymbol{r})$

Self-Consistency achieved?

No $n_{i+1}(r) \rightarrow n_i(r)$

Yes

Electronic Structure Theory 101



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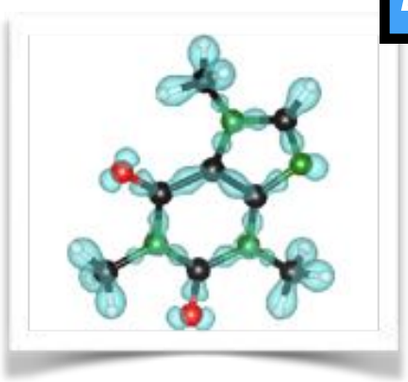

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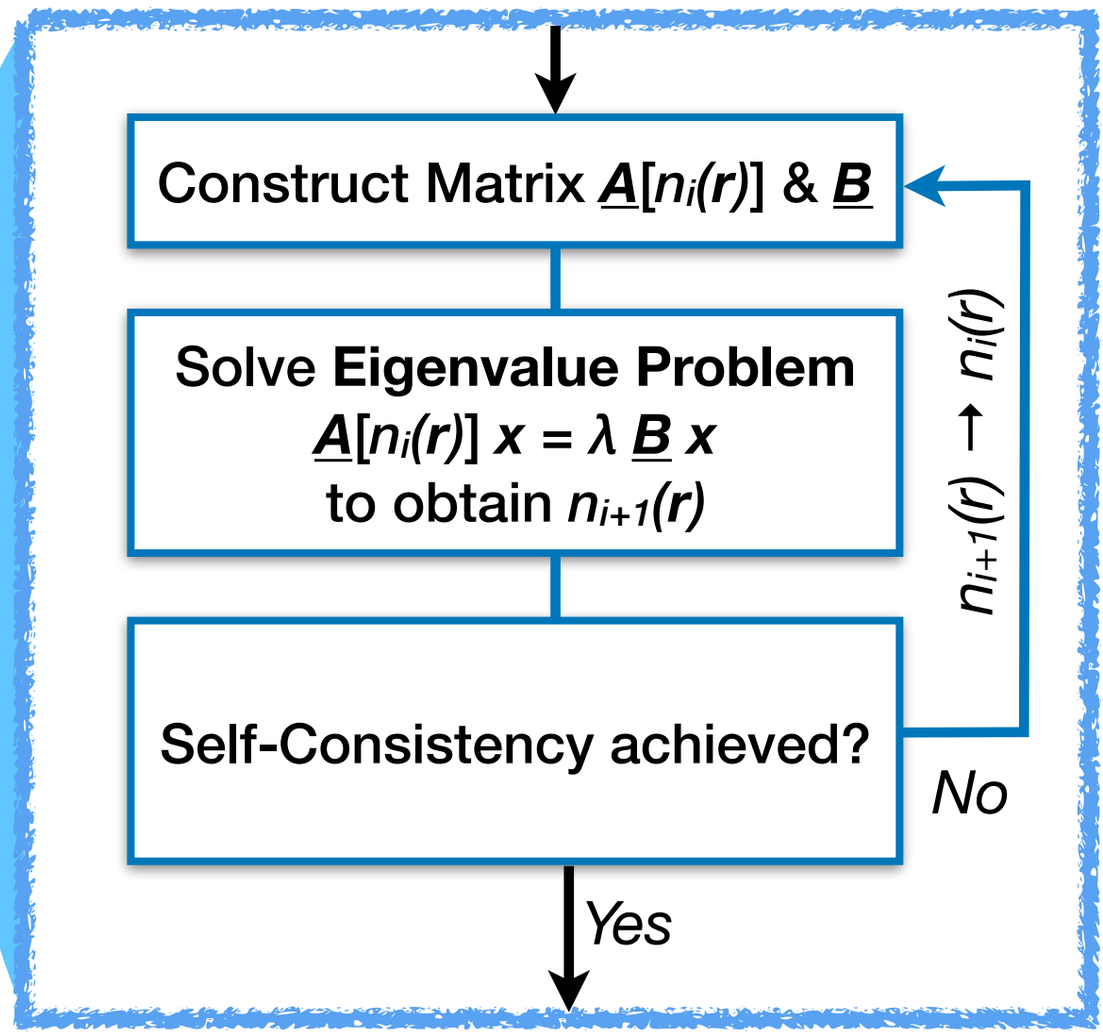
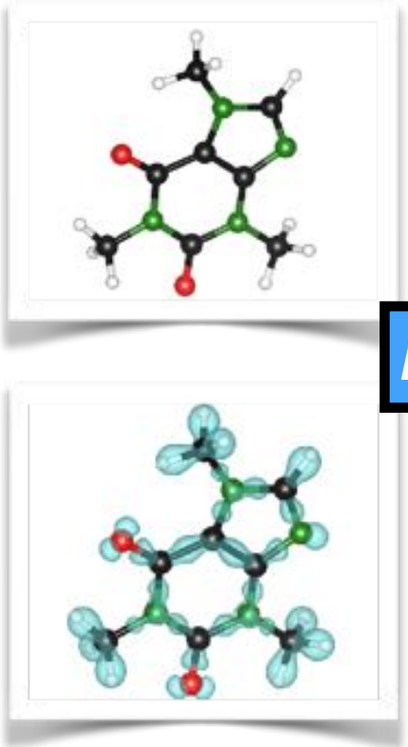


A series of different eigenproblems with *same* $\underline{B}$ are solved one after another.

Electronic Structure Theory 101

Update Geometry



Geometry & Species

Electronic Structure Theory

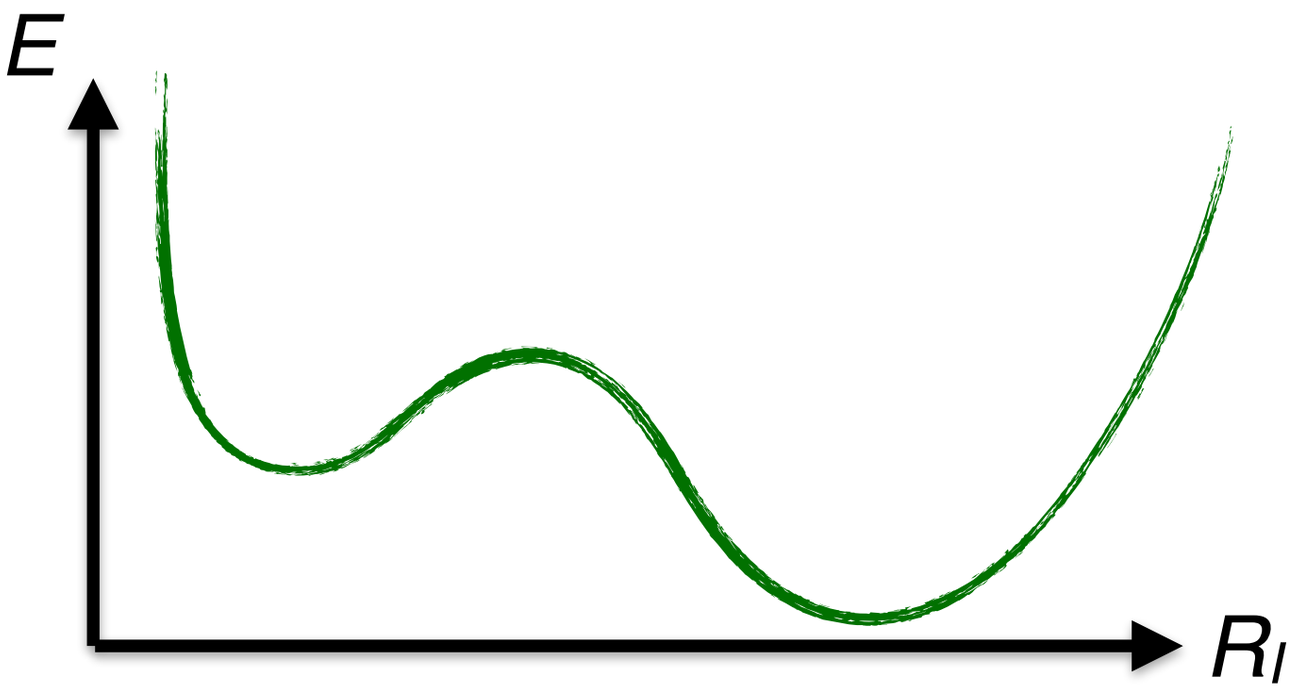
Electronic Structure

Compute Energy *E* and Forces *F* on Atoms

⇒ Materials' Properties

A series of different, but similar electronic structure theory problems are solved one after another.

Exploring the Potential-Energy Surface



The *Potential-Energy Surface (PES)* describes the **dependence** of the **energy** *E* on the *M* **nuclear positions** $\boldsymbol{R_I}$.

The *Potential-Energy Surface (PES)* determines the **dynamics** of the **nuclei**.

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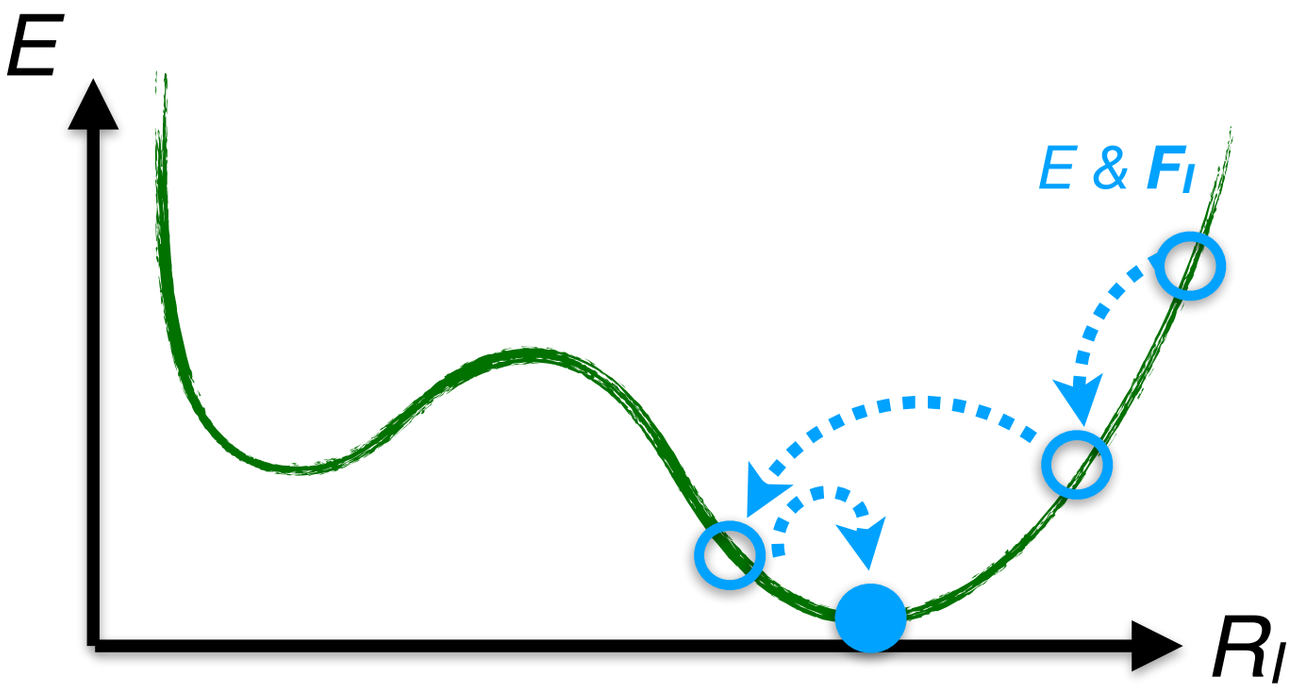

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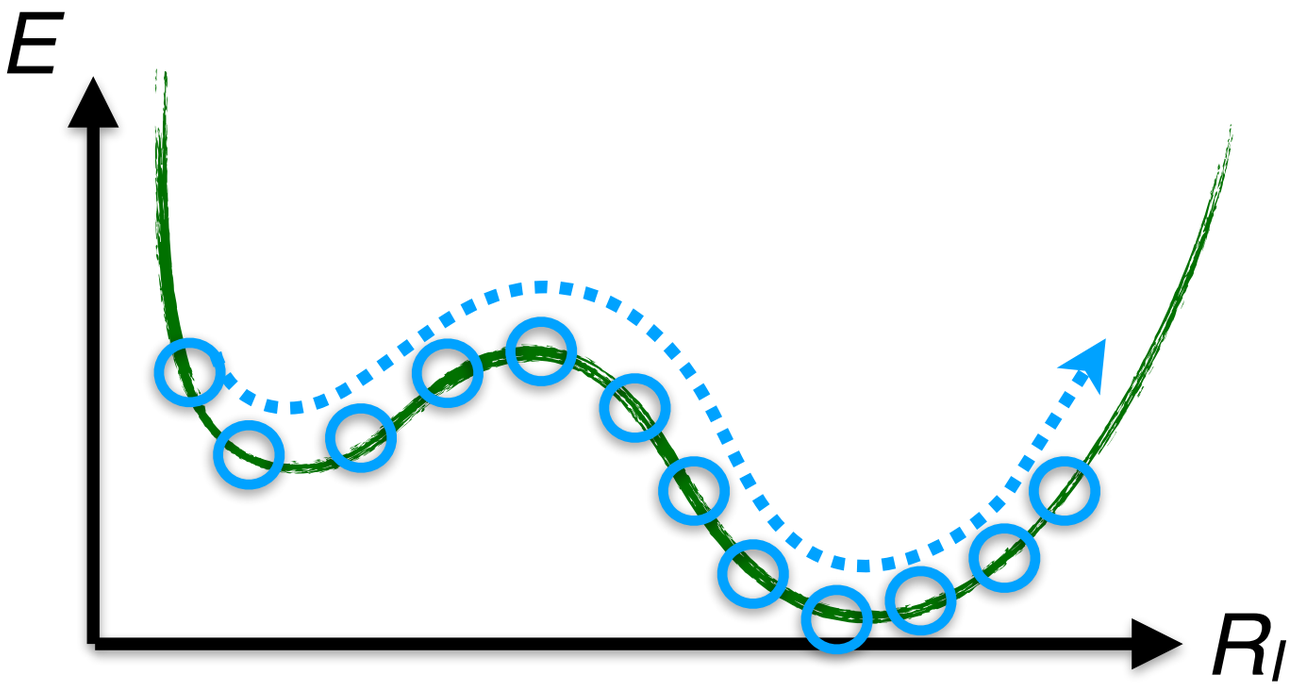
- **Iterative Minimization ("Relaxation"):** Find the *minima* of the PES

  ⇒ Most probable configuration(s), static properties, stabilities,…

Exploring the Potential-Energy Surface



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- ***Ab initio* Molecular Dynamics:** Iteratively integrate the equations of motion

  ⇒ **Quantitative explore the full Dynamics!**

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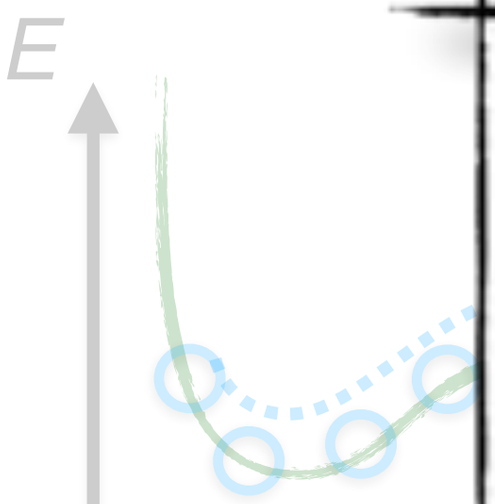

