MuST - A high performance computing software package for the ab initio study of materials

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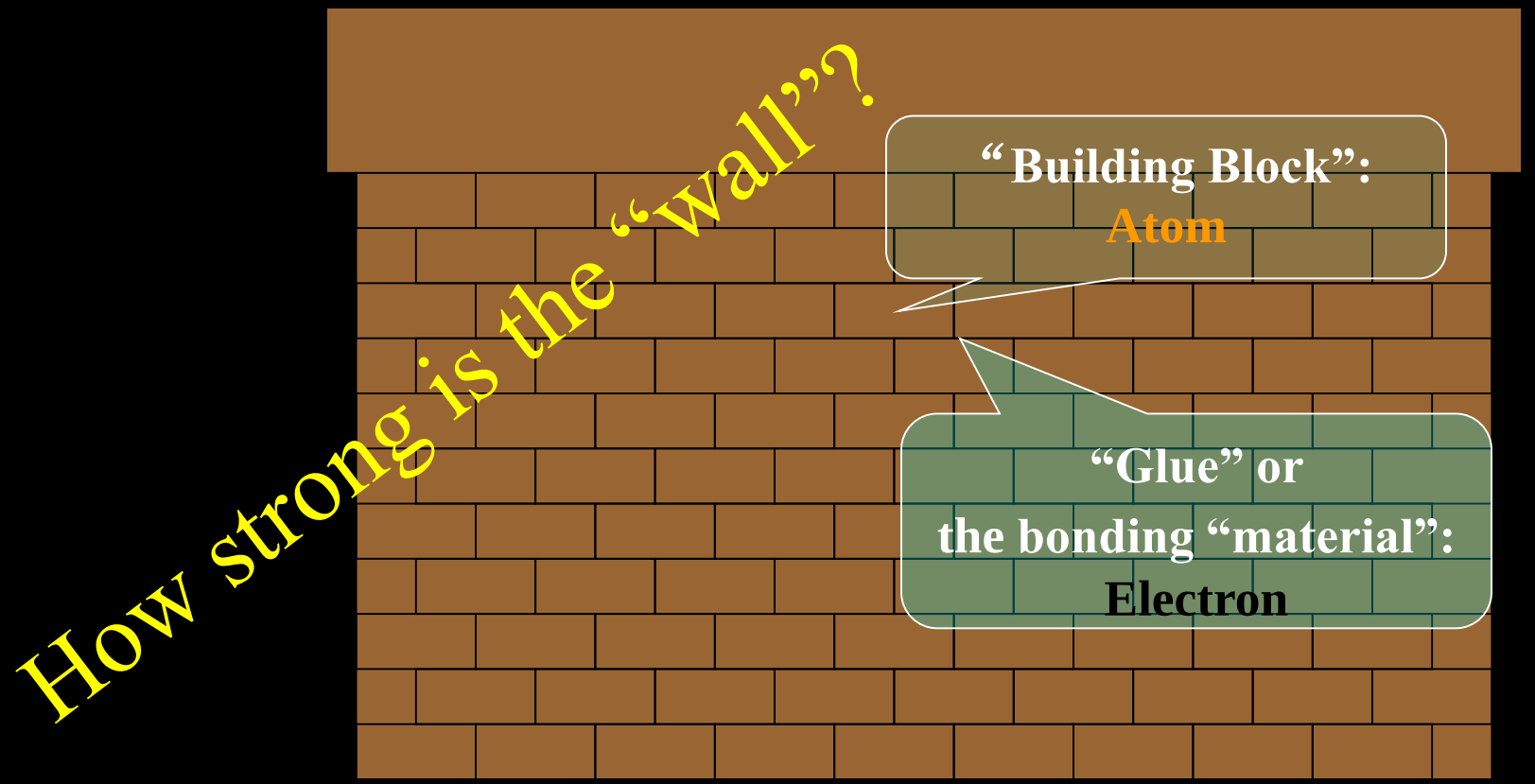
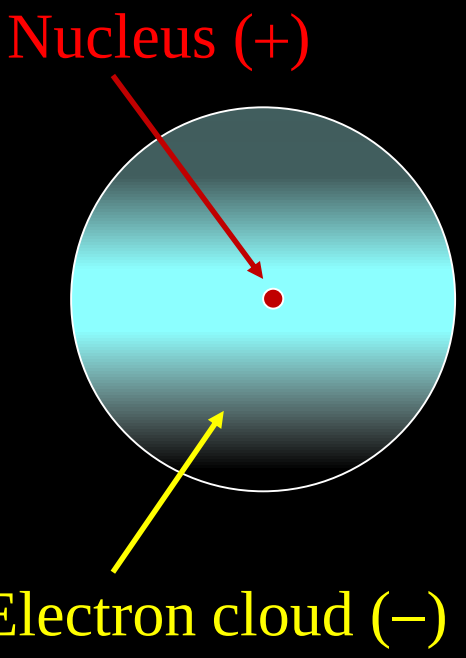
Outlines

- A brief overview of *ab initio* electronic structure calculation
- What is MuST
  - Multiple scattering theory approach to the Kohn-Sham equation
  - Ordered structures
  - Disordered structures
  - Strongly correlated systems with disorders
- Petascale performance of MuST
- Summary

Computational Materials Science



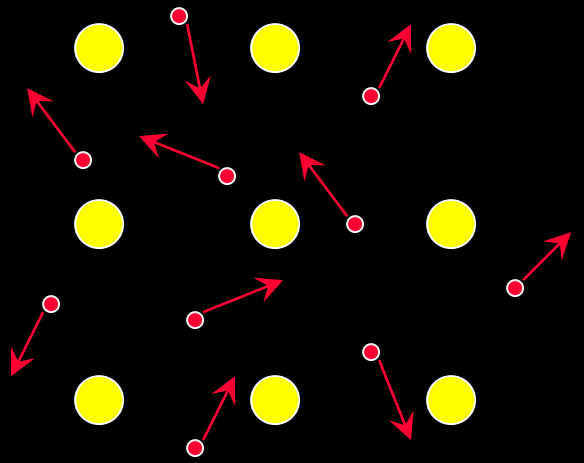


Physical properties of matter, such as whether it is metal or non-metal, magnetic or non-magnetic, its mechanical strength, and so on, are determined by the behavior of the electrons (*electronic states*), since the majority space in a material is occupied by electrons.

Quantum Mechanical Approach to Solid State Materials

Electron: ● **Nucleus:** ●

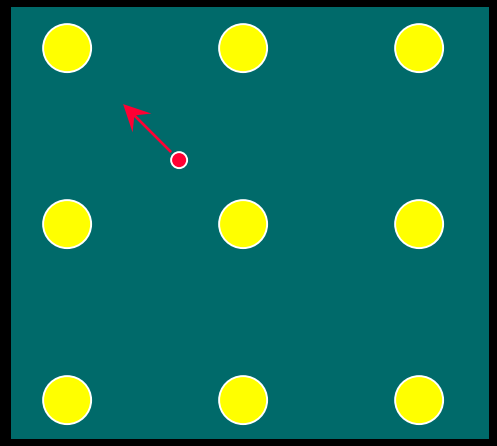
Many-electron problem



electron-electron interaction
electron-nucleus interaction
many-electron Schrödinger equation

Density Functional Theory

One-electron problem



One electron swims in a "swamp,"
described by potential: $V_{\text{eff}}[\rho(\mathbf{r})]$
with Kohn-Sham equation