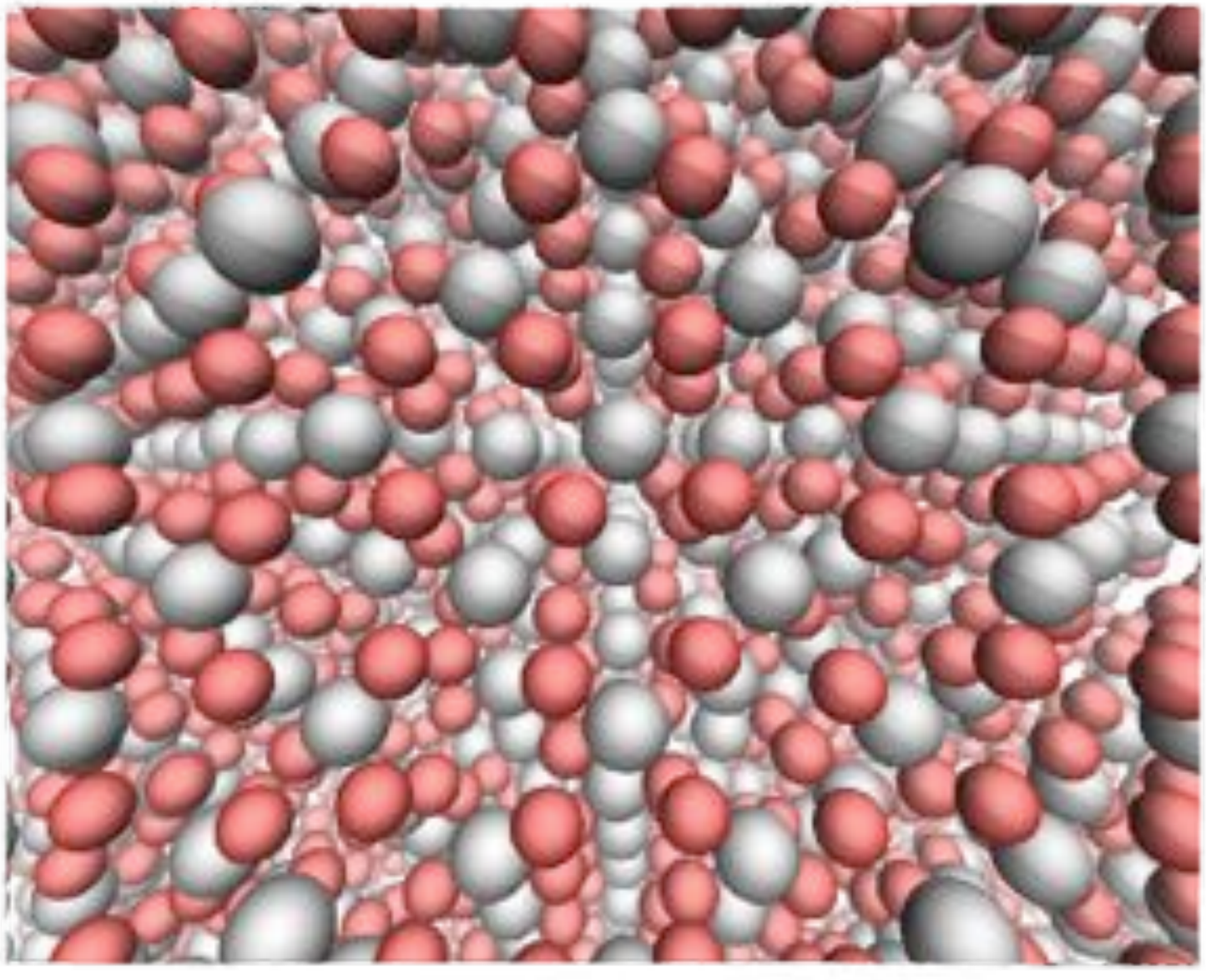

Surface (PES)

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Surface (PES)

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- **Iterative Mini**
- **Transition-Sta** **inima of the PES**
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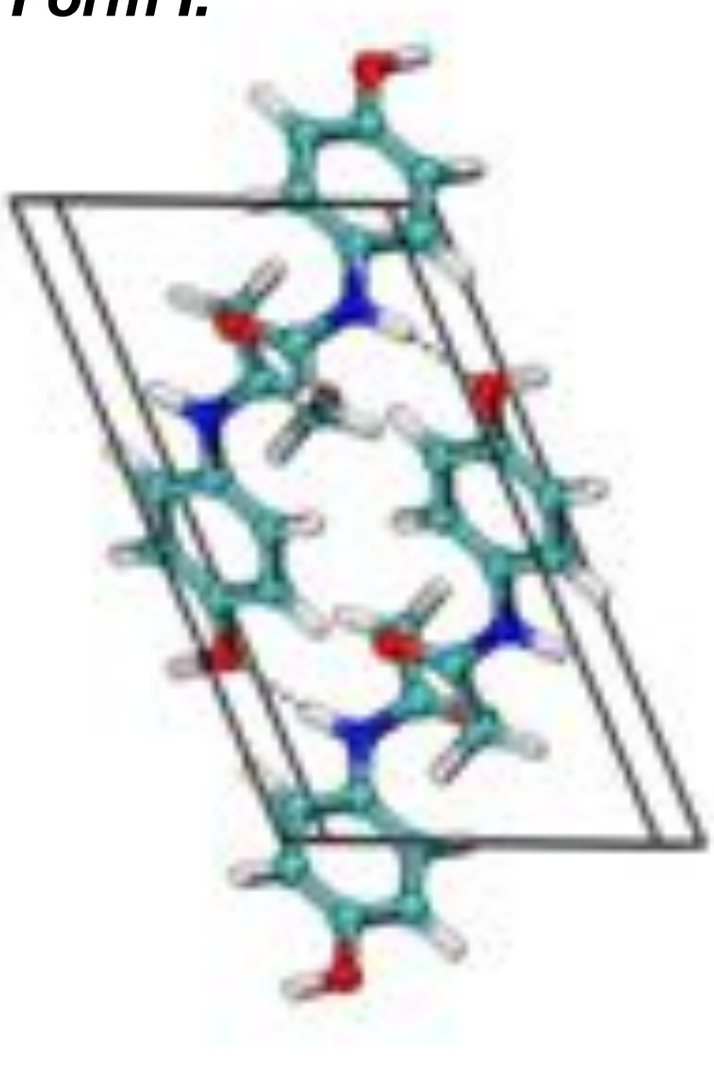
Example A: Paracetamol

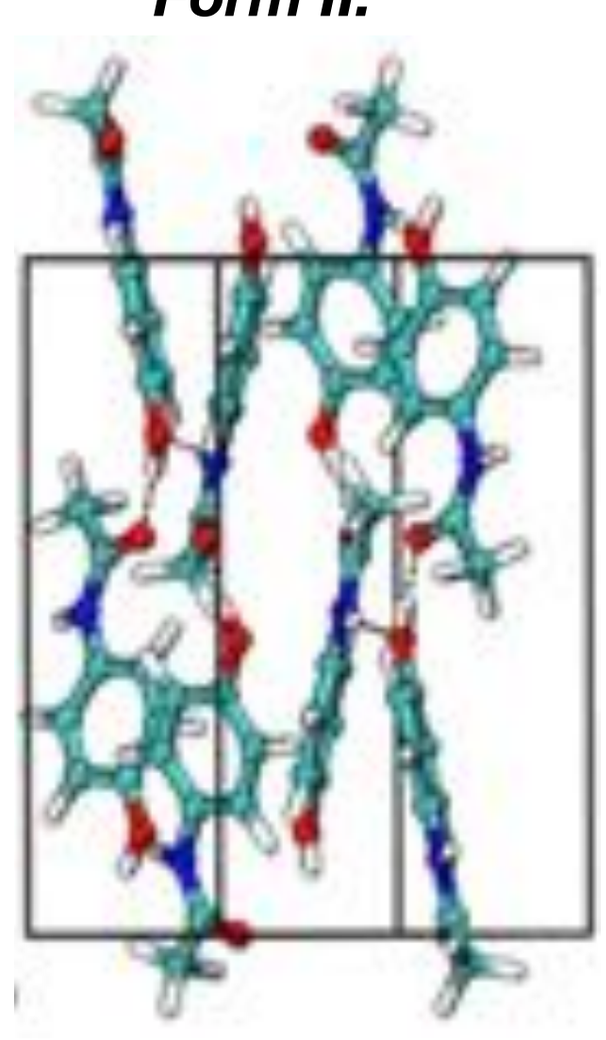
H. Shang, et al., New J. Phys., ***DOI:****10.1088/1367-2630/aace6d*

Paracetamol exists in **two** different **polymorphs:**
"Same paracetamol molecules, different crystalline order"

Form I:



Form II:



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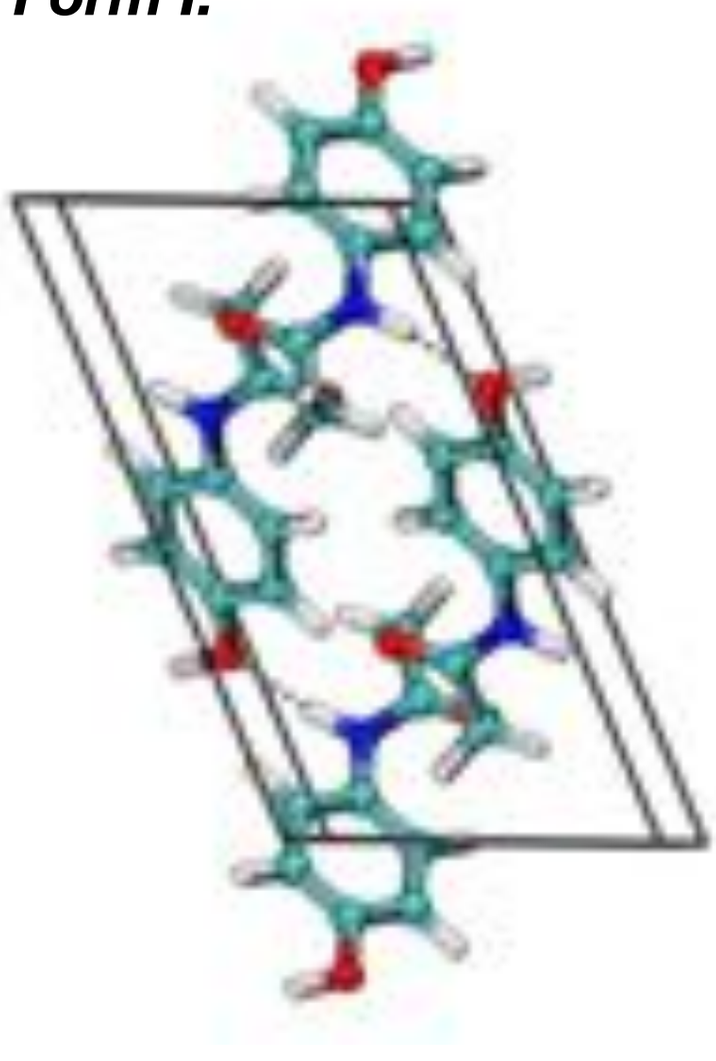

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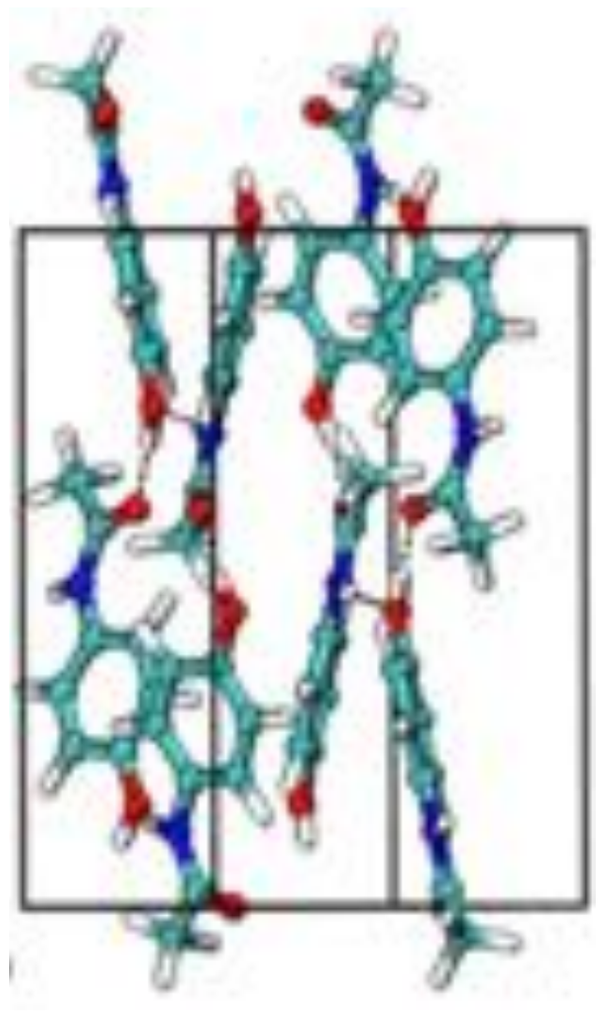
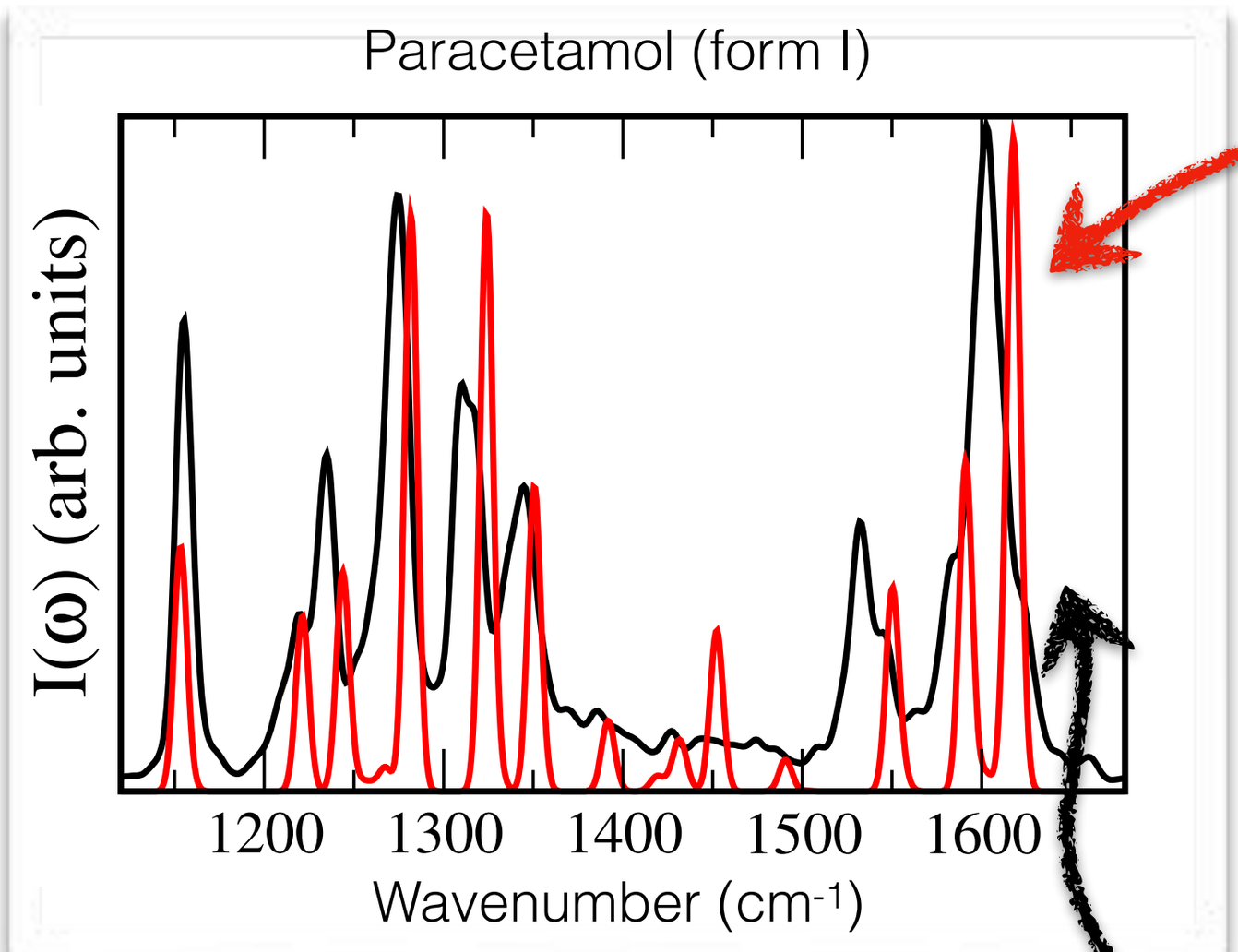


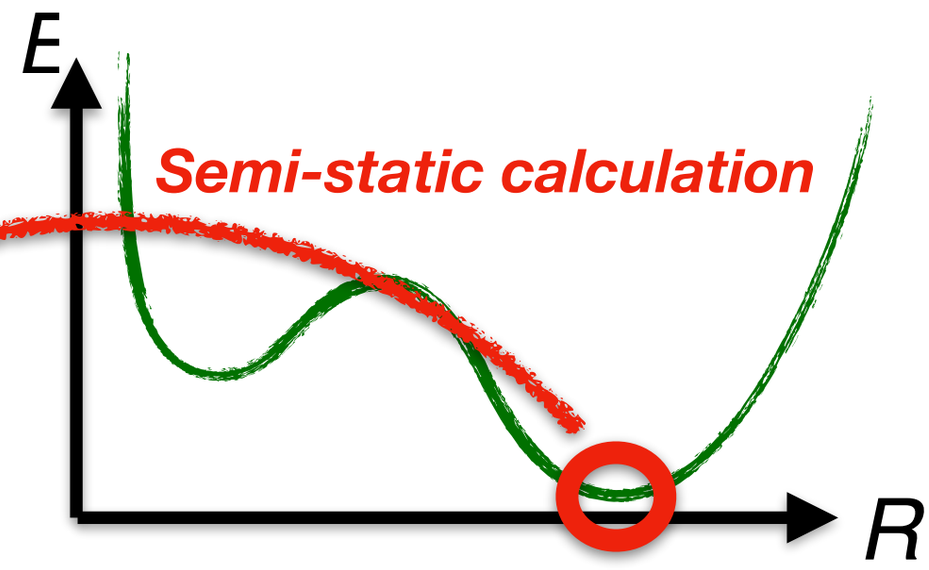
The two forms differ in their physo-chemical properties, e.g., *solubility.*