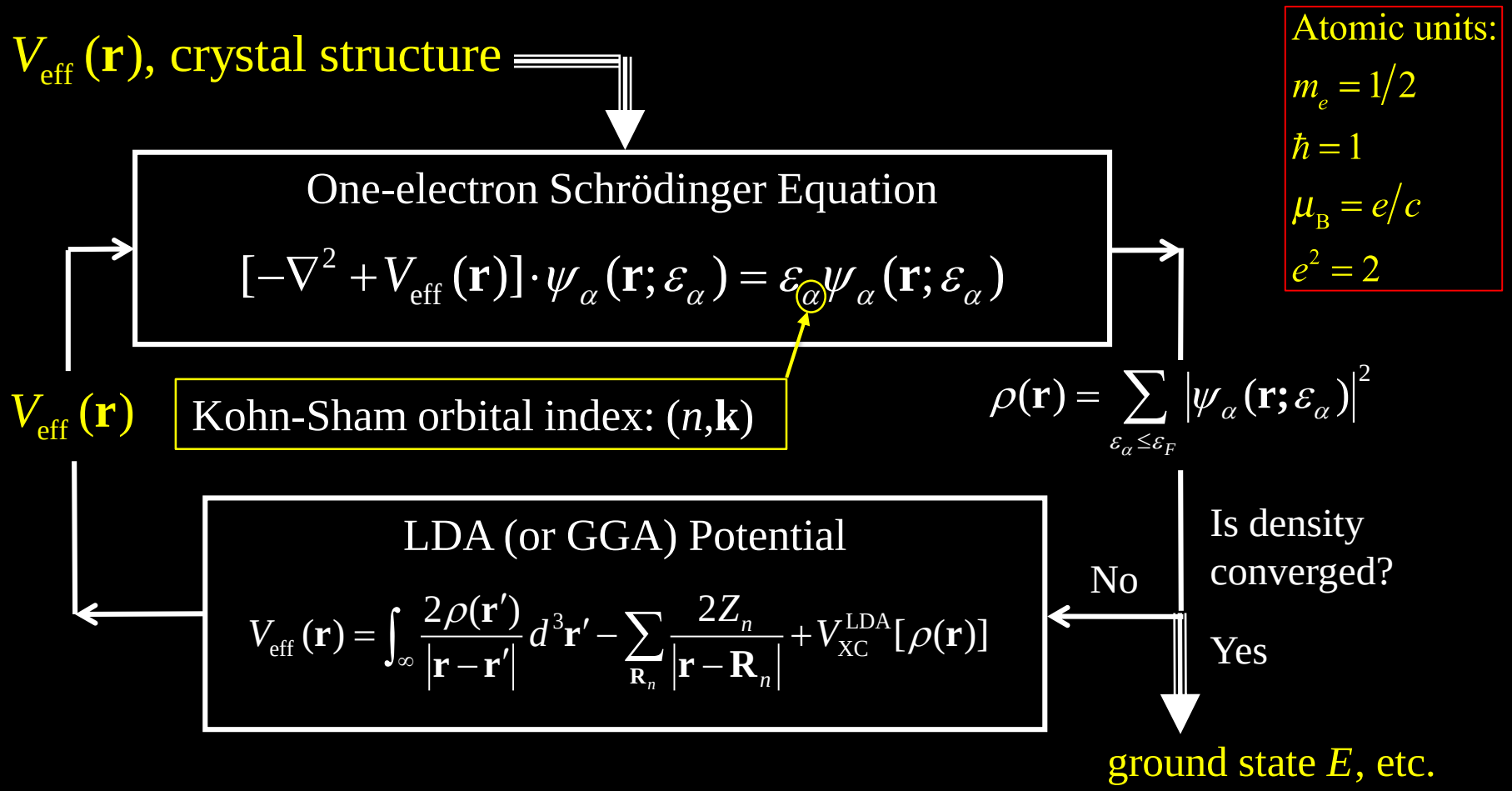
$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 + e^2\int_\infty \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}' - e^2\sum_{\vec{R}_n}\frac{Z_n}{|\mathbf{r}-\mathbf{R}_n|} + V_{\text{xc}}[\rho]\right)\psi_\alpha(\mathbf{r}) = \varepsilon_\alpha\psi_\alpha(\mathbf{r})$$

Prof. Walter Kohn
Awarded the Nobel Prize
in Chemistry in 1998

Find $\rho(\mathbf{r}) = \sum_\alpha |\psi_\alpha(\mathbf{r})|^2$ so that
Kohn-Sham equation is satisfied

$\psi_\alpha(\mathbf{r})$ is called Kohn-Sham orbital

The Self-consistent Process in an *Ab initio* Electronic Structure Calculation



Atomic units:

$m_e = 1/2$

$\hbar = 1$

$\mu_B = e/c$

$e^2 = 2$

$$E[\rho] = \int_{-\infty}^{\varepsilon_F} \varepsilon\rho(\varepsilon)d\varepsilon - \int_\infty \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}d^3\mathbf{r}' - \int_\infty V_{\text{XC}}^{\text{LDA}}(\mathbf{r})\rho(\mathbf{r})d^3\mathbf{r} + E_{\text{XC}}^{\text{LDA}}[\rho]$$

Ab initio Methods

They differ in the way of calculating the electron density $\rho(\mathbf{r}) = \sum_{\varepsilon_\alpha \le \varepsilon_F} \left|\psi_\alpha(\mathbf{r};\varepsilon_\alpha)\right|^2$

- Band structure approach: Solving the Kohn-Sham equation to obtain the Kohn-Sham orbital $\psi_\alpha(\mathbf{r};\varepsilon_\alpha)$
  - Pseudopotential methods
    - Planewave basis (VASP, QuantumEspresso, Abinit, etc.)
    - Multi-grid, Finite elements
  - All-electron methods, usually using local orbital basis
    - FLAPW (WIEN2K, ELK, FLEUR, FLAIR, etc)
    - KKR (MuST, JuKKR, SPR-KKR, Akai-KKR)
      - also known as multiple scattering theory approach
      - theoretically it gives the exact solution of the Kohn-Sham equation
    - LMTO, EMTO, etc

$$[-\nabla^2 + V_{\text{eff}}(\mathbf{r})]\cdot\psi_\alpha(\mathbf{r};\varepsilon_\alpha) = \varepsilon_\alpha\psi_\alpha(\mathbf{r};\varepsilon_\alpha)$$

- Green function approach: Calculating the Green function of the Kohn-Sham equation, instead of solving the Kohn-Sham equation
  - KKR (MuST, JuKKR, SPR-KKR, Akai-KKR)

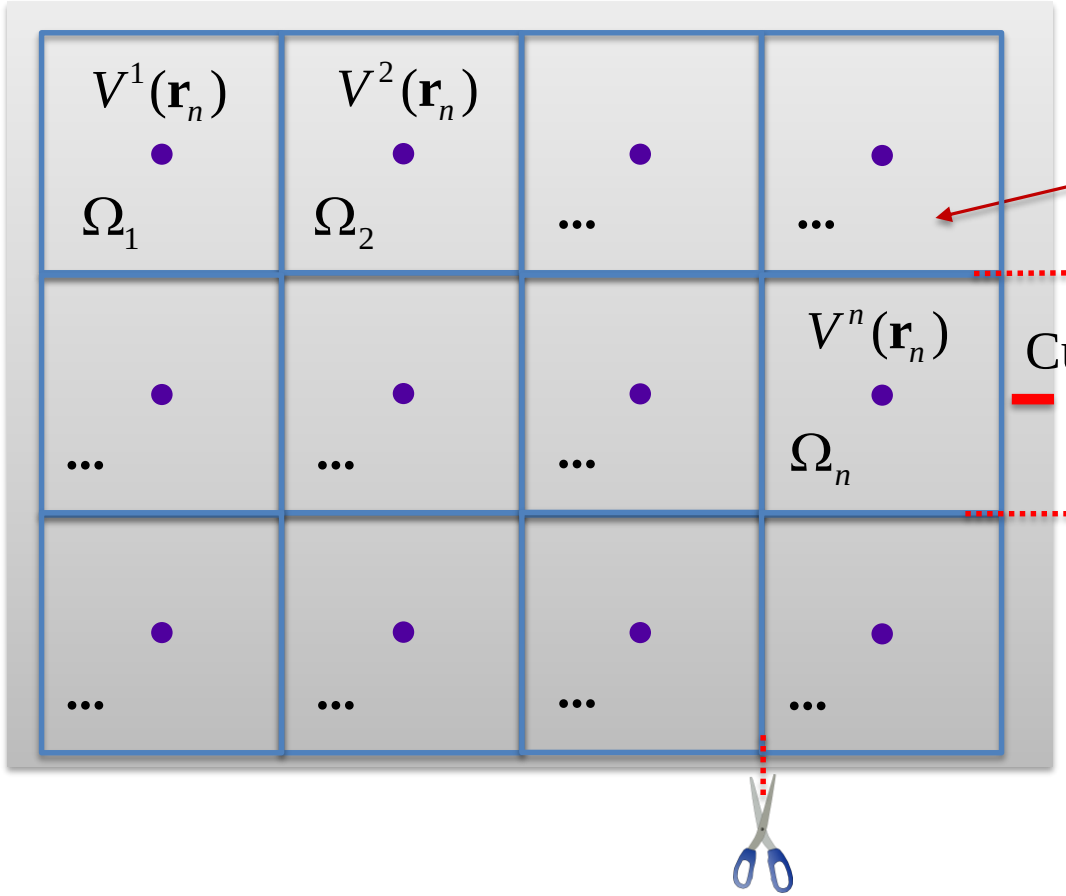
$$\rho(\mathbf{r}) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_F} G(\mathbf{r},\mathbf{r};\varepsilon)\,d\varepsilon.$$

From Solid to Atom

In the point of view of multiple scattering theory

Density function theory with LDA/GGA approximation enables us to find the electron density of the ground state of solids

This is achieved by solving the Kohn-Sham equation, which is an one-electron Schrödinger equation with effective potential $V_{\text{eff}}(\mathbf{r})$



$$V^n(\mathbf{r}_n) = \begin{cases} V_{\text{eff}}(\mathbf{r}), & \text{if } \mathbf{r} \in \Omega_n; \\ 0, & \text{else.} \end{cases}$$

$$\mathbf{r}_n = \mathbf{r} - \mathbf{R}_n$$

$$V_{\text{eff}}(\mathbf{r}) = \sum_n V^n(\mathbf{r}_n)$$

$V^n(\mathbf{r}_n)$: single site scattering potential.