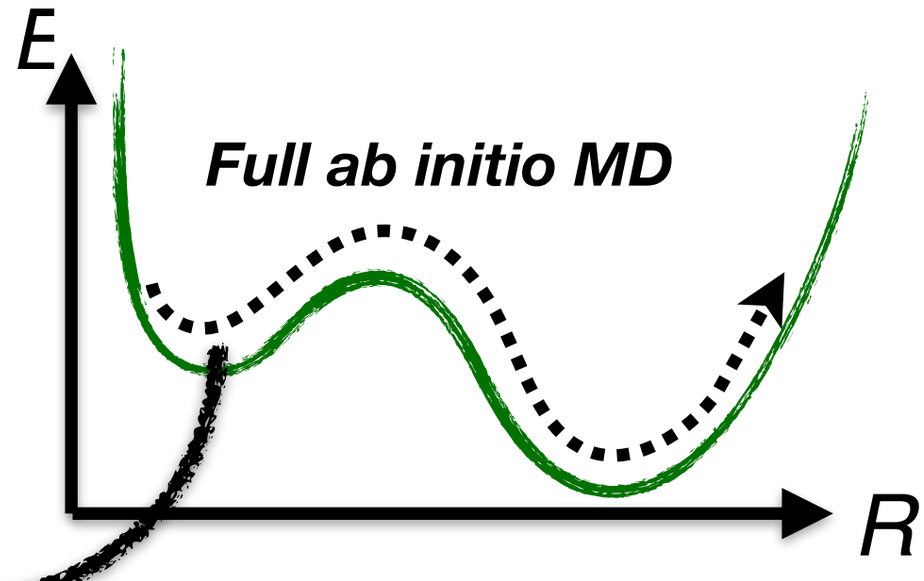
Example A: Paracetamol

H. Shang, et al., New J. Phys. **20**, 073040 (2018).

Raman Spectra *describing the response to* ***electric fields*** *typically used to differentiate between* ***two polymorphs.***







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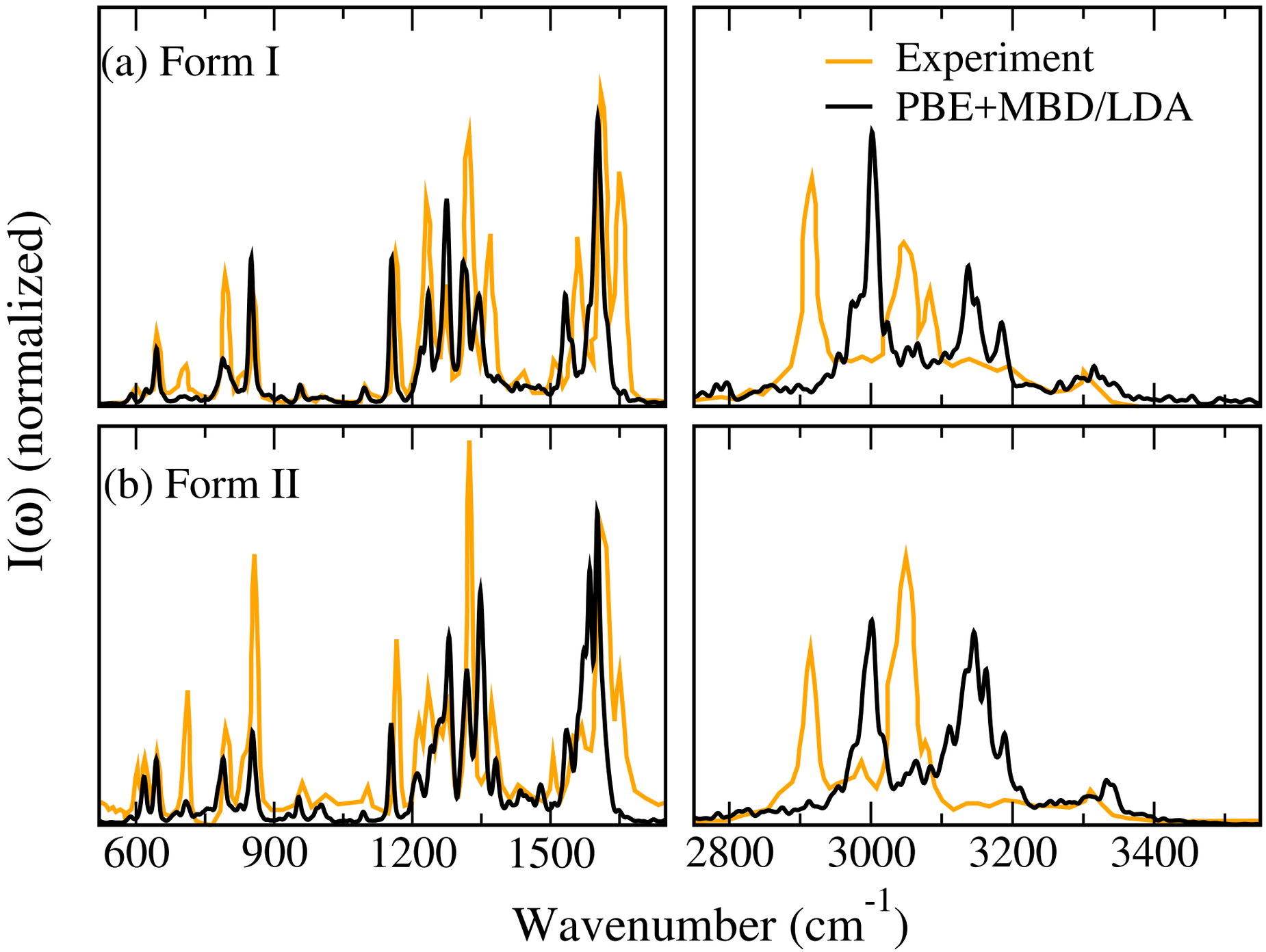
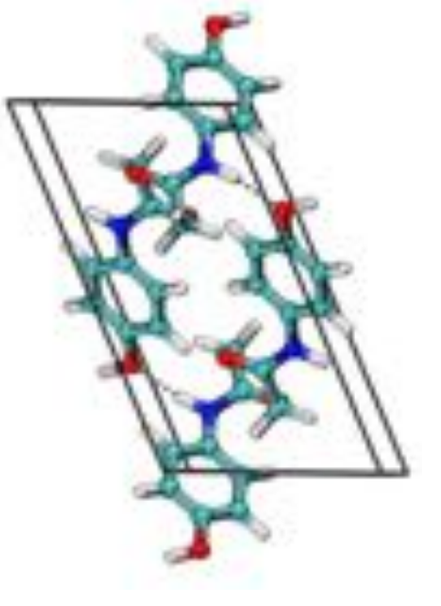
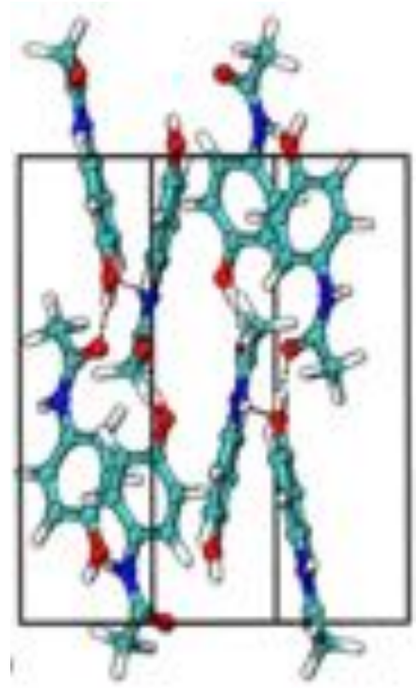
Exp.: J. B. Nanubolu and J. C. Burley. *Mol. Pharm.*, **9**,1544 (2012).

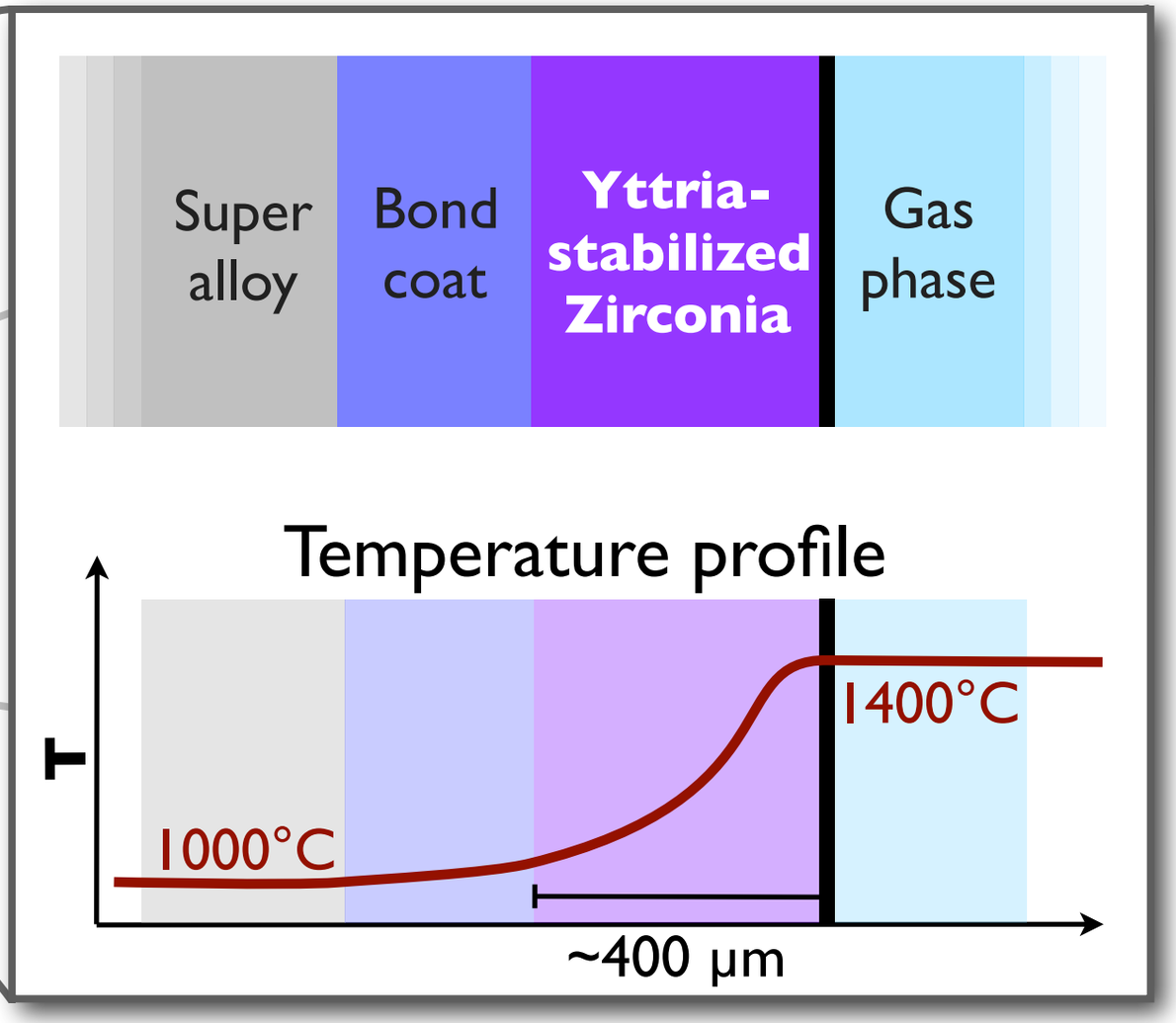






Example B: Thermal-Barrier Coatings

CFM 56-7 airplane engine

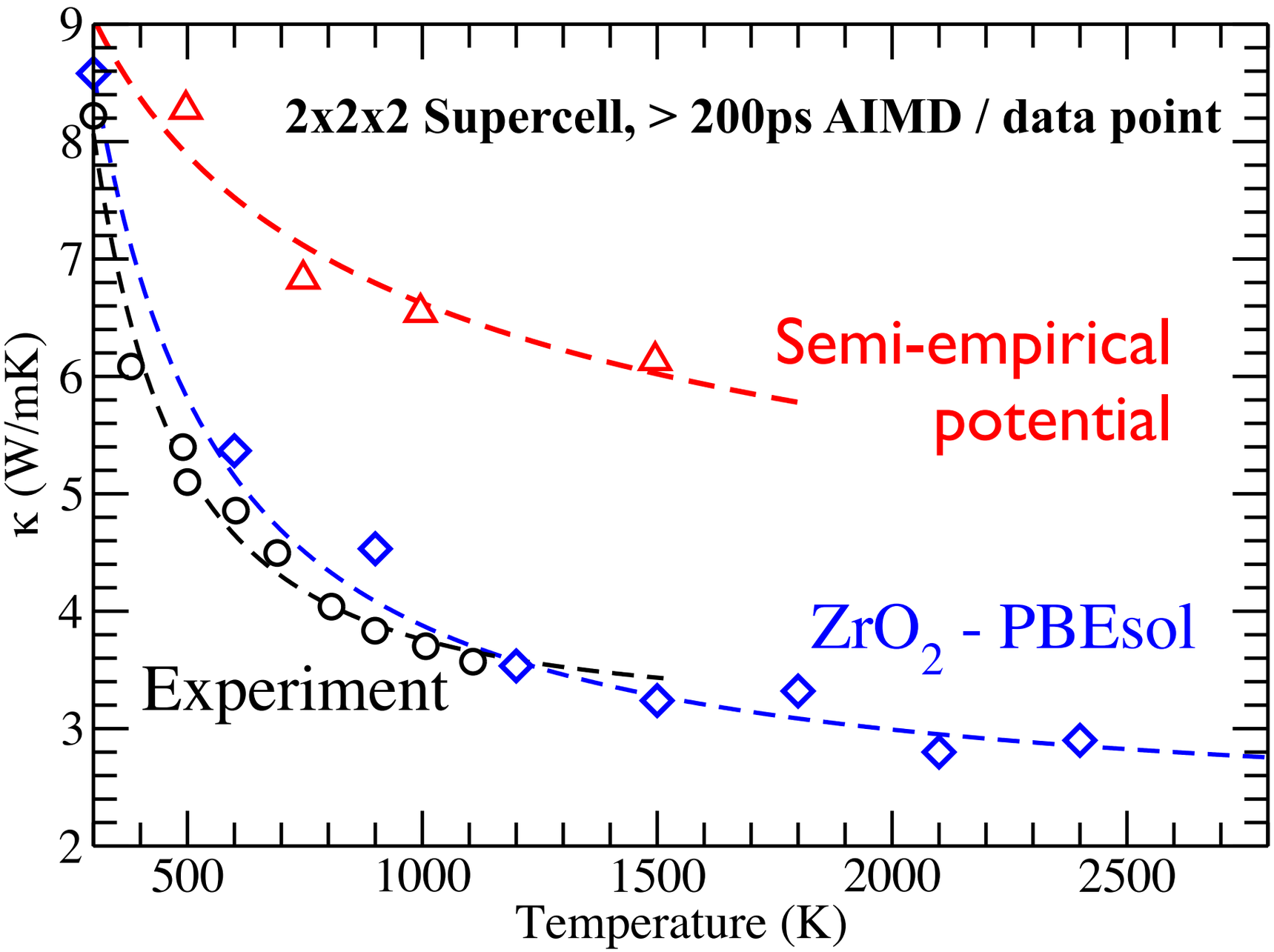


Suppressing heat transport in **thermal barrier coatings** has driven the fuel-efficiency increase over the last 30 years.

D. R. Clarke & C. G. Levi, *Ann. Rev. Mat. Res.*, **33**, 383 (2003).

THERMAL CONDUCTIVITY OF ZIRCONIA

C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).



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Semi-empirical MD:

P. K. Schelling, and S. R. Phillpot,
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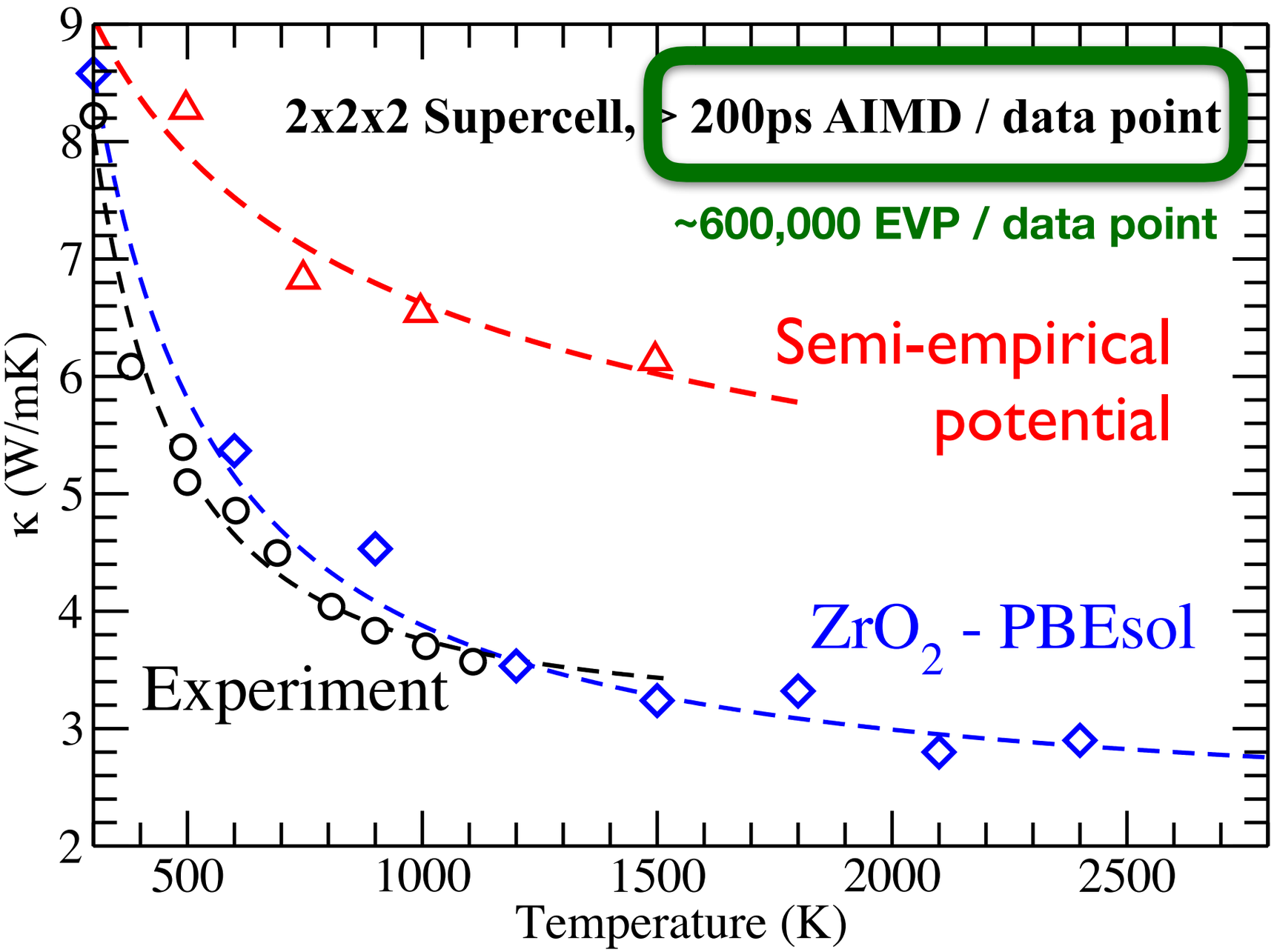

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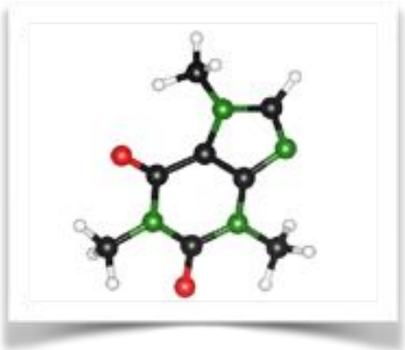
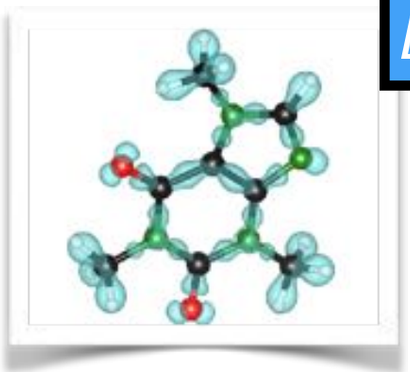


Geometry & Species



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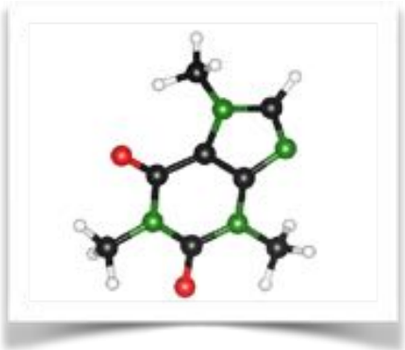
Compute Energy *E* and Forces *F* on Atoms

⇒ Materials' Properties

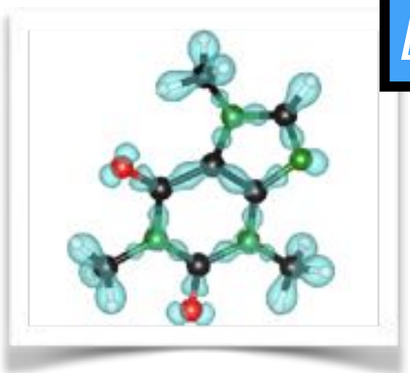
A series of **different**, but **similar** **eigenvalue problems** are solved one after another.

A series of **different**, but **similar** **electronic structure theory problems** are solved one after another.

Update Geometry



Geometry & Species



Electronic Structure Theory

Electronic Structure

Compute Energy *E* and Forces *F* on Atoms

⇒ Materials' Properties

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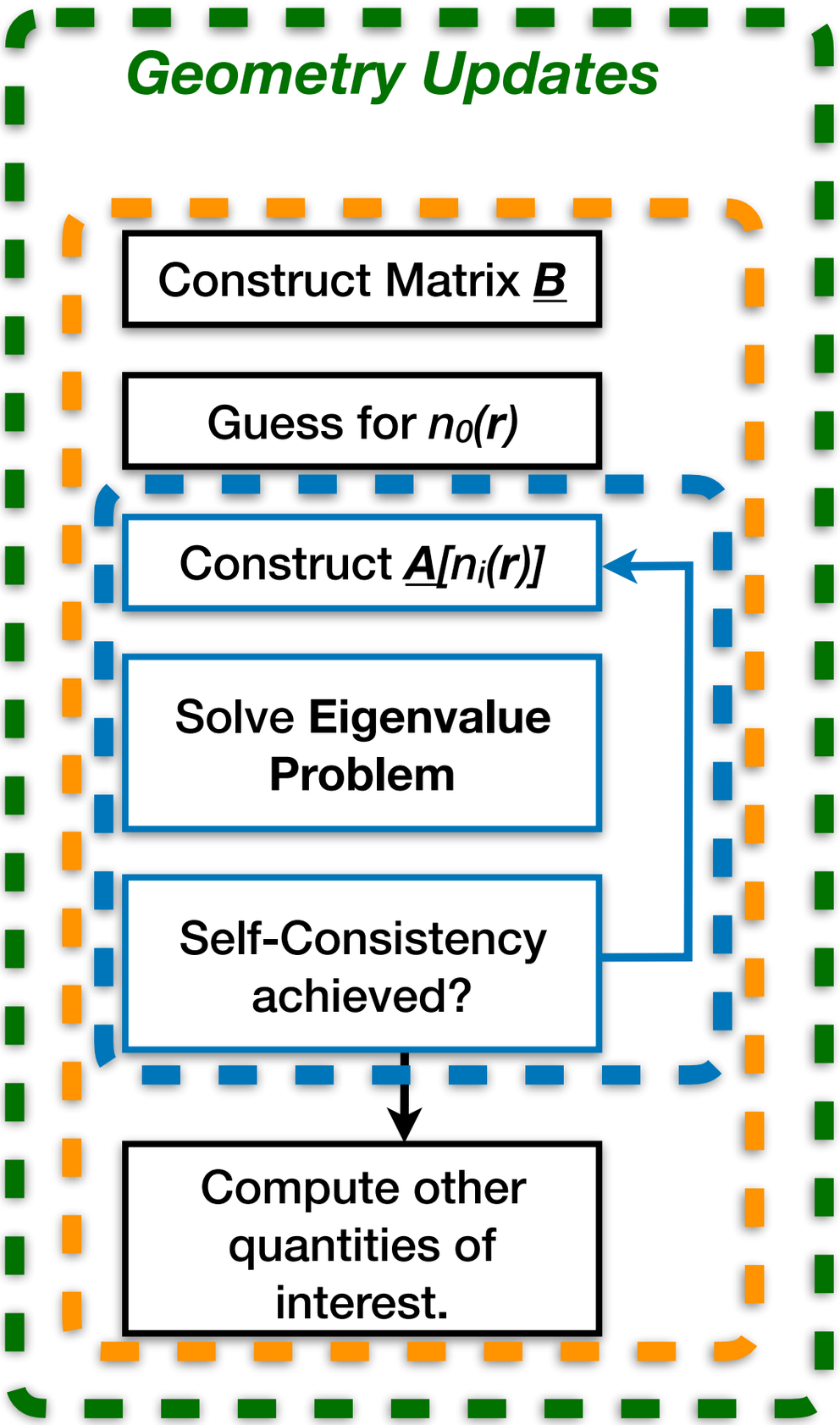
A series of **different**, but **similar** **electronic structure theory problems** are solved one after another.

This Talk: How can this be exploited within **ELPA** to accelerate applications.

Overview:



These are **several** self-concistency cycles.

What can we do across many electronic structure theory calculations?

Hypothesis: For **similar** problems, **similar numerical** settings and **code paths** should be **most efficient.**

Typical Approach: **Manually test** different settings or choose (possibly automatically) by **educated guess.**

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ELPA's Autotuning Solution: **Explicitly** test **different** (combination of) **settings** and then choose the **optimal one.**
Possible settings **include:**

Code Paths:
ELPA 1
or
ELPA 2
solver?

Optimized Kernels:
Generic, AVX2, or AVX512 kernel?

Hybrid MPI/MP Parallelization:
Number of threads / core

GPU offload:
Which routines should make use of GPUs?

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This requires ELPA to *"remember"* settings and timings from earlier calls across one run.

Necessary Technology:

API Redefinition

Old ELPA API

```
! Solve evp, return eigenvalues and eigenvectors
if(ph%elpa_solver == 2) then
   success = elpa_solve_evp_real_2stage_double(ph%n_good,ph%n_states_solve,&
                ham,bh%n_lrow,eval,evec,bh%n_lrow,bh%blk,bh%n_lcol,&
                ph%elpa_comm_row,ph%elpa_comm_col,bh%comm)
else
   success = elpa_solve_evp_real_1stage_double(ph%n_good,ph%n_states_solve,&
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                ph%elpa_comm_row,ph%elpa_comm_col,bh%comm)
endif
```

from elsi_elpa.f90 *in ELSI*

- **Traditional *Scalapack-esque* interface**
- **Stable and Here-to-Stay:**
  All pre-2017 features are and will be accessible also in future
- **This includes all internal accelerations and kernels.**
- **New (optional) post-2017 features not accessible via the old API**

New ELPA API

- **Object-oriented**
- **Get/Set API**
- **Mandatory and Optional Arguments are set separately**
- **Actual ELPA call has simple syntax**
- **ELPA Object survives iterations and cycles**

```
! Create ELPA object
elpa => elpa_allocate()

! Set MANDATORY parameters decribing the matrix and it's MPI distribution
call elpa%set("na", na, success)
call elpa%set("nev", nev, success)
call elpa%set("local_nrows", na_rows, success)
call elpa%set("local_ncols", na_cols, success)
call elpa%set("nblk", nblk, success)
call elpa%set("mpi_comm_parent", mpi_comm_world, success)
call elpa%set("process_row", my_prow, success)
call elpa%set("process_col", my_pcol, success)
success = elpa%setup()

! Set OPTIONAL run-time options
call elpa%set("solver", elpa_solver_2stage, success)

! Use ELPA
call elpa%eigenvectors(a, ev, z, success)
~
```

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```

ELPA is able to store and exploit information across calls.

Example: Autotuning

- **Usual setup**
- **Attach Autotuning**
- **Run your loops**
- **Set optimal settings once identified**

```
! Setup ELPA using the new API
succes = elpa%setup()

! Autotuning setup
tune_state => elpa%autotune_setup(ELPA_AUTOTUNE_MEDIUM, ELPA_AUTOTUNE_DOMAIN_REAL, error)

! Loop of ELPA calls
do i=1, scf_cycles
  ! Autotuning still running?
  unfinished = elpa%autotune_step(tune_state)

  ! Use optimal setup once finished
  if (.not.(unfinished)) then
    call elpa%autotune_set_best(tune_state)
  endif

  ! ELPA cal
  call elpa%eigenvectors(a, ev, z, error)

enddo
```

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Manual Settings or Predefined Options

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Manual Settings or Predefined Options

Autotuning can be used during production iterations.

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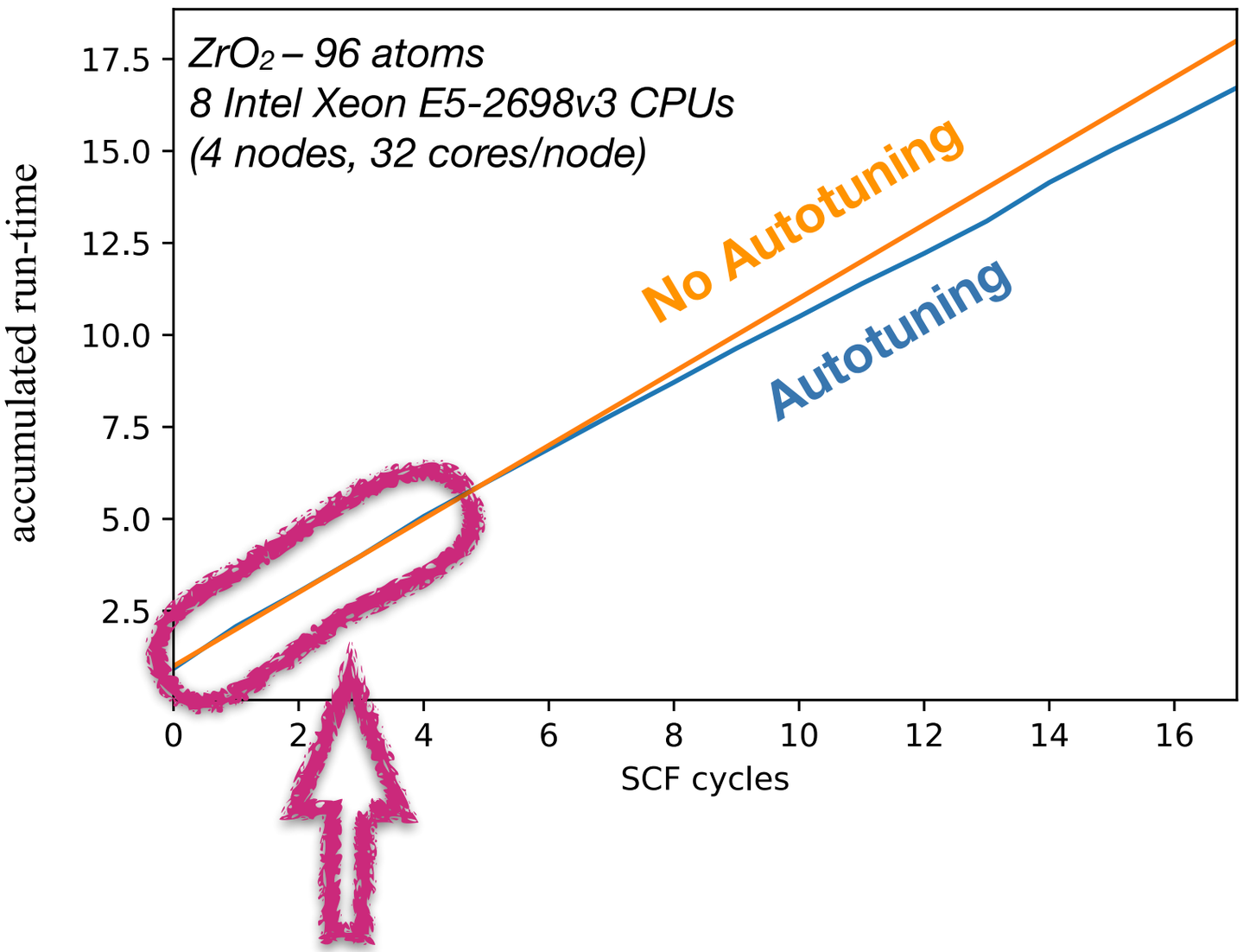
ELPA_AUTOTUNE_FAST