$\rightarrow$ single site scattering t-matrix, $\underline{t}^n(\varepsilon)$.

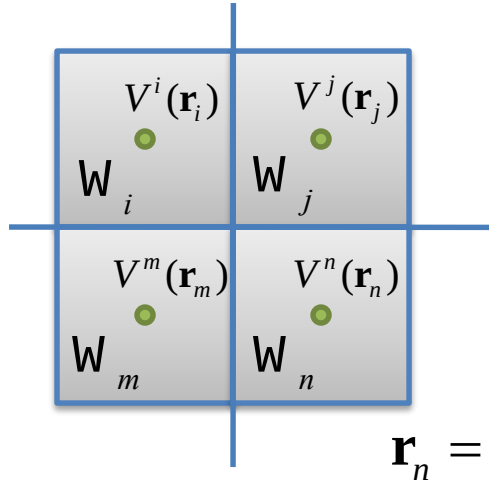
Multiple Scattering Theory (MST) Approach

- Also known as the KKR method, or Green function method
- The Kohn-Sham effective potential is considered as a collection of non-overlapping electronic scattering potentials centered at each atom
- The Kohn-Sham orbital wavefunctions (i.e., the Bloch waves) are the standing save solution of the one-electron multiple scattering processes
- Unlike other *ab initio* methods (e.g. FLAPW), it is Not based on Rayleigh-Ritz variation
- Allows convenient calculation of the Green function
  - No need for band structure calculation
  - No wavefunction normalization and orthogonalization
  - MST methods: KKR, LSMS, KKR-CPA, etc.

single scattering matrix multiple scattering matrix

$$V^n(\mathbf{r}_n) \rightarrow \underline{t}^n(\varepsilon) \rightarrow \underline{\tau}^{nm}(\varepsilon) \rightarrow G(\mathbf{r}_n,\mathbf{r}_n;\varepsilon) \rightarrow \rho(\mathbf{r}) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_F} G(\mathbf{r}_n,\mathbf{r}_n;\varepsilon)\,d\varepsilon$$

$$V^n(\mathbf{r}_n) = V_{\mathrm{eff}}(\mathbf{r}), \quad \text{for } \mathbf{r} \in \Omega_n$$



$$\mathbf{r}_n = \mathbf{r} - \mathbf{R}_n$$

What is MuST?

MuST stands for **Mu**ltiple **S**cattering **T**heory

- Multiple scattering theory is a method for solving the Kohn-Sham equation, which is an one-electron Schrödinger equation describing the electronic structure in solids
- Specifically, it calculates the Green function of the Kohn-Sham equation, and determine the electron density by taking the imaginary part of the Green function

MuST is a computational tool for *ab initio* electronic structure calculations

- So called *ab initio*, it implies that the electronic structure is determined based on fundamental physical law, which in this case is quantum mechanics, rather than on empirical models with adjustable parameters
- Other popular ab initio software packages include VASP, WIEN2K, ELK, Abinit, Quantum Espresso, etc., which are based on different methods (other than multiple scattering theory) for solving the Kohn-Sham equation.

Obtaining the package

```
$ git clone https://github.com/mstsuite/MuST
```

A directory called `MuST` is created in your local space

MuST: A Multiple Scattering Theory based Computational Framework for the First Principles Study of Disordered Materials

- A collaborative 3-year project funded by NSF CSSI program
  - involving researchers from CMU, LSU, MTSU, and ORNL, and collaborators from Germany and China
- A computational framework based on scalable approach to the first principles studies of random alloys and disorder effects in quantum materials
- Built on the research codes developed at ORNL and PSC
  - DFT based ab initio codes: KKR, KKR-CPA, LSMS
  - Effective medium methods: DMFT, DCA, TMDCA
- An open software package available on GitHub (https://github.com/mstsuite/MuST)

Wiki page:
https://github.com/mstsuite/MuST/wiki/Must-Wiki

Youtube channel:
https://www.youtube.com/channel/UCvlVeAb_m4kvBa-3_q43TIQ

MuST Team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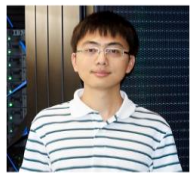
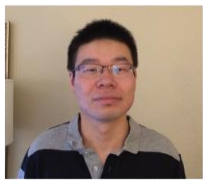

Xianglin Liu


Liviu Chioncel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Equation of state, elastic constants and force for Mo

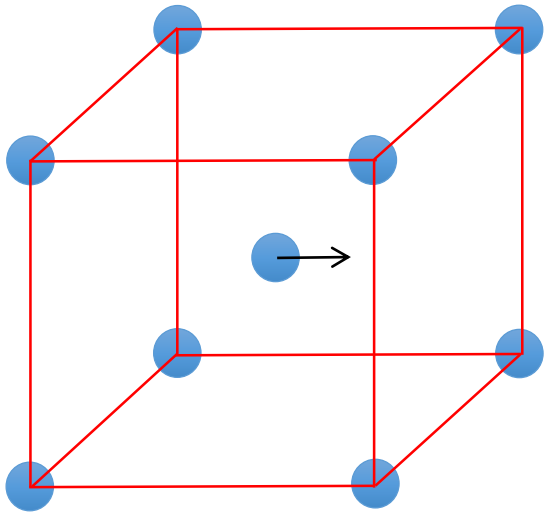
Mo	a (Bohr)	B (GPa)	B′(GPa/Bohr^3)	c′(GPa)	c_{11}(GPa)	c_{12}(GPa)	c_{44}(GPa)
Exp.	5.947	261.00		152.95	463.70	157.80	109.20
MuST	5.975	258.09	2.21	168.93	483.33	145.48	131.13
WIEN2k	5.973	263.47	3.99	147.45	460.07	165.17	103.15
EMTO	5.991	254.21	4.89	169.80	480.61	141.01	131.02
VASP	5.978	263.08	3.15	148.57	461.18	164.03	102.56

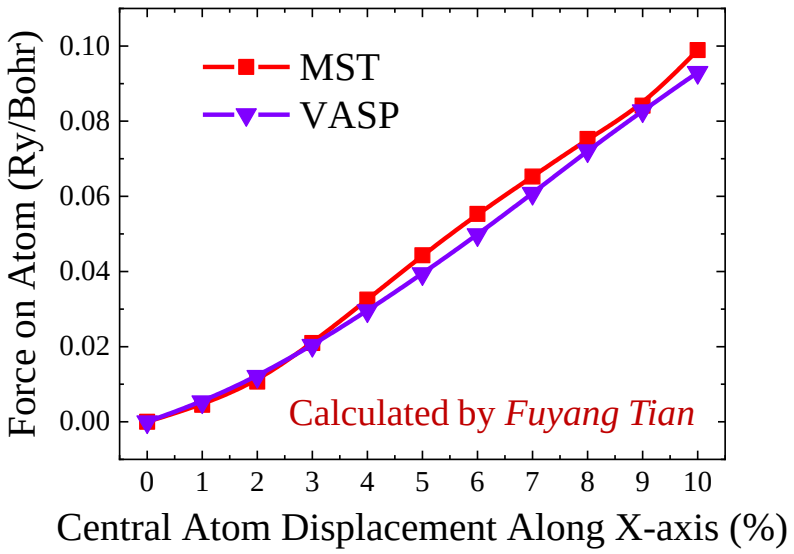
The results are provided by *Fuyang Tian*

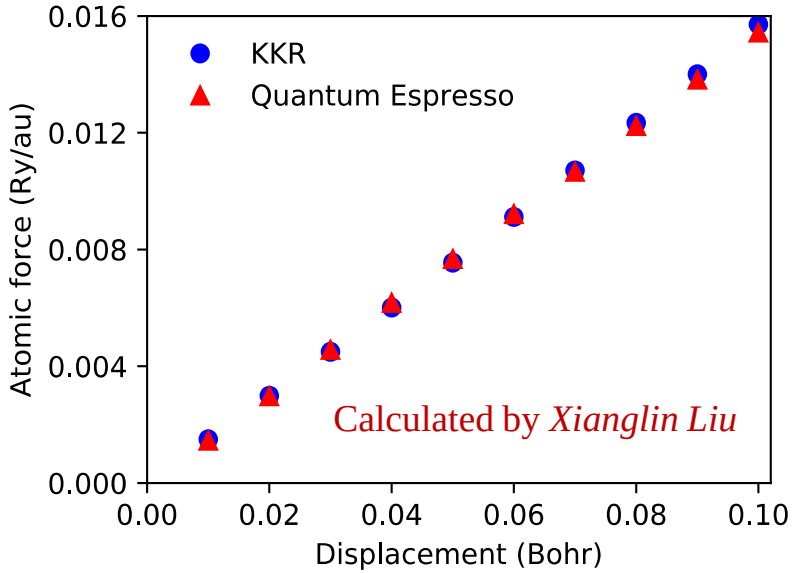
In MST and EMTO: *4s4p* are treated as semi-core states

In WIEN2K and VASP: *4s4p* are treated as valence states

The Hellmann-Feynman force on Mo atoms







Relativistic Effects in Materials

- Magnetic anisotropy, arising from the spin-orbit coupling effect
- Magneto-optical effects
- Bond length contraction

A Recall of Bohr's Model

Bohr orbital radius: $R_n = \frac{n^2}{m_e Z e^2}$

Speed of electron: $v_n = \frac{\hbar Z e^2}{n}$.