Reasonable domain-specific presets such as ELPA_AUTOTUNE_FAST available, more to come…

Autotuning with ELPA_AUTOTUNE_FAST

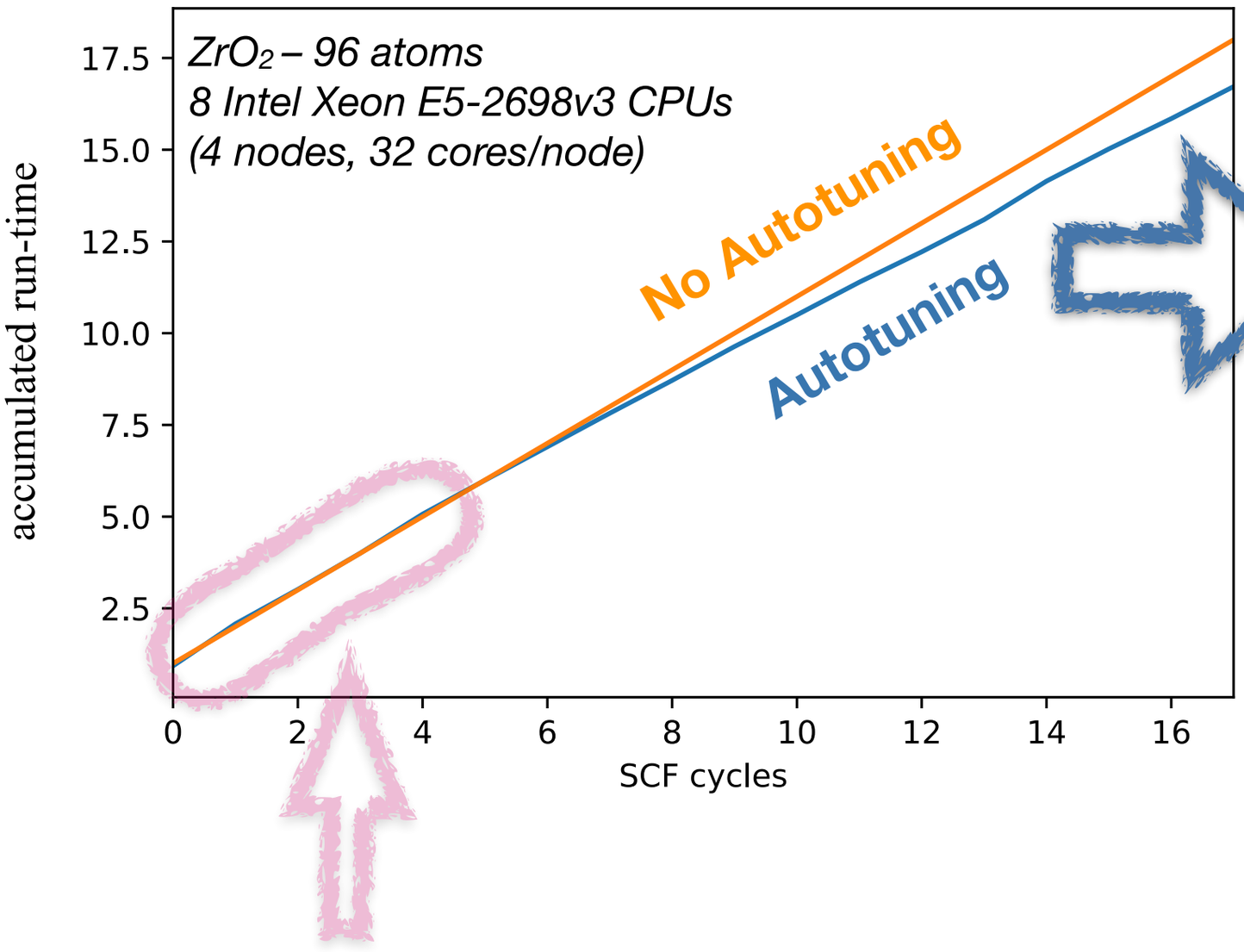
Accumulated Runtimes:



Slight computational overhead observed in the **first couple** of iterations…

Autotuning with ELPA_AUTOTUNE_FAST

Accumulated Runtimes:

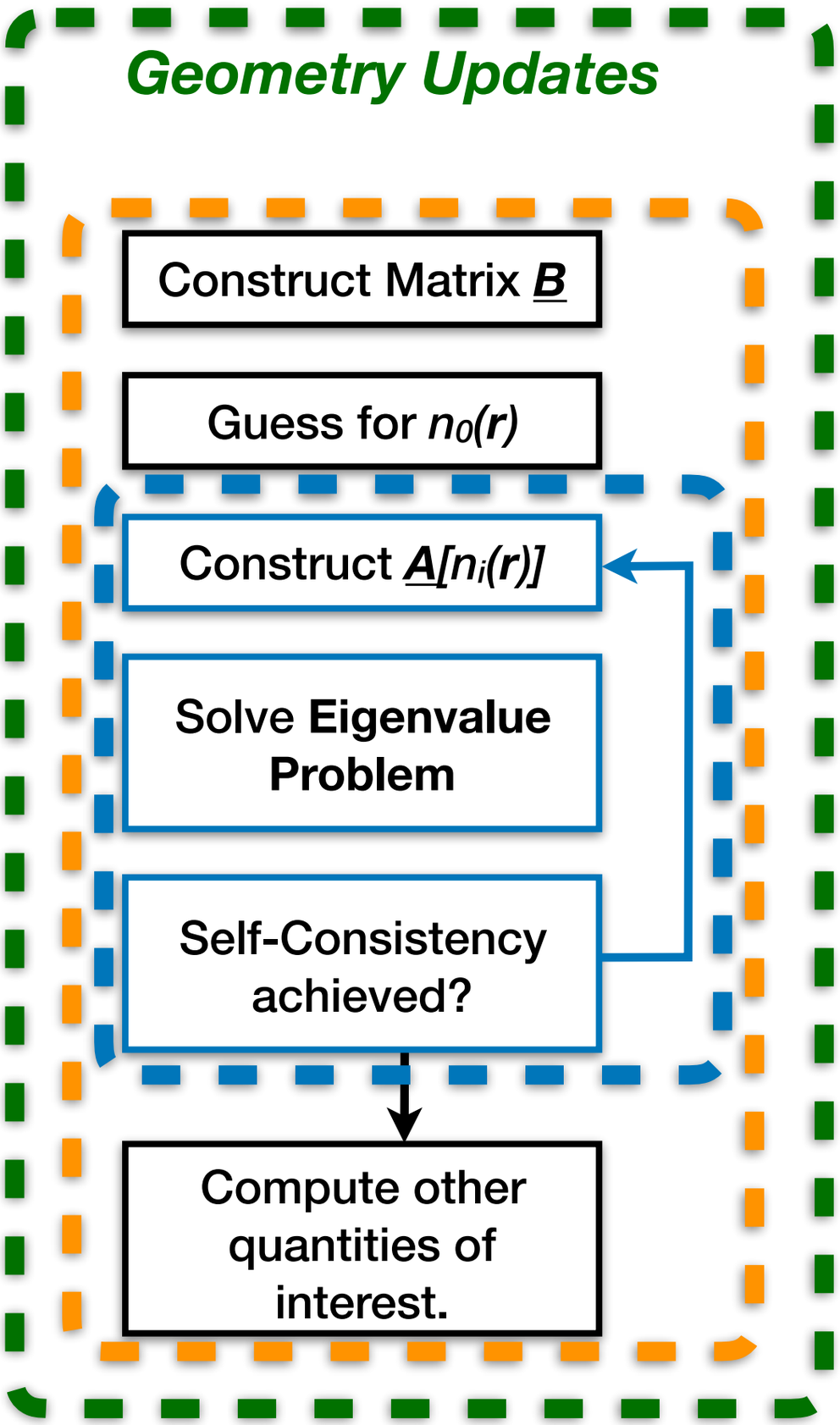


Slight computational overhead observed in the first couple of iterations…

Autotuning beneficial in the long-run

- Autotuning can already be **beneficial** in a **single-run!**
- **Generally,** autotuning can eventually leads to a speed-up between **15-20% per SCF iteration.**
- Autotuning speed-up retained across geometry changes (MD-ready!).

Overview:



These are **several** self-concistency cycles.

⇒ **(A)** Exploit ELPA-Autotuning
for **a series** of calculations

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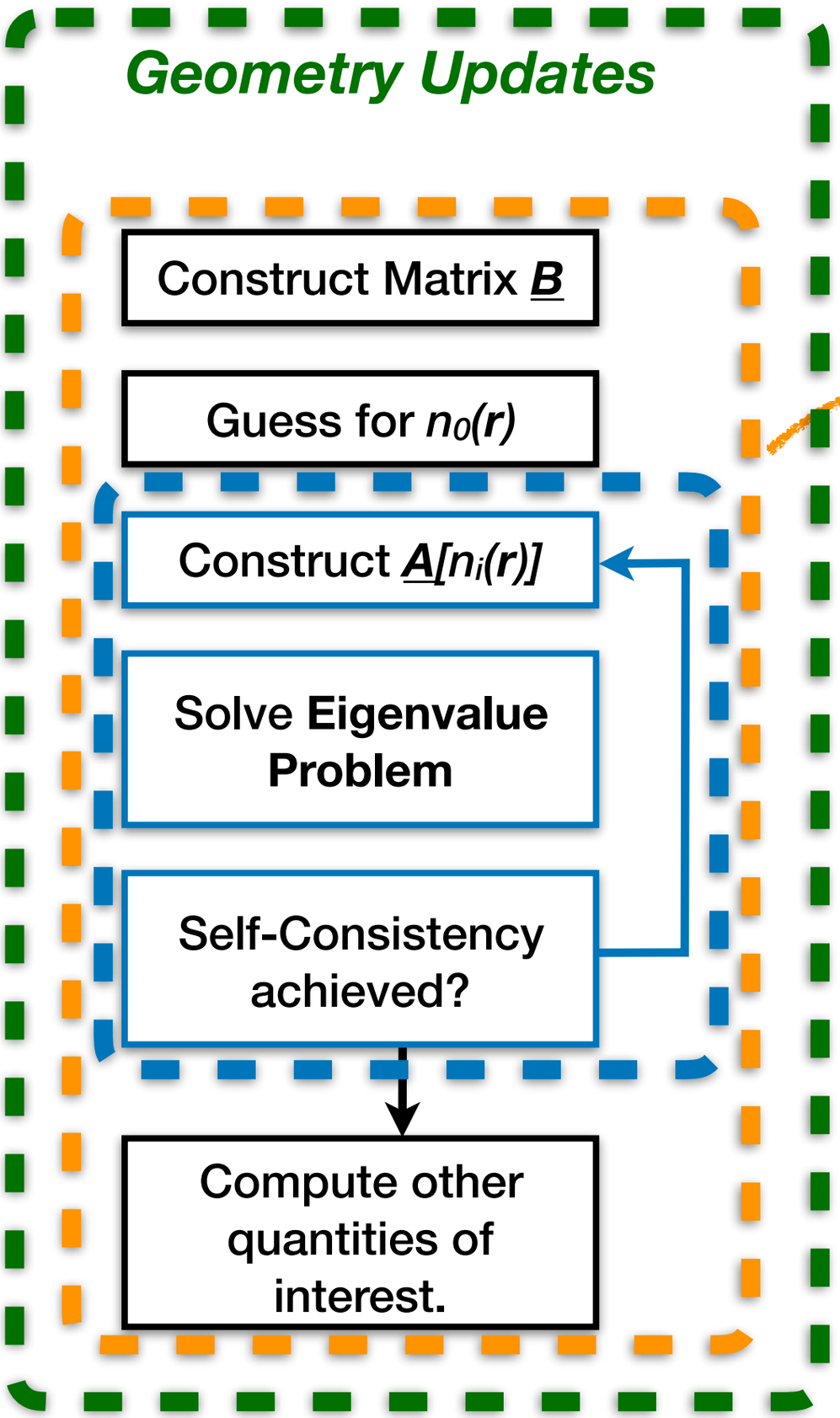

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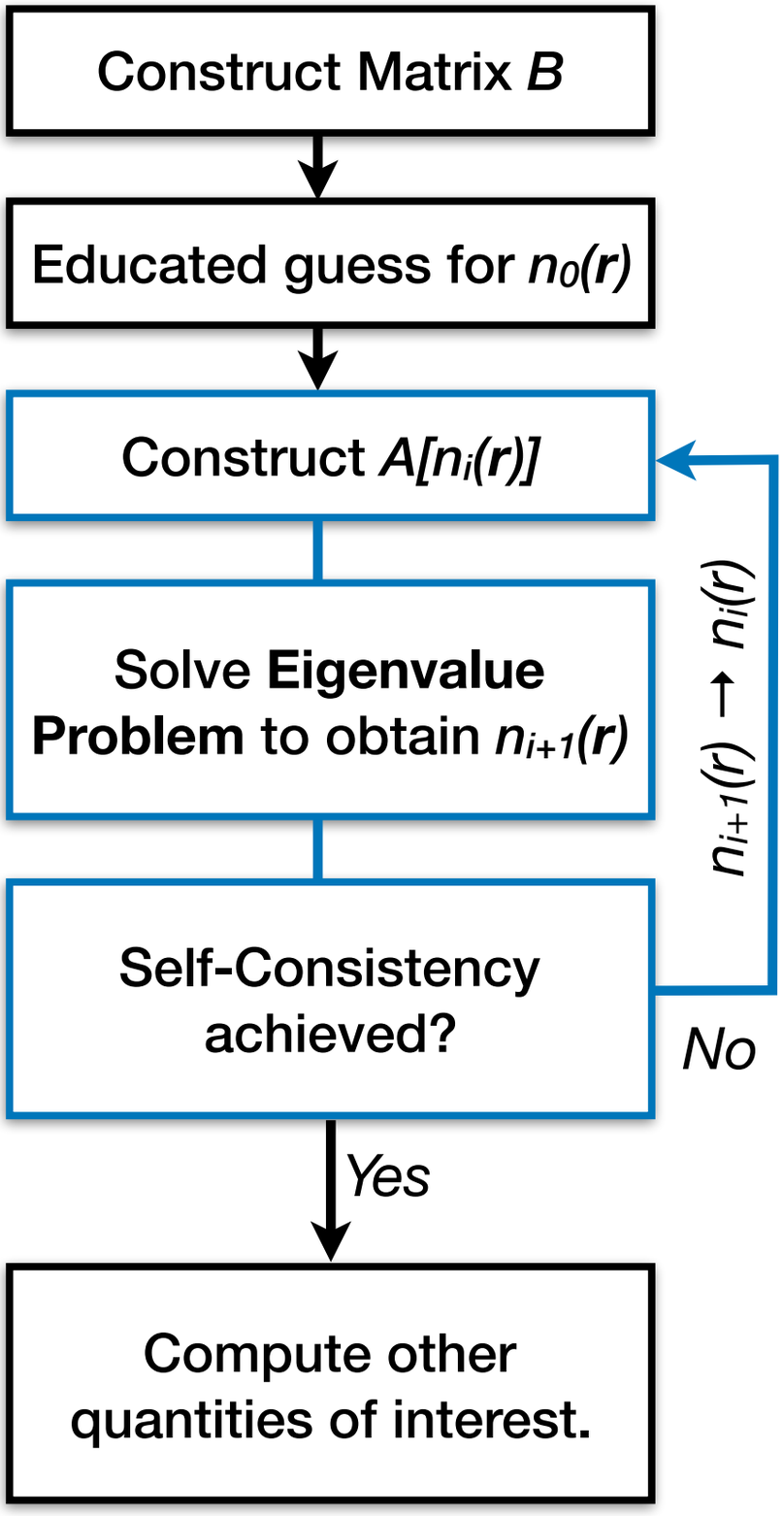
The Self-Consistency Cycle



Some Remarks:

- **Typical number of iterations:** 10-100
- **Convergence accelerated by mixing schemes**
- **Convergence/Self-concistency monitored via:**
  - Change in **density** $n_i(\mathbf{r})$
  - Change in **energy** $E_i(\mathbf{r})$
  - Change in **forces** $\boldsymbol{F_I}$
  - Change in **eigenenergies** ε_i