In particular for $n = 1$, $v_1 = \alpha Z c$, $Z \approx \frac{1}{\alpha} = 137$.

Relativistic effect: $R_{rel} = R_{non\text{-}rel}\sqrt{1 - \frac{v^2}{c^2}}$

- Color of gold (Z=79)

  the 5*d* orbital is raised in energy and the 6*s* orbital is lowered in energy, so that the 5*d* to 6*s* absorption occurs in the blue region of the spectrum, resulting in a yellowish color for light reflected from gold. In addition, its resistance to tarnishing and corrosion are also the consequences of special relativity, due to contraction of the 6*s* outer shell.

- Low melting temperature of mercury (Z=80)

  It was demonstrated recently (Schwerdtfeger *et al*, 2013) that nonrelativistic mercury would be a solid at room temperature, while a scalar-relativistic approach allows to reproduce the melting temperature very well. The contraction of the outer electron orbital makes mercury reluctant to form bonds. It is this lack of electron bonding between mercury atoms that makes it melt and boil at such low temperatures.

Kohn-Sham-Dirac Equation

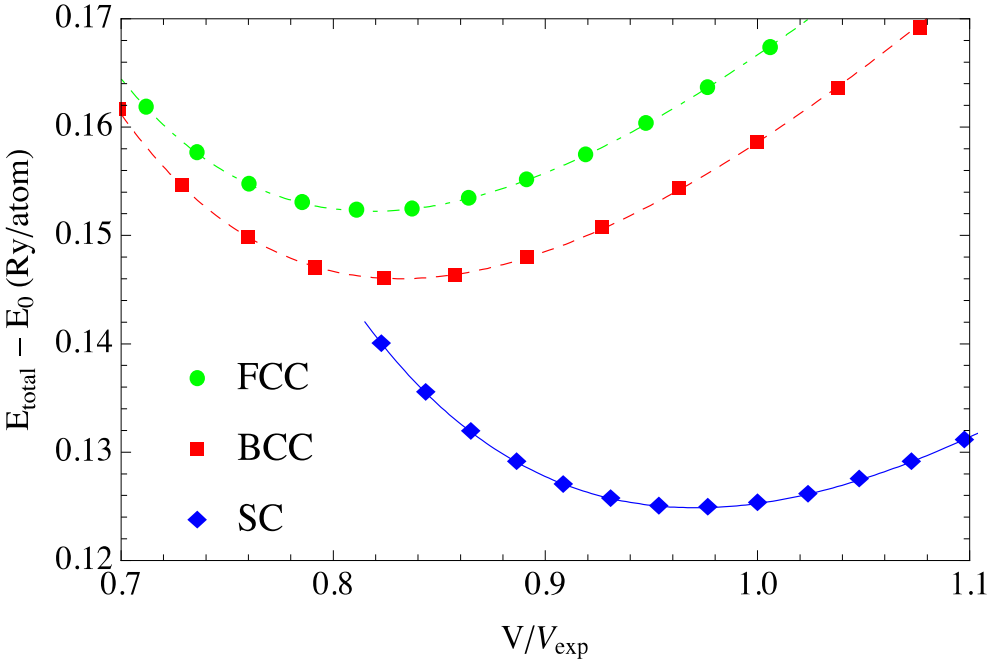
$$\left[c\underline{\boldsymbol{\alpha}} \cdot \left(-i\nabla + \mu_B \mathbf{A}_{\text{eff}}(\mathbf{r}) \right) + (\underline{\beta} - 1)\frac{c^2}{2} + V_{\text{eff}}(\mathbf{r}) \right] \underline{\psi}(\mathbf{r};\varepsilon) = \varepsilon \underline{\psi}(\mathbf{r};\varepsilon)$$

An Investigation of Polonium (Z = 84)

- Highly toxic and radioactive
- Only element with simple cubic structure at ambient condition
- Due to its high *Z*, relativity effects need to be taken into account
- It is generally believed that the SC structure is driven by relativity

Relativistic KKR calculation

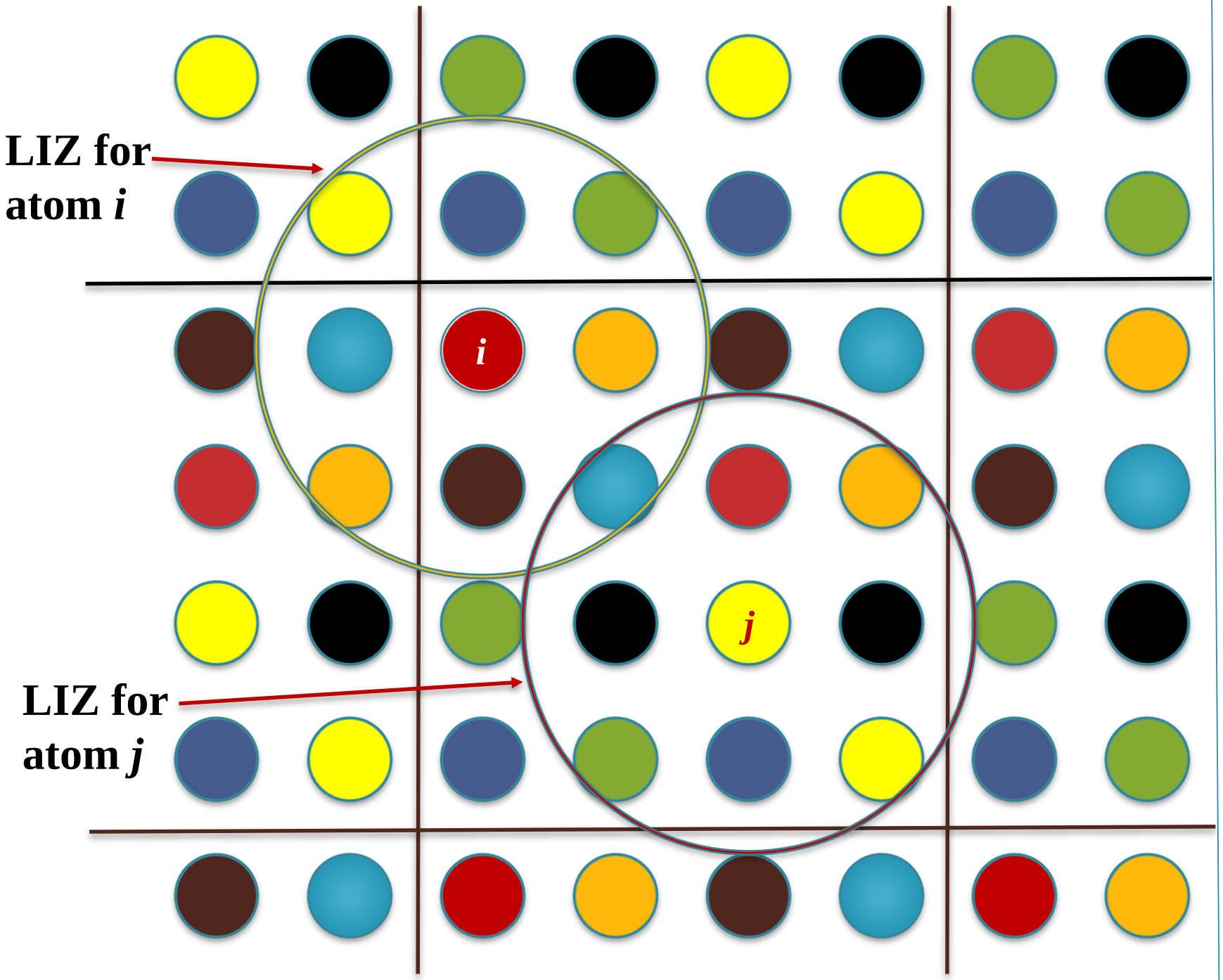
- Both valence and core states are calculated fully-relativistically
- Full-potential multiple scattering theory (KKR method)
- LDA potential
- Good agreement with other methods and experiment results.



Method	a(Å)	B_0(GPa)
MuST (LDA+Dirac)	3.327	55.1
TB+SO	3.29	51
LDA+SO, FLAPW (1)	3.323	42.3
LDA+SO, FLAPW (2)	3.334	47.35
GGA+SO, FLAPW	3.34	
LDA, PP	3.28	56
Experiment	3.359 (1) 3.345 (2)	

Ab initio Approaches to Random Alloys

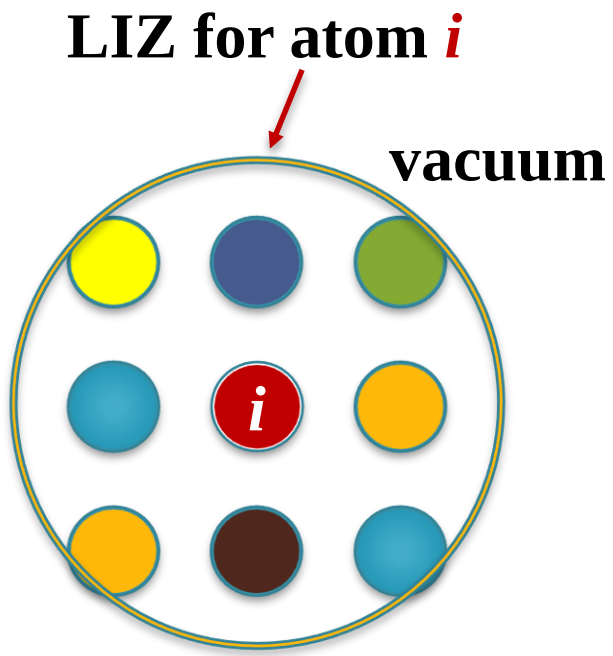
- Supercell approach
  - LSMS (linear scaling allow to study very large unit cell containing 10,000 atoms or more)
- Cluster expansion approach, e.g., special quasi-random structures (SQS)
  - KKR + SQS
- Effective medium approach with coherent potential approximation (CPA)
  - KKR-CPA



Locally Self-consistent Multiple Scattering (LSMS) Method

The LIZ cluster with M atoms is embedded in vacuum

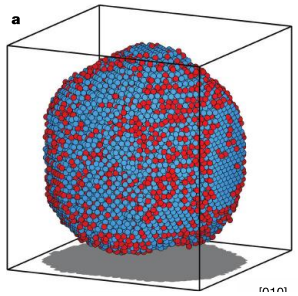
$$\underline{\tau}^{11}(\varepsilon) = \begin{bmatrix} \underline{t}_1^{-1}(\varepsilon) & \cdots & -\underline{g}_{1M}(\varepsilon) \\ \vdots & \ddots & \vdots \\ -\underline{g}_{M1}(\varepsilon) & \cdots & \underline{t}_M^{-1}(\varepsilon) \end{bmatrix}^{-1}_{11}$$

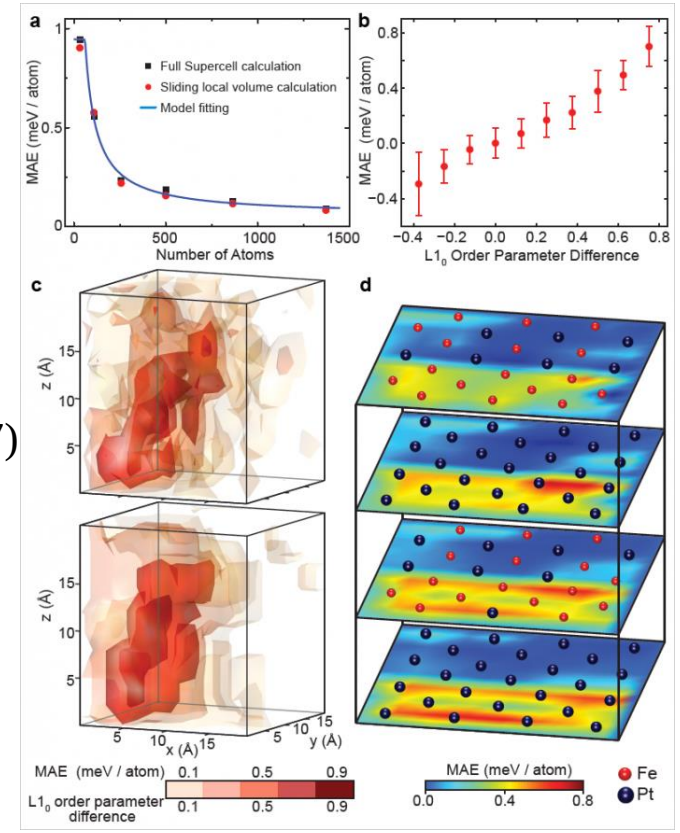


Locally Self-consistent Multiple Scattering (LSMS) Method

- Linear scaling is made possible by ignoring the multiple scattering processes outside a finite region (LIZ) centered at each atom
  - Computational cost depends (~ O[M^3])on the size of the LIZ (M atoms)
  - Computational cost depends linearly (~ O[N]) on the number of atoms in the unit cell (N atoms)
  - Intrinsically parallel over the atoms in the unit cell
- Allows to perform *ab initio* calculations for >100,000 atoms
- Gordon Bell Prize Winner in Year 1998 and Year 2009 for exceeding teraflop and petaflop performance, respectively.
- Computer World Smithsonian Award (Year 2000)
- One of the 8 scientific application projects selected recently by Center for Accelerated Application Readiness (CAAR) for **Frontier**, which is DoE's Exascale supercomputer to become available in 2021, and open to users in 2022.

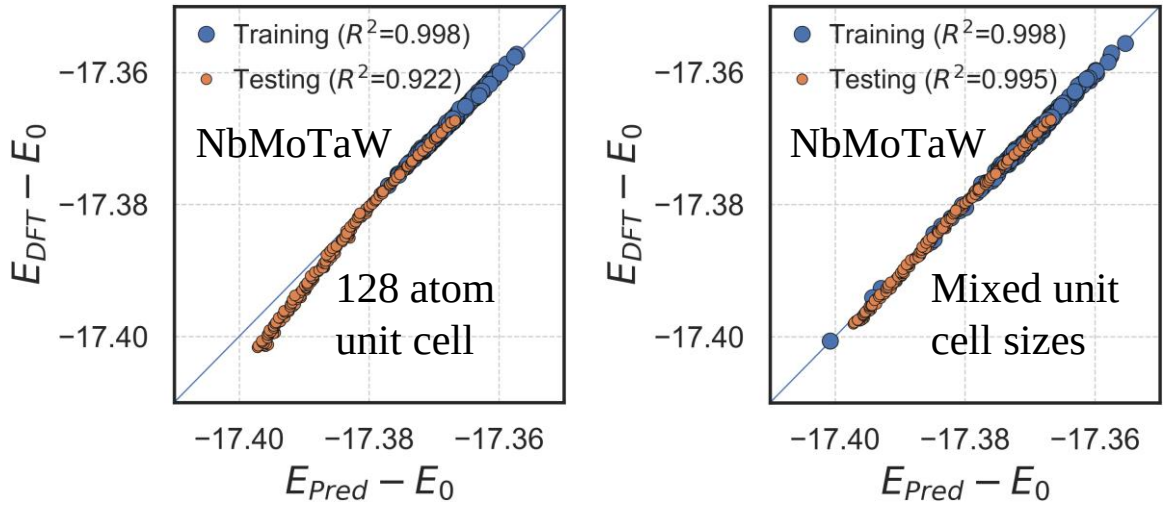
First Principles Calculations for Materials with Complex Structures





Magnetism in FePt.
Nature **542**, 75 (2017)

The experimentally determined coordinates of 6,569 Fe and 16,627 Pt atoms in an FePt nanoparticle are used as direct input for the DFT calculations, with the LSMS method, of material properties such as atomic spin and orbital magnetic moments and local magnetocrystalline anisotropy.



Xianglin Liu, et al, https://arxiv.org/abs/1906.02889

The use of the linear-scaling LSMS greatly improves the calculation speed of the energies, allowing the use of a larger DFT dataset and the direct evaluation of the configurations to construct a data-driven framework, which includes a learned effective Hamiltonian, for the study of multicomponent high entropy alloys.