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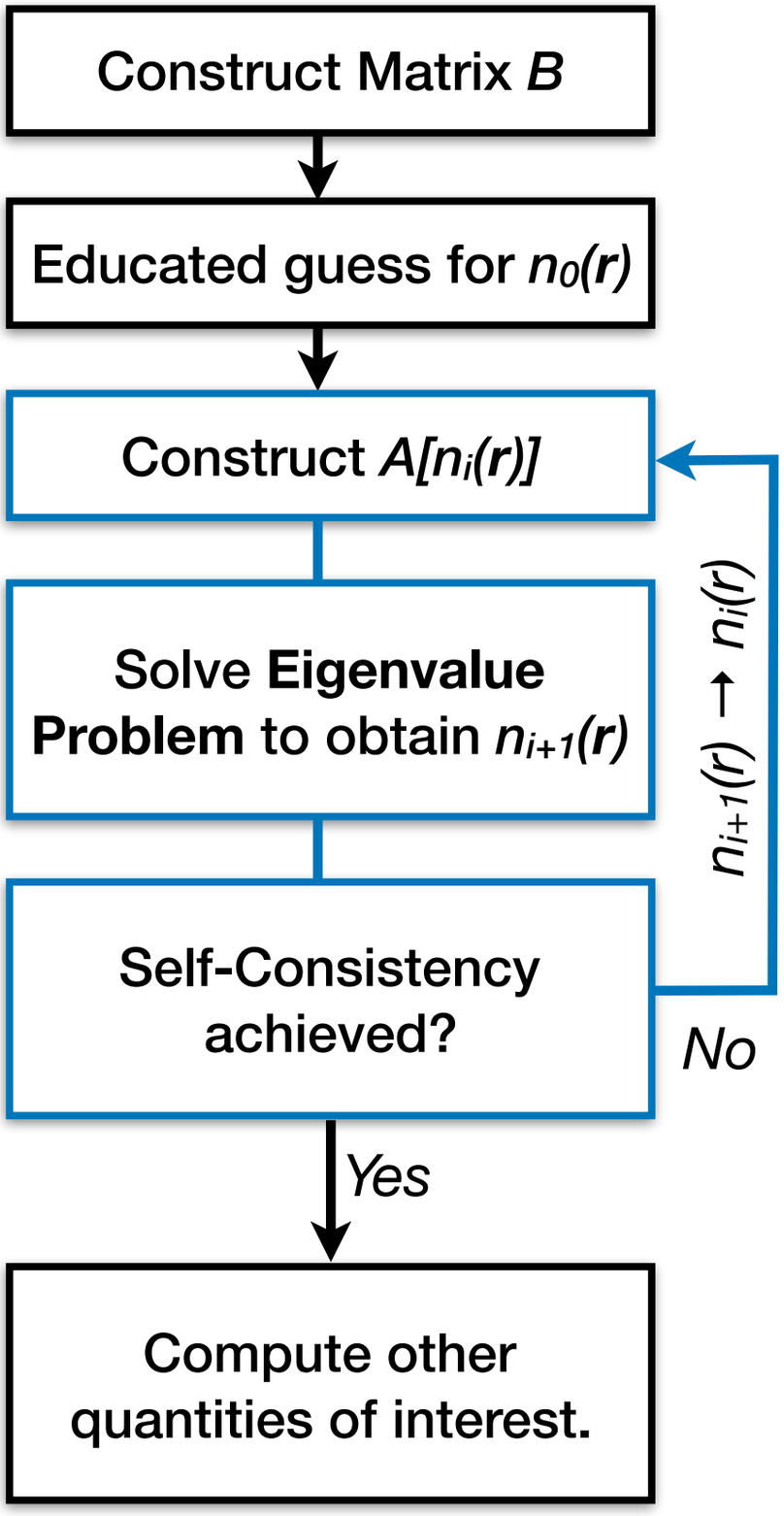

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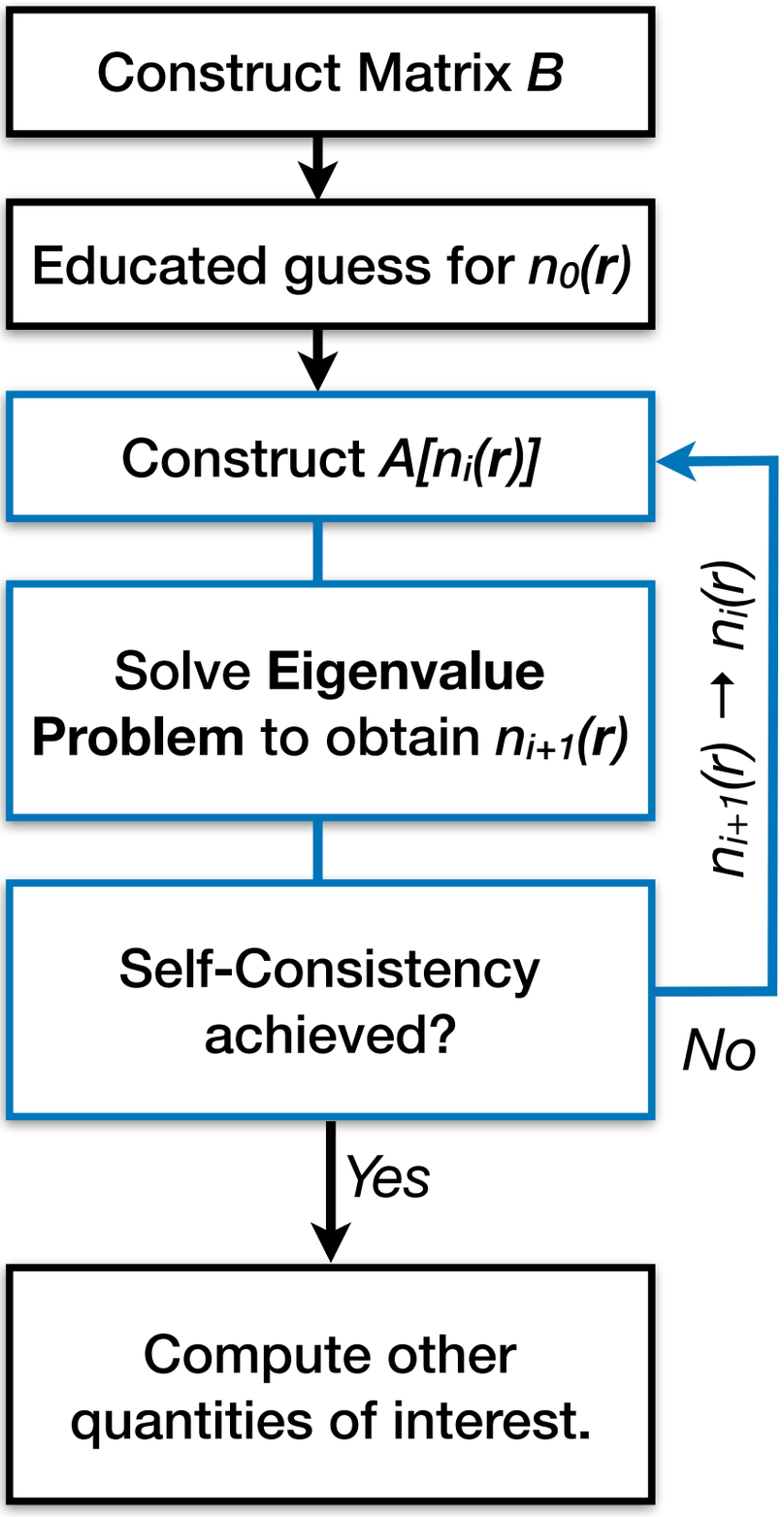

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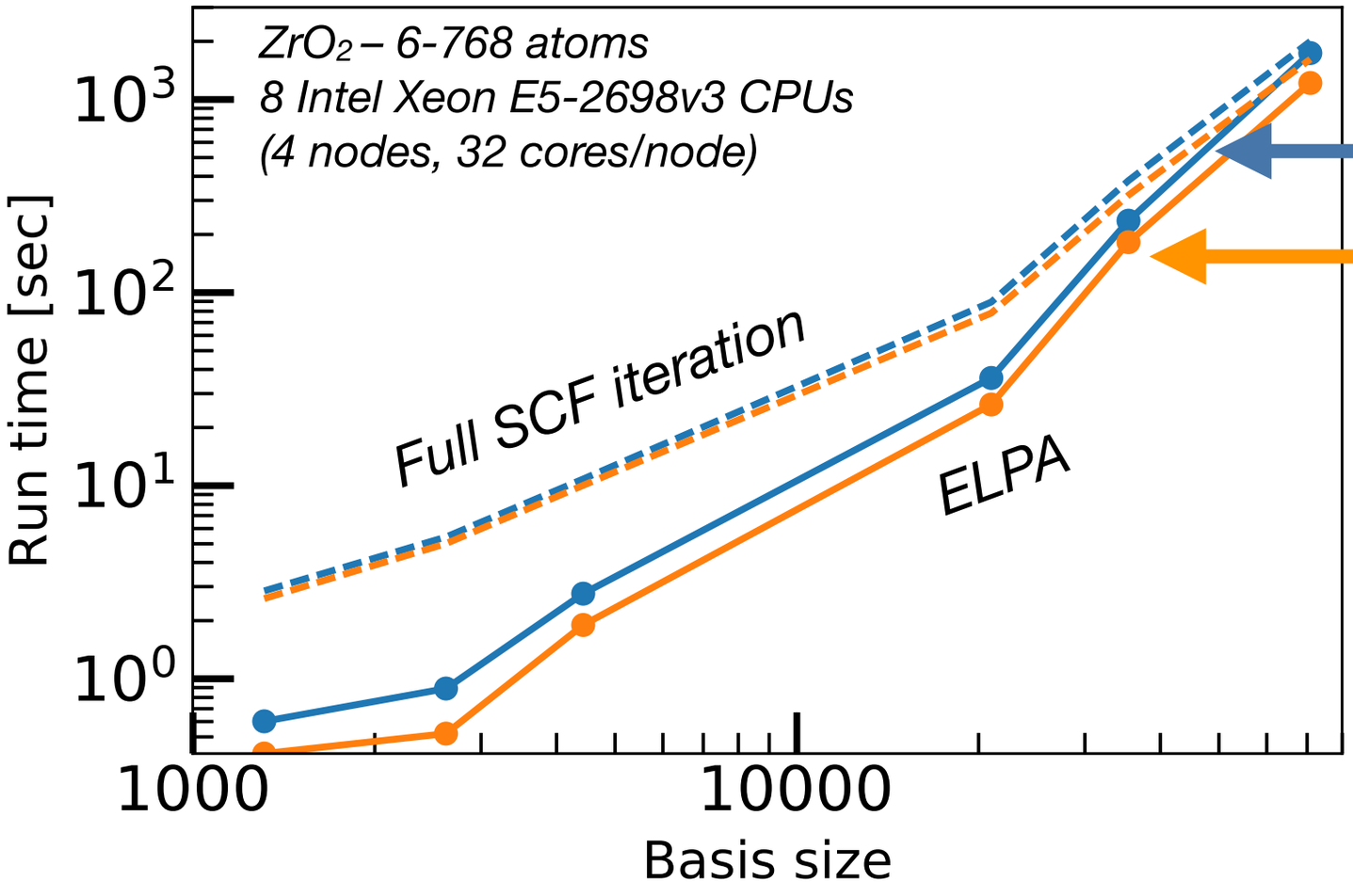
  Intensive & Non-Variational

IDEA:
Use mixed precision to reduce computational cost
Perform the first self-consistency cycles
with cheaper single precision routines.

Mixed Precision Calculations

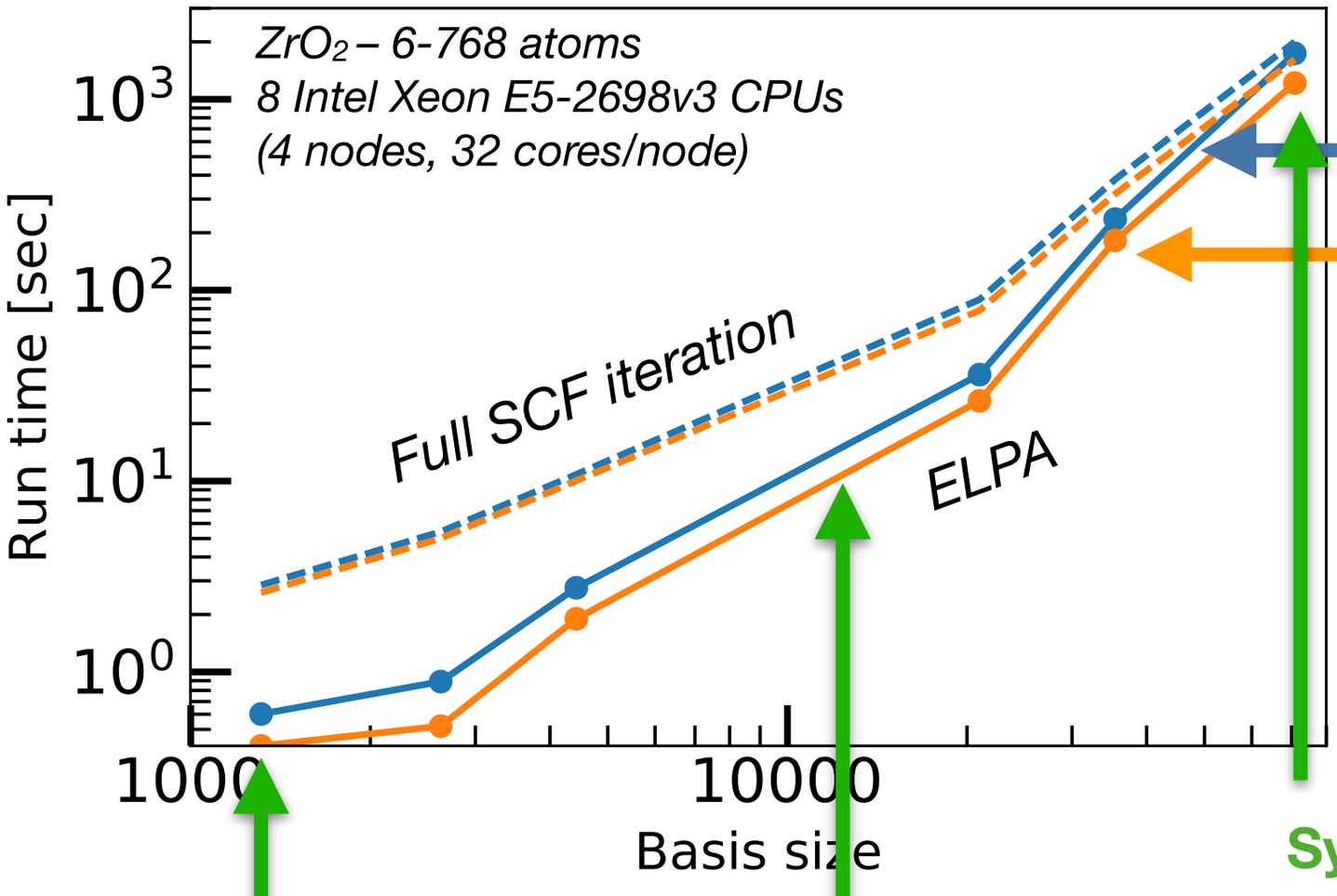


Standard double precision (DP)

Single Precision (SP)

- SP routines ~20% faster
- **Eigenvalue problem** dominates comp. cost for larger systems.