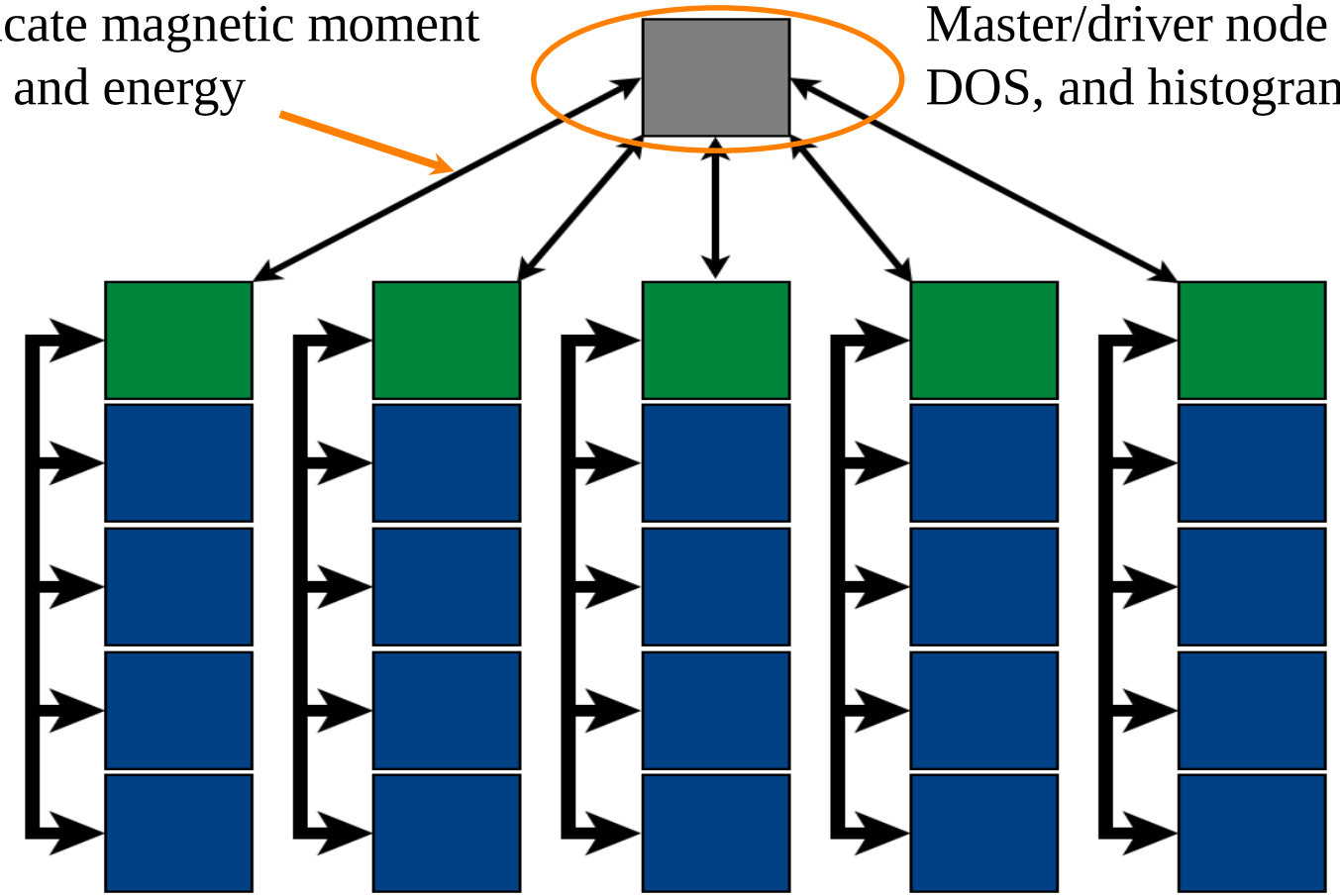
In this study, the energy data is trained using Bayesian Ridge regression. The testing data set consists of 200 different 1024-atom supercell structures.

Ab Initio Magnetic Materials Simulation at Petascale

Wang-Landau Monte-Carlo: $Z(\beta) = \sum_{\{x_i\}} e^{-\beta H(\{x_i\})} = g_0 \int g(E) e^{-\beta E}\, dE$

Communicate magnetic moment directions and energy

Master/driver node controlling WL acceptance, DOS, and histogram



LSMS is used to compute the energy of each spin orientation configuration sample

16 Fe atoms (2x2x2 cell)

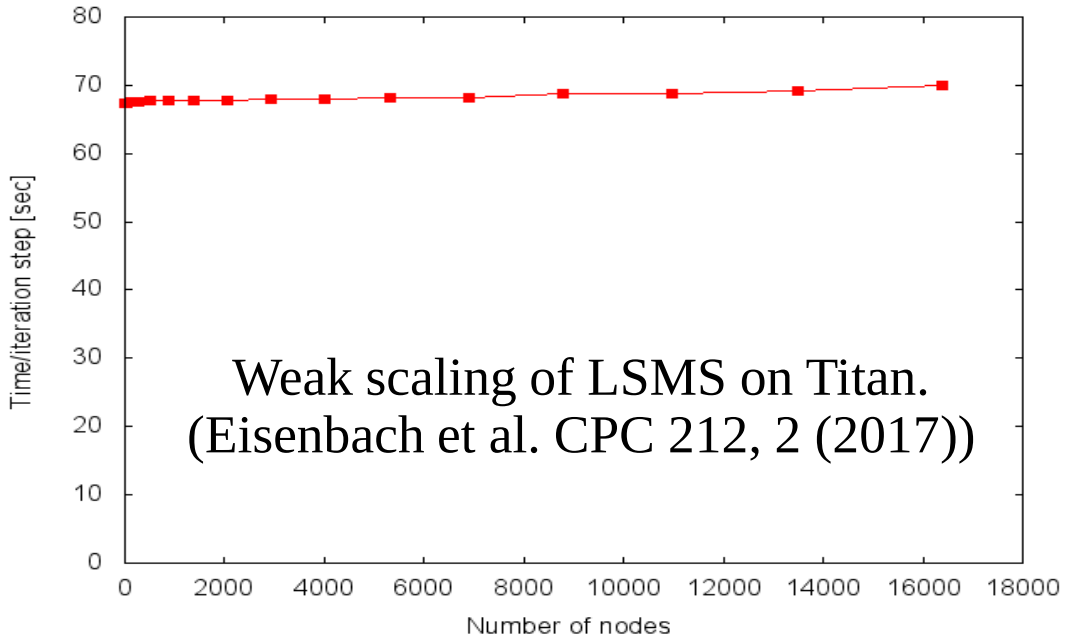
T_c=670K,

250 Fe atoms (5x5x5 cell)

T_c=980K, compared to experimental value 1050K

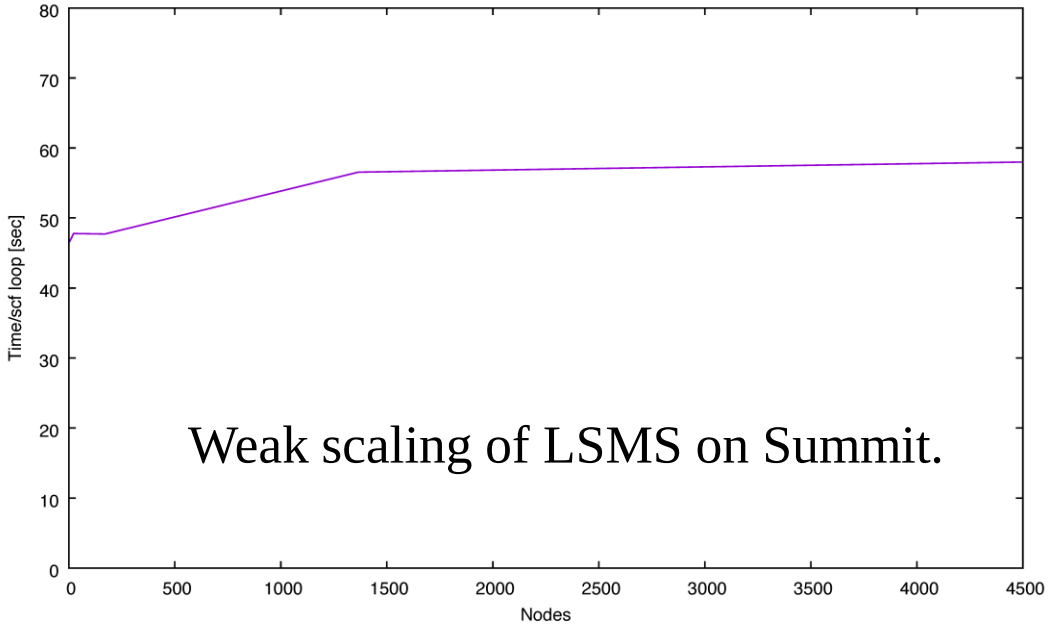
1024-atom simulation: 18,561 Titan nodes (99% of Titan). **14.5** PFLOPS accelerated with 3.5 MW-H vs **1.86** PFLOPS CPU only with 25.7 MW-H

Scalability of LSMS Method



Weak scaling of LSMS on Titan.
(Eisenbach et al. CPC 212, 2 (2017))

- Utilizing the GPU accelerators for a bulk iron calculation
- 16 atoms on 4 nodes: 67.343 wall-clock seconds per SCF iteration
- 65536 atoms on 16384 nodes: 69.988 wall-clock seconds per SCF iteration
- Parallel scaling efficiency: 96% across the machine

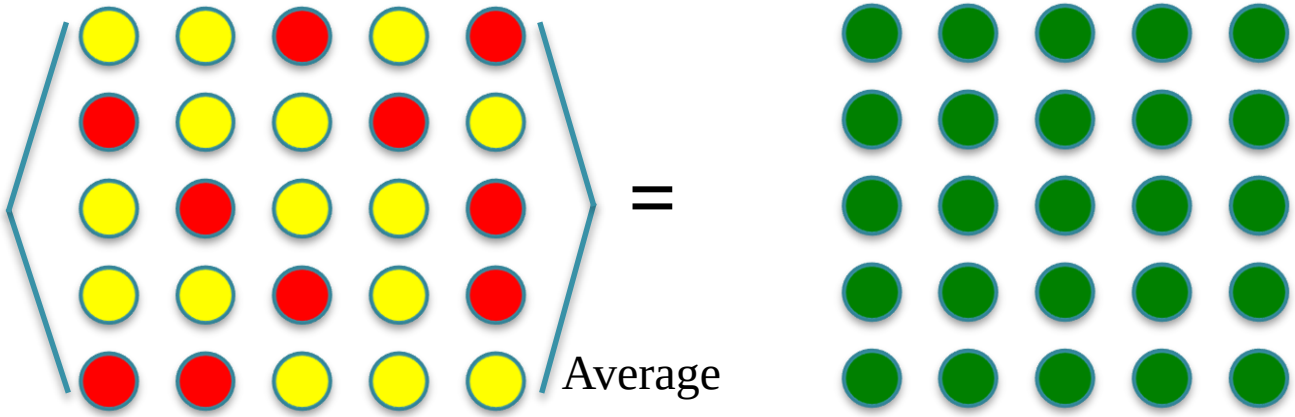


Weak scaling of LSMS on Summit.

- Strong scaling of LSMS for a 128 atom test case on both Titan and Summit from 2 to 64 GPUs. The ratio of execution time for 2 GPUs is 4.6
- Weak scaling of LSMS on Summit using GPUs from 3 nodes for 128 atoms to 4500 nodes (98% of the full machine) for 216,000 atoms

atom 1: atom 2: CPA medium:

The effective medium "atom" is described by its single site scattering *t*-matrix

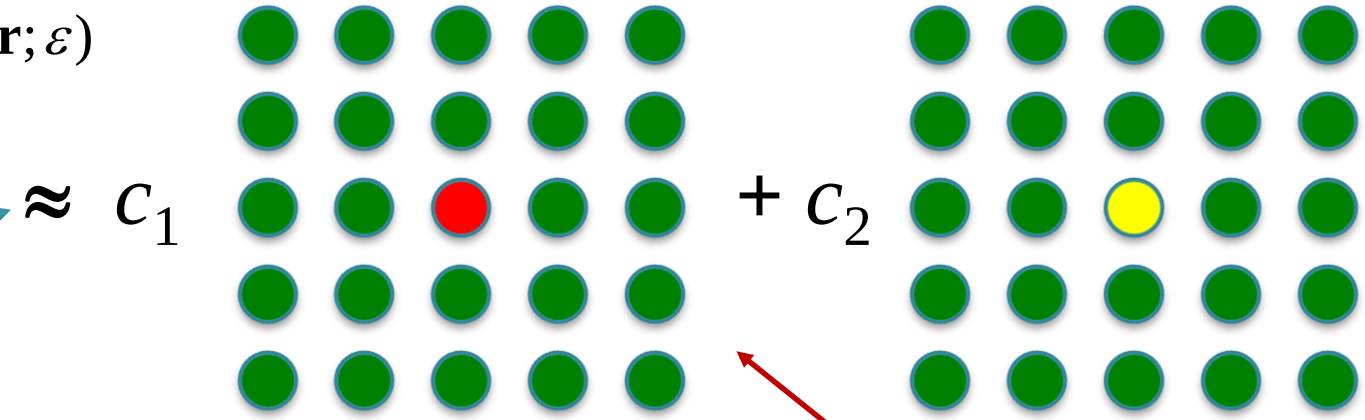


KKR-CPA Method

Coherent potential approximation (CPA) allows to find an effective medium that gives configurational averaged properties of a random alloy

$$\langle G(\mathbf{r},\mathbf{r};\varepsilon)\rangle_{\text{ave}} = \sum_{\alpha=1}^{N_\alpha} c_\alpha G_\alpha(\mathbf{r},\mathbf{r};\varepsilon)$$

Single-site approximation



$$\rho_\alpha(\mathbf{r}) = -\frac{1}{\pi}\,\text{Im}\int_{-\infty}^{\varepsilon_F} G_\alpha(\mathbf{r},\mathbf{r};\varepsilon)\,d\varepsilon \qquad \rho(\mathbf{r}) = \sum_{\alpha=1}^{N_\alpha} c_\alpha \rho_\alpha(\mathbf{r})$$

These are a single impurity problem, and can be solved with 1 atom per unit cell calculation

Take CuZn as an example

CuZn is also known as *brass*.

According to Wikipedia: Although forms of brass have been in use since prehistory, its true nature as a copper-zinc alloy was not understood until the post-medieval period.

Brass has long been a popular material for decoration for its bright gold-like appearance, e.g. for drawer pulls and doorknobs. It has also been widely used for all sorts of utensils due to many properties, such as low melting point, workability (both with hand tools and with modern turning and milling machines), durability, electrical and thermal conductivity.

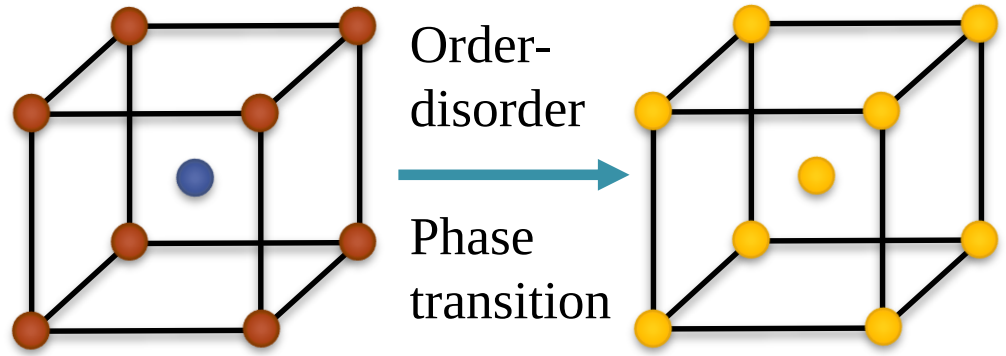
At zero temperature (T = 0 K), CuZn exists as an ordered intermetallic compound in B2 structure (β' phase). As T increases and reaches around 730 K, the materials becomes a random alloy in A2 structure (β phase).

T < 730 K

Cu:

Zn:

β' Phase (B2)