Mixed Precision Calculations



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- **SP** routines **~20%** faster
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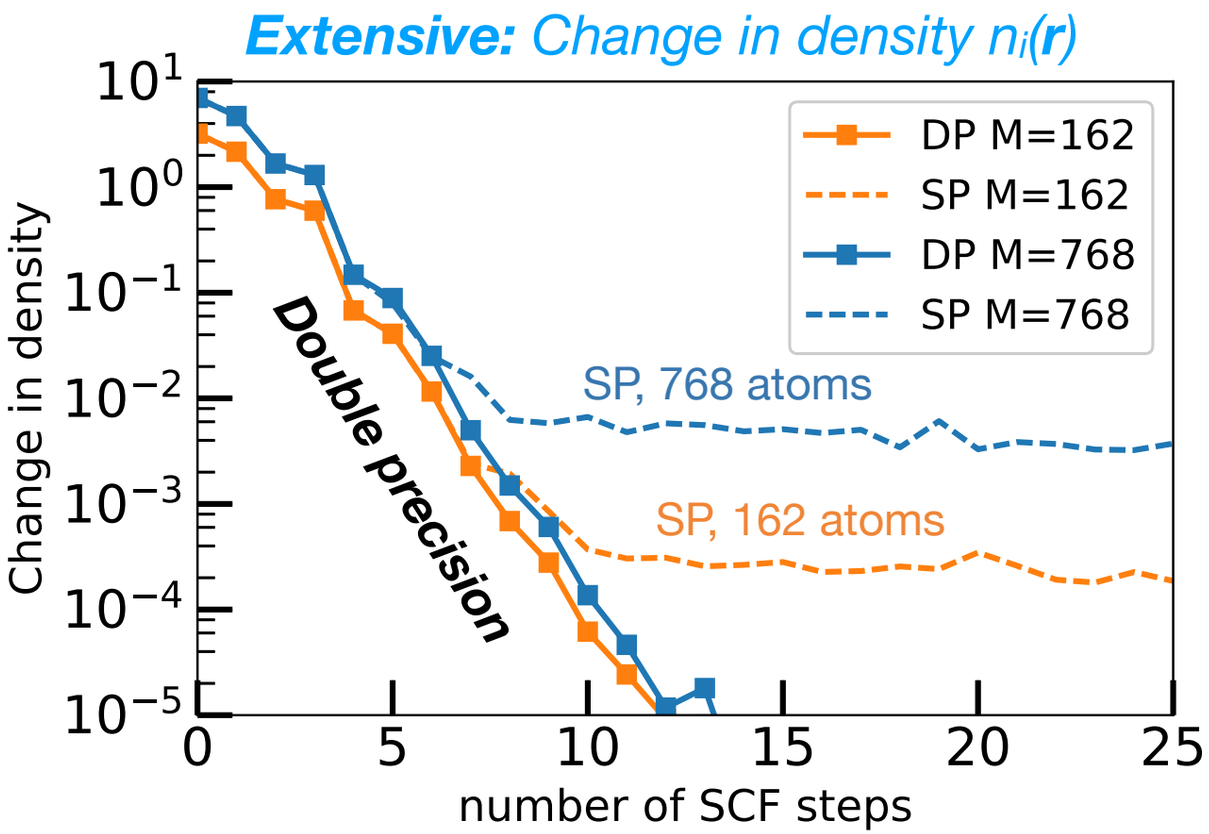
System size needed to model **atomic defects** in the **crystal.**

System size needed for a **thermal conductivity** calculation in **pristine** ZrO_2.

System size needed for a **relaxation** (“PES minima search”).

How far can we go?

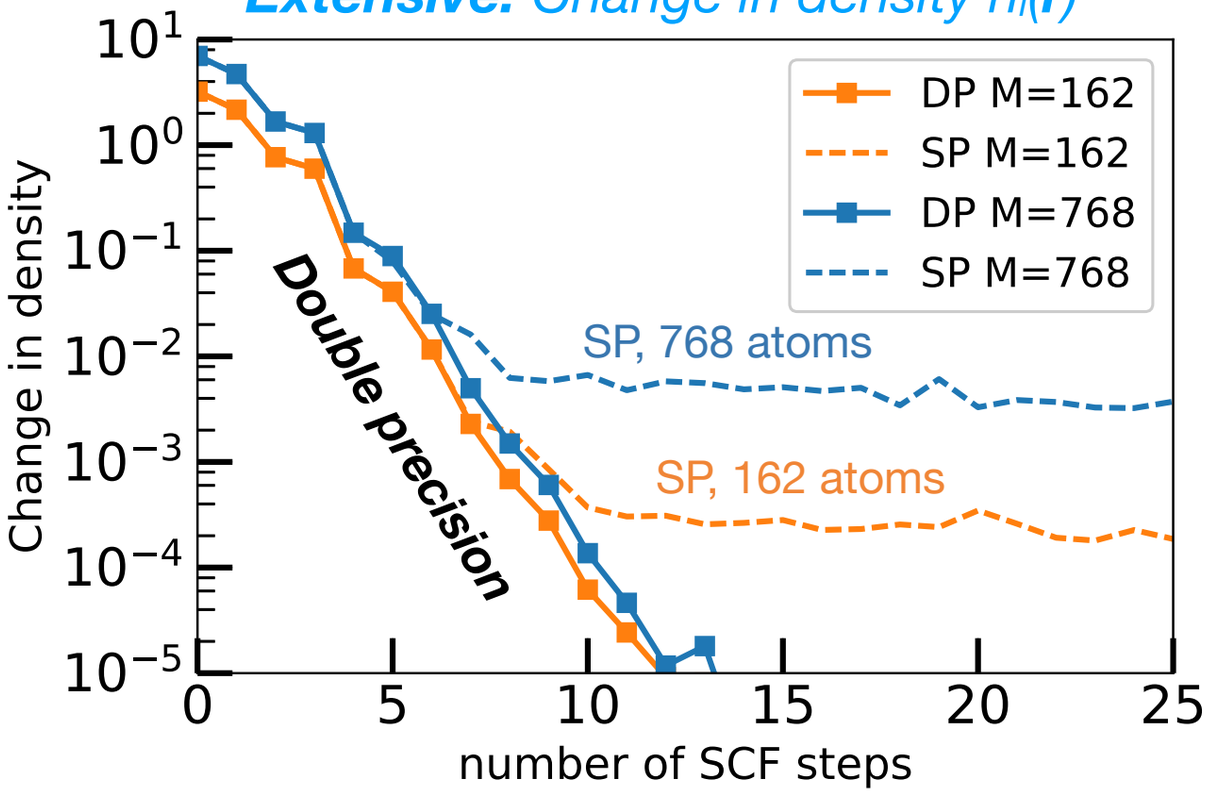


Monitoring the convergence of the self-consistency cycle

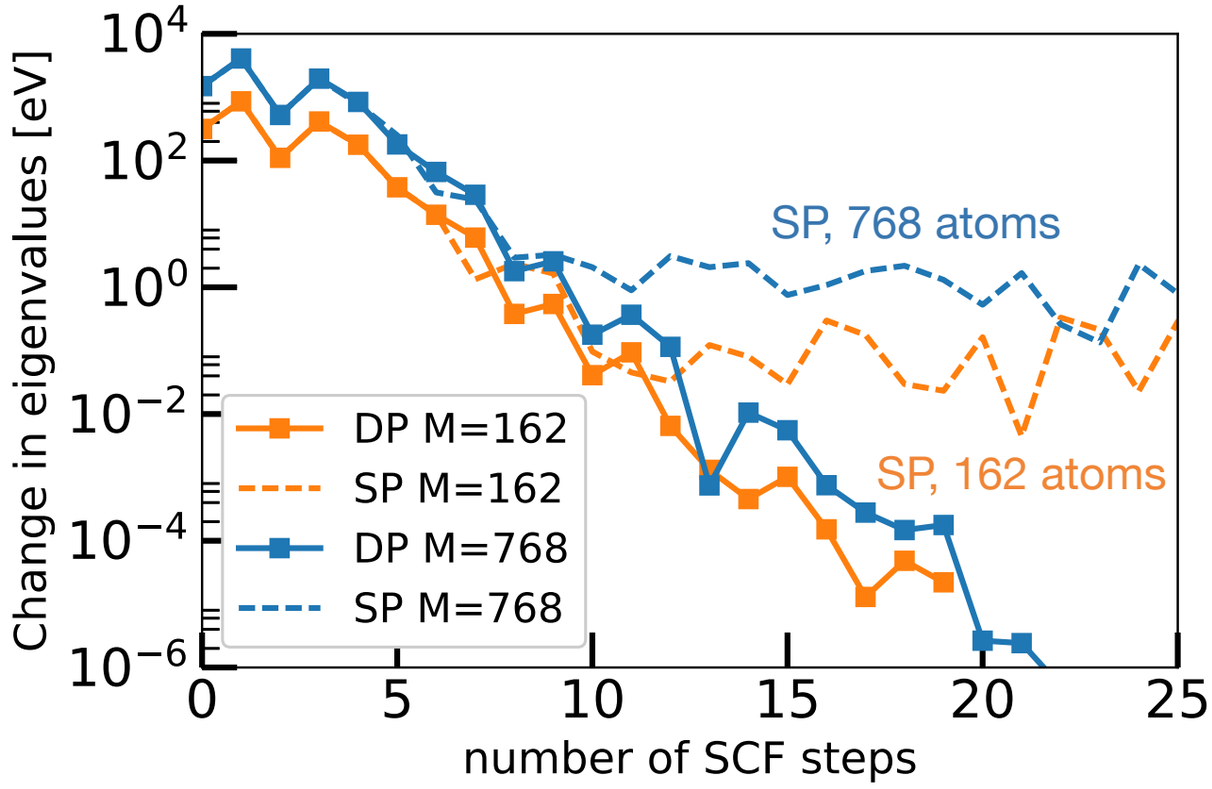
- **Single-Precision** routines **do not allow** to reach **convergence.**
- ***"First"*** few iterations **can be performed** with **single-precision** without loss of accuracy.
- Break-down point of **single-precision** routines system-size-dependent.

How far can we go?

Extensive: *Change in density $n_i(\mathbf{r})$*



Intensive: *Change in* ***eigenenergies*** ε_i



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⇒ Intensive Quantities naturally less affected by system-size dependence.

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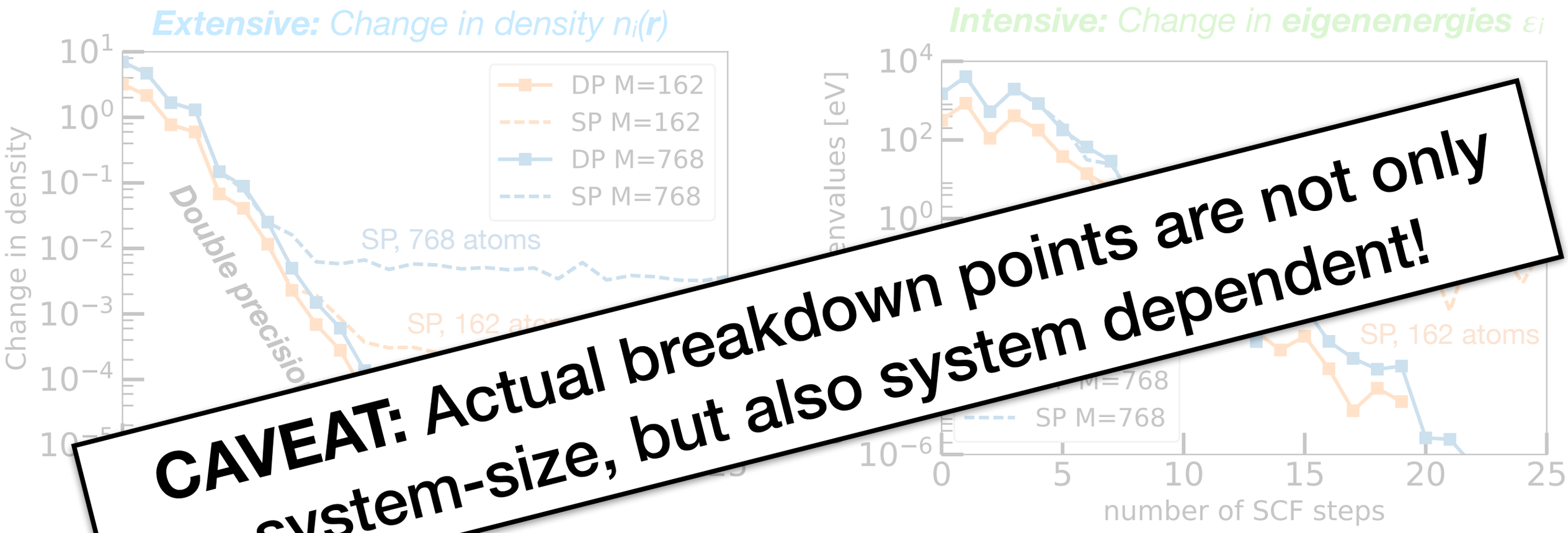

CAVEAT: Actual breakdown points are not only system-size, but also system dependent!

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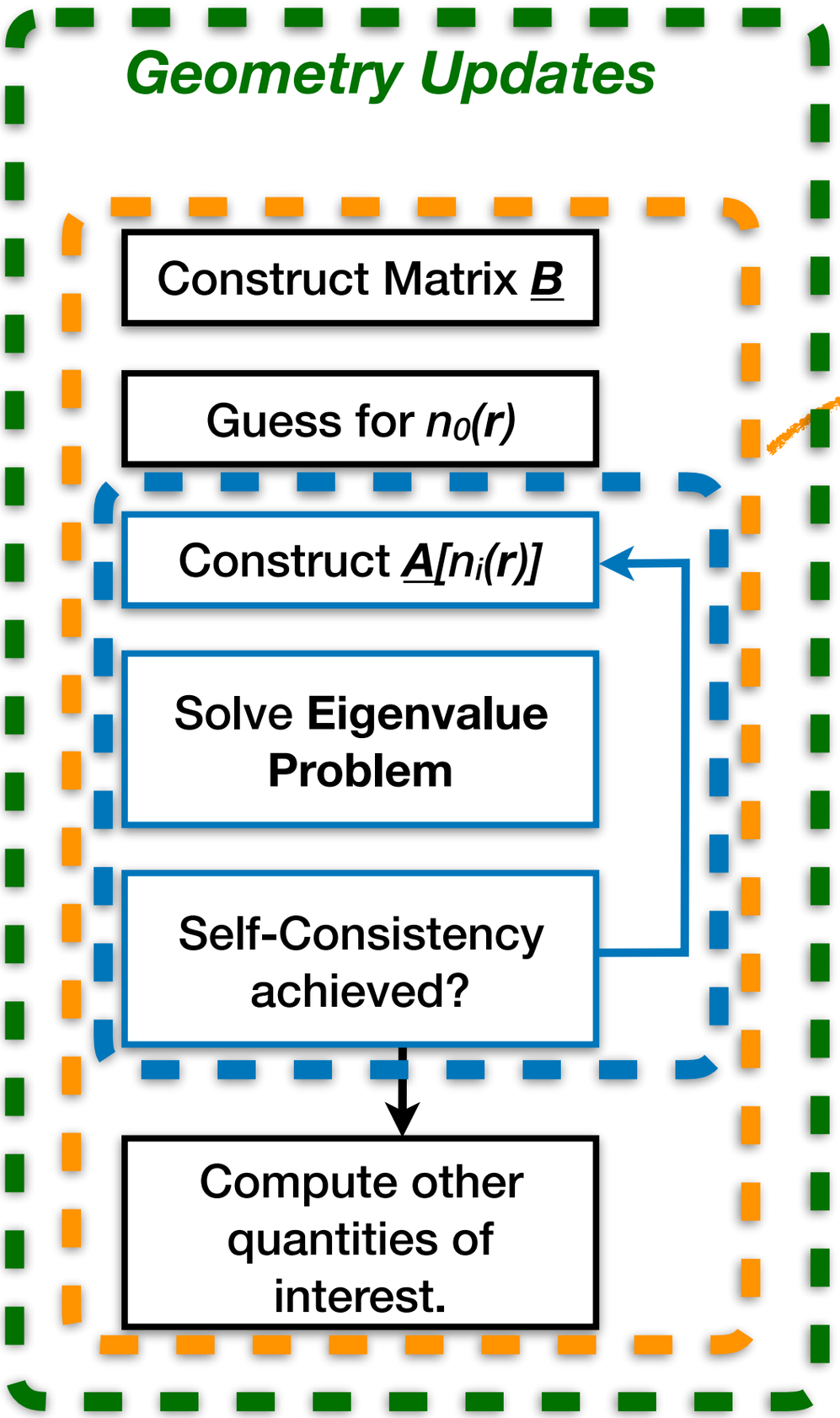

These are **several** self-concistency cycles.