Order-disorder

Phase transition

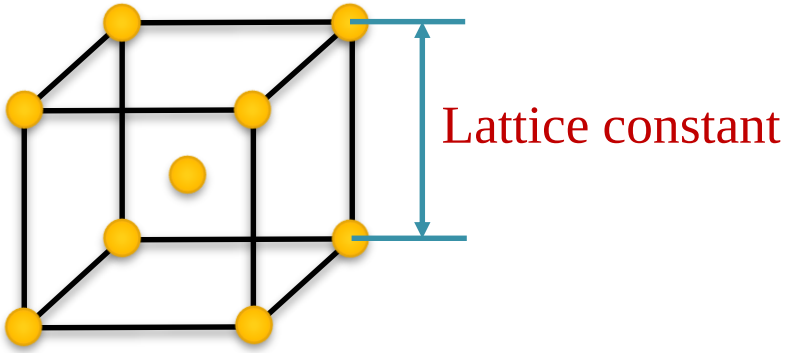
T > 730 K

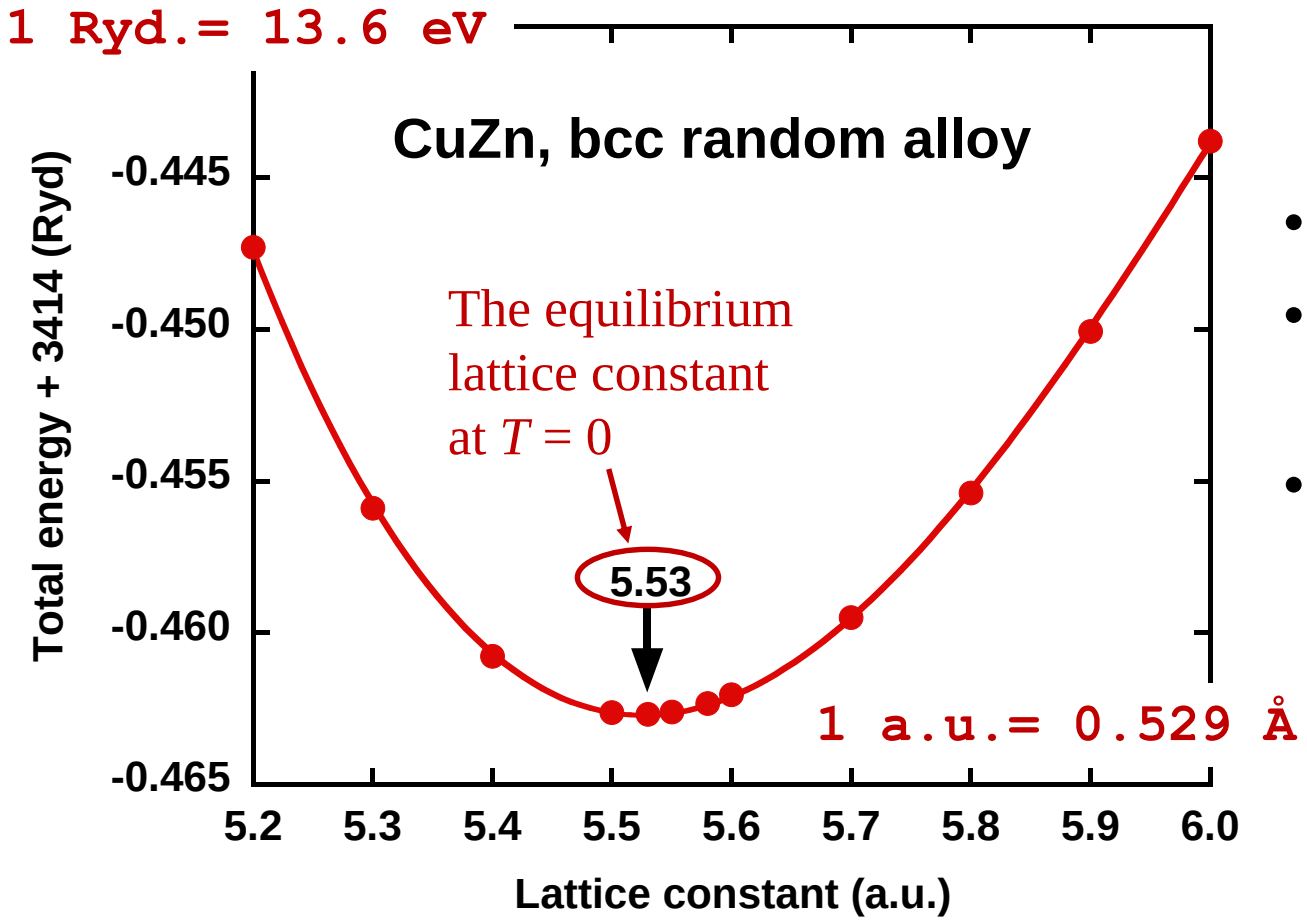
Cu/Zn:

β Phase (A2)

BCC structure

A plot of the total energy versus the lattice constant

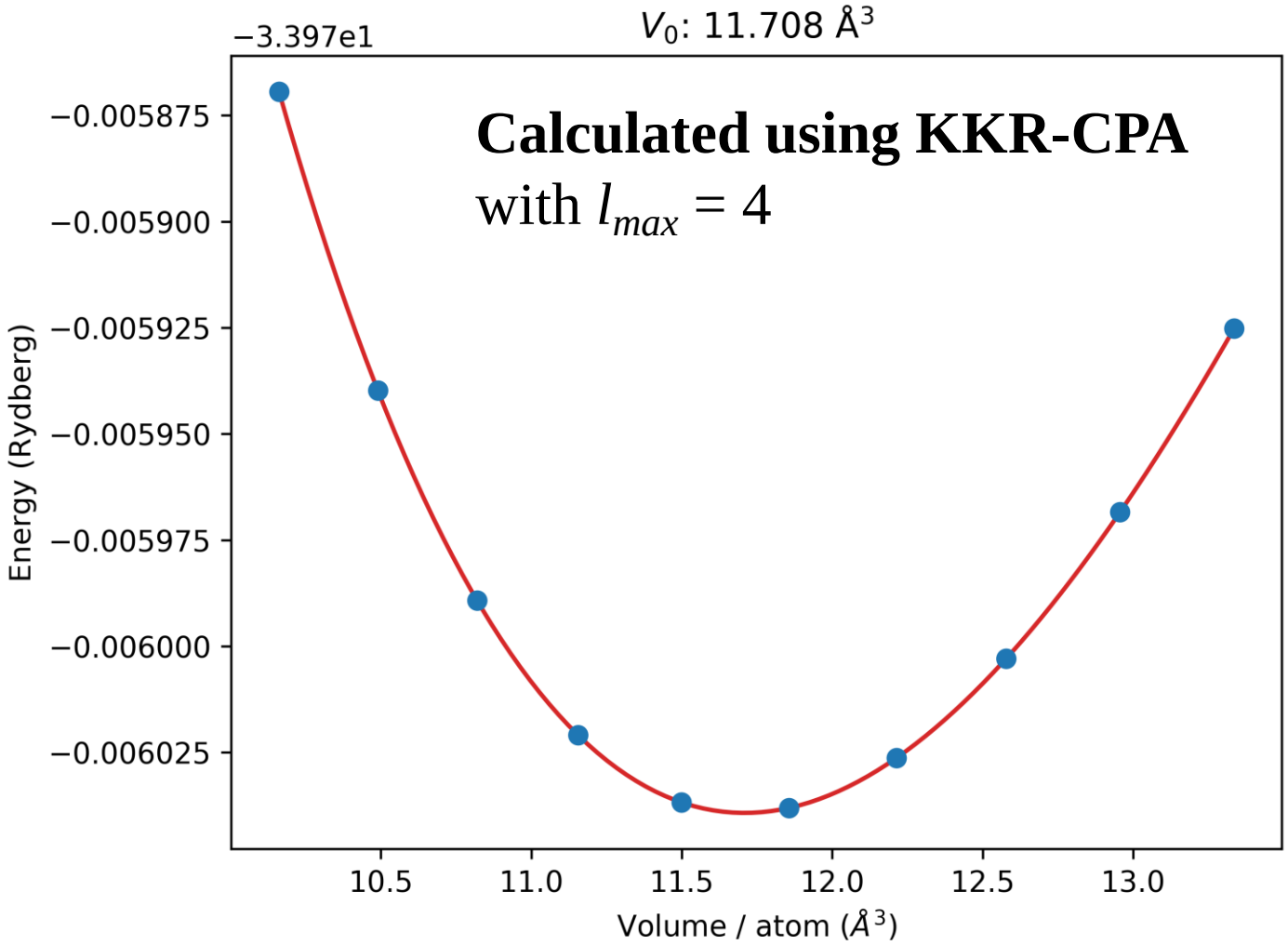




What we can learn from the total energy results

- Equilibrium crystal structure at $T = 0$
- Equilibrium lattice constant of the crystal structure at $T = 0$
- Mechanical properties of the alloy
  - Faster (slower) increase in energy when the lattice is stretched or compressed from its equilibrium state is an indication of harder (softer) material

Al-Cr-Fe-Co-Ni High Entropy Alloys



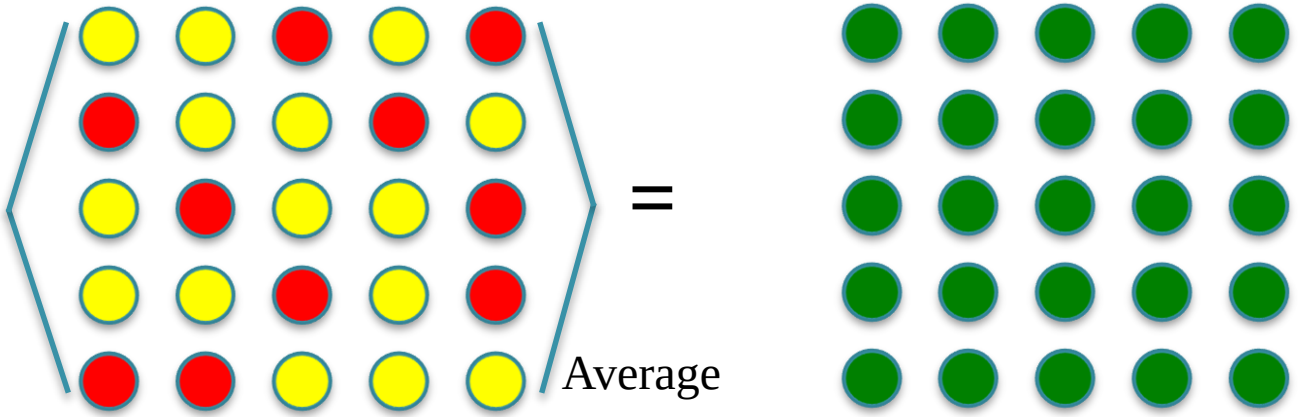
- This is spin-polarized ab initio calculation with only 1 atom in the unit cell
- The concentration of each chemical element can be chosen arbitrarily