⇒ **(A)** Exploit ELPA-Autotuning
for **a series** of calculations

This is **one** self-concistency cycle.
(**Several** Eigenvalue Problems)

⇒ **(B)** Exploit **Single/Double Precision routines**
in ELPA-AEO for **a series** of Eigenvalue Problem

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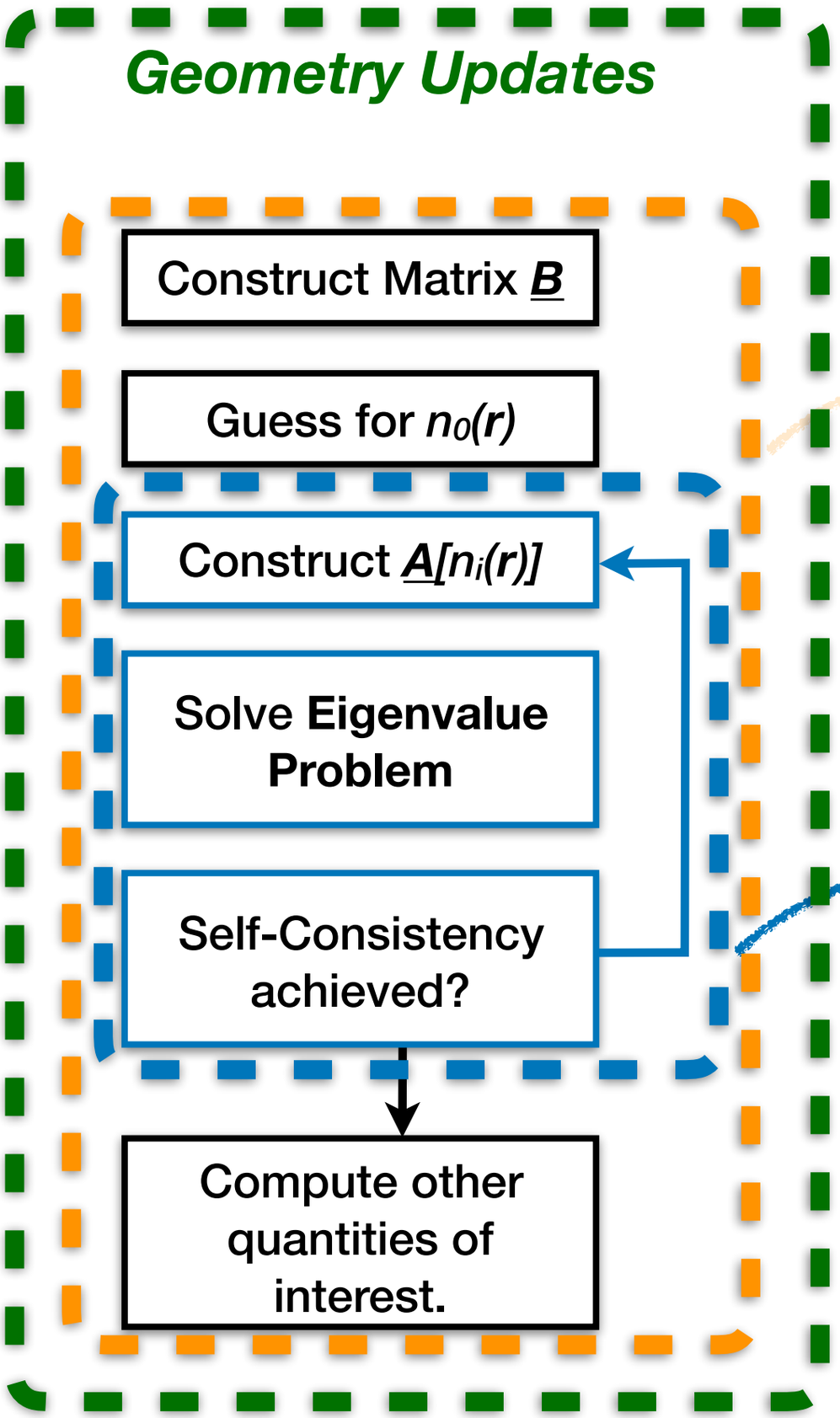

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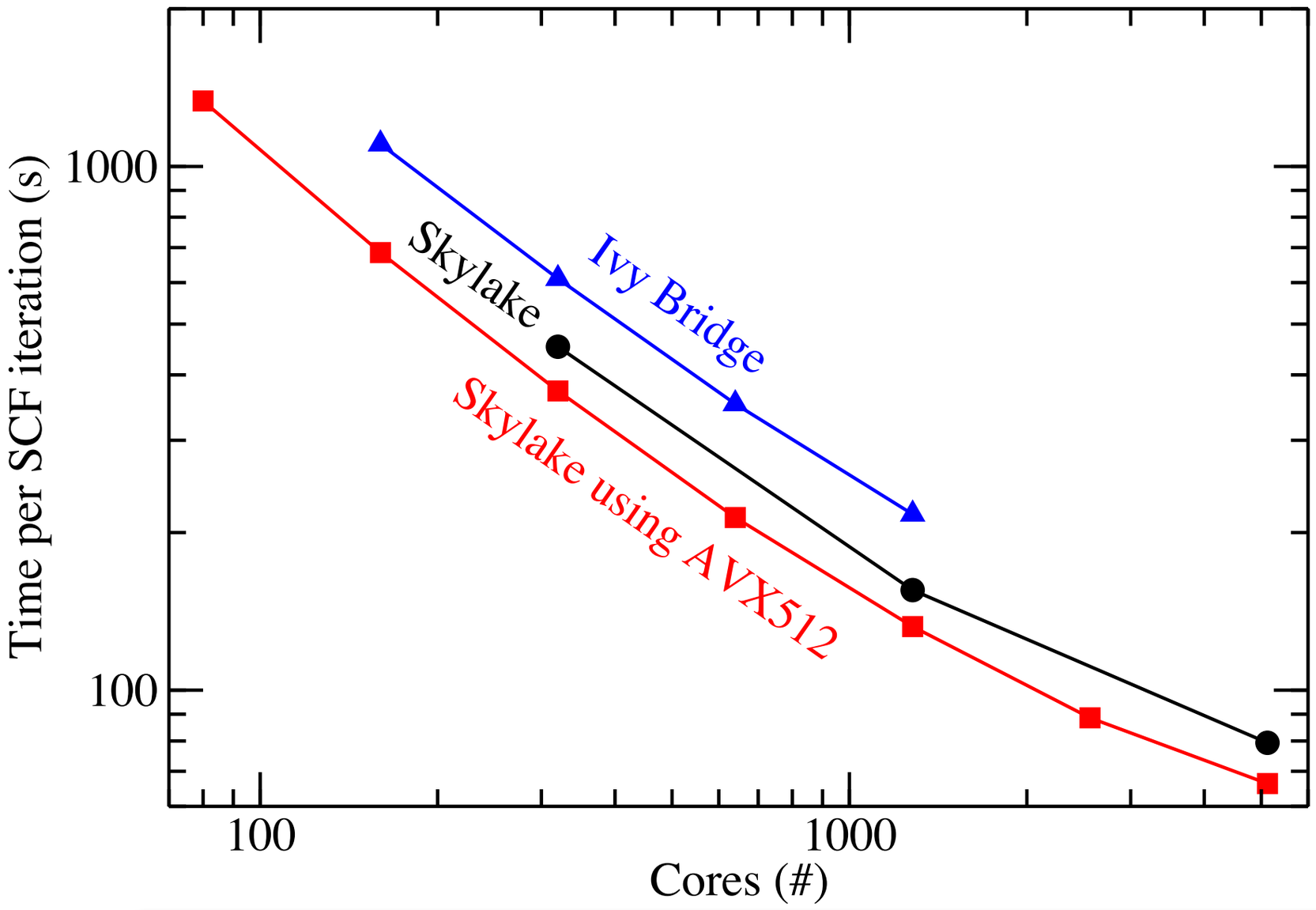
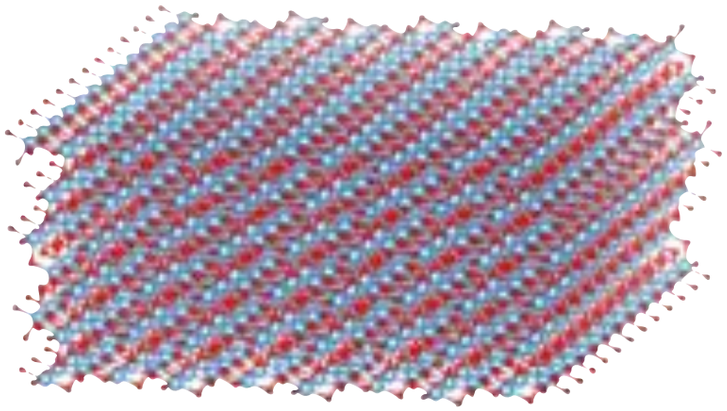
Accelerating One Iteration

Ivy Bridge: Hydra@MPCDF – 20 cores/node
Skylake: Cobra@MPCDF – 40 cores/node



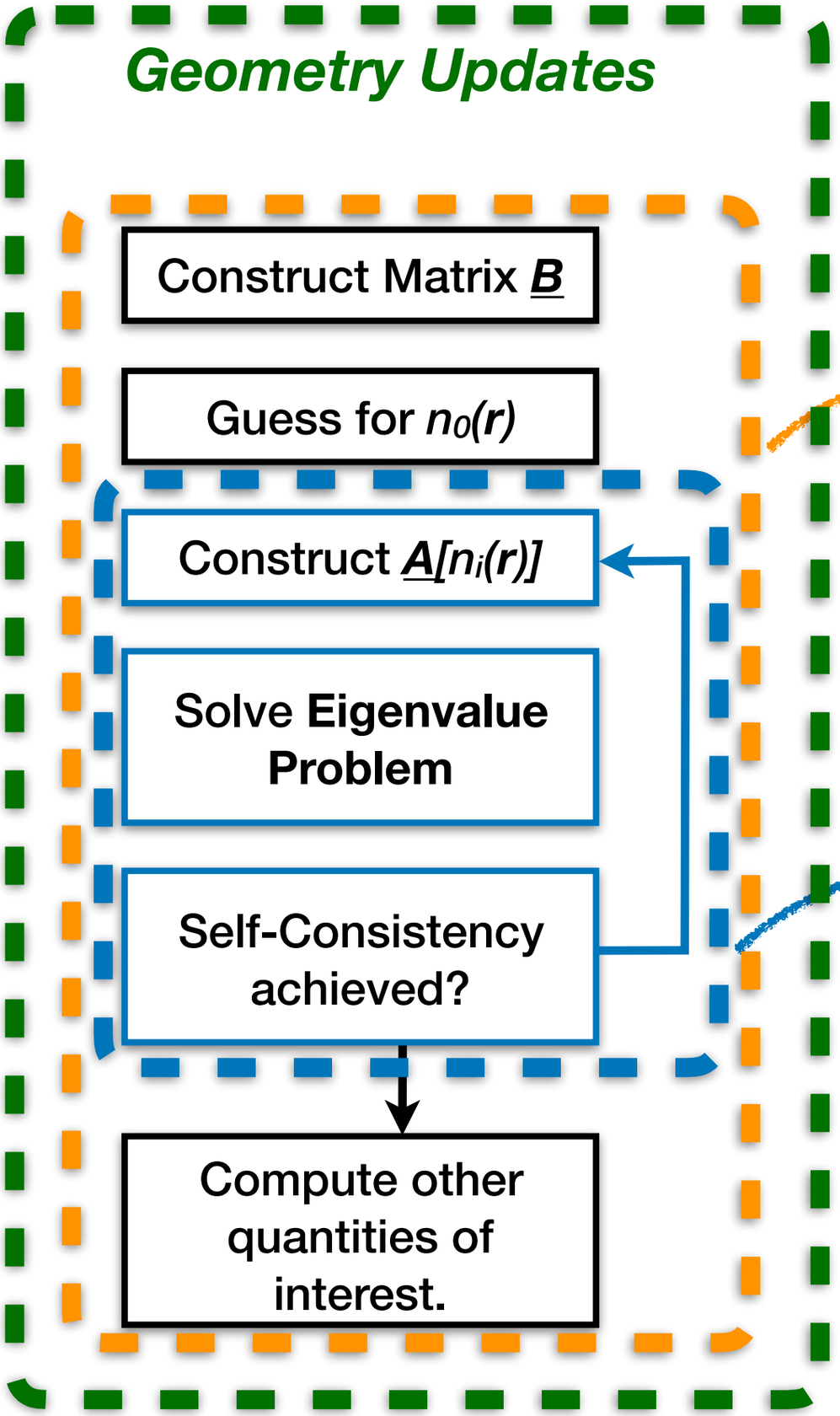


TiO_2 slab/surface with
3,500 atoms and
100 Å vacuum

⇒ Optimizations in ELPA

directly translate into an application speed-up.

SUMMARY:



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⇒ **(C)** Exploit **optimizations** in ELPA-AEO for **single** Eigenvalue Problem

Acknowledgments

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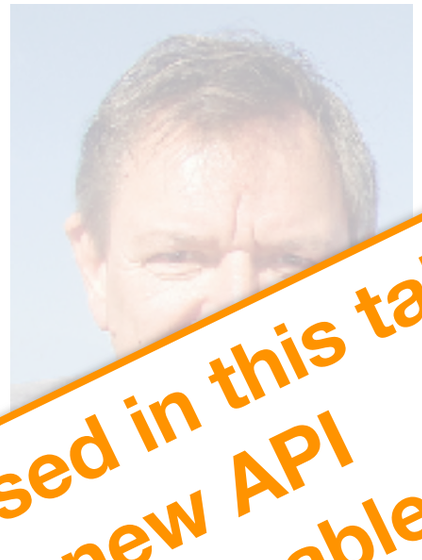

Matthias Scheffler

All features discussed in this talk, including the new API are available and usable in ELSI.

The ELSI project

http://

BERGISCHE UNIVERSITÄT WUPPERTAL

MAX PLANCK COMPUTING & DATA FACILITY

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Victor Yu

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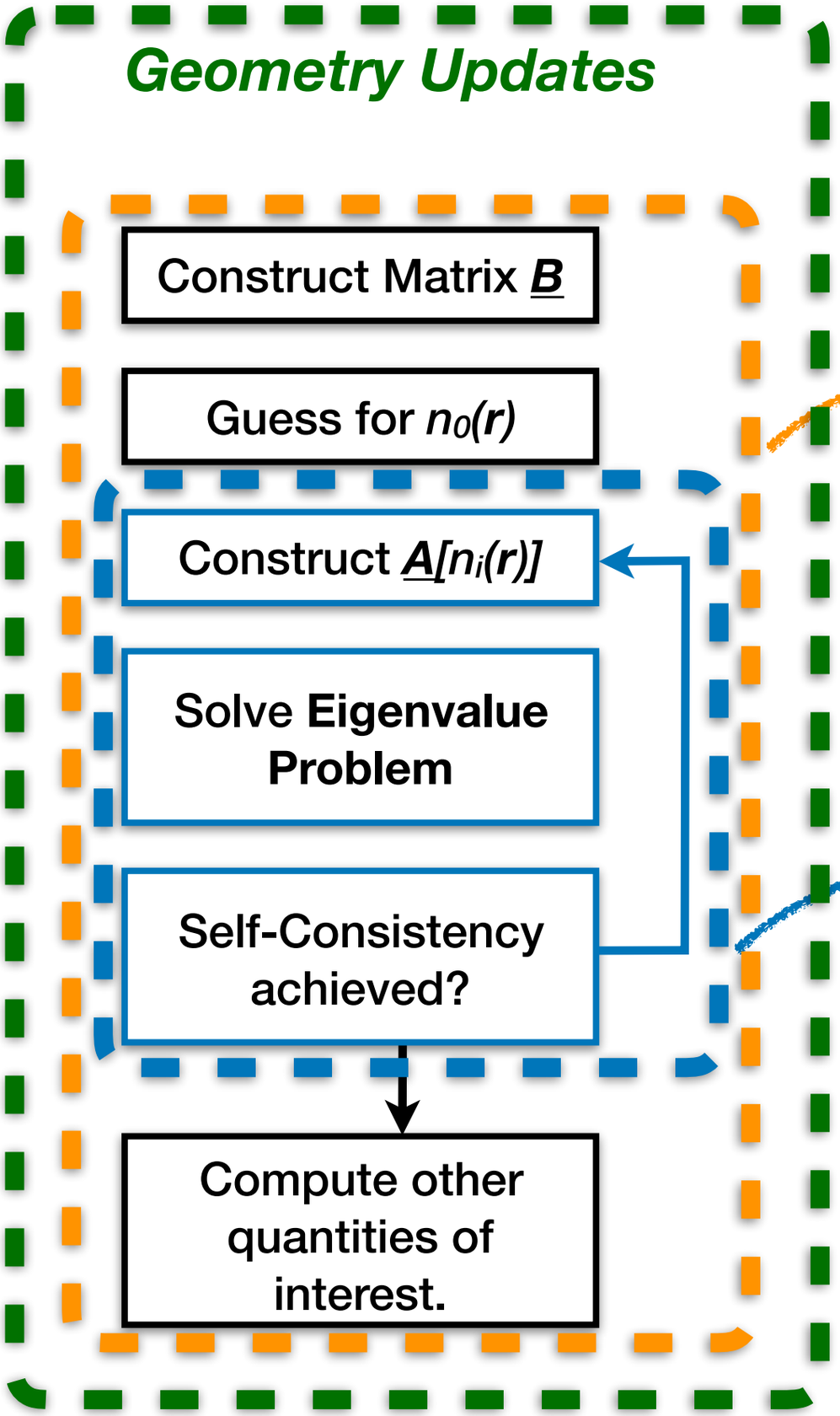

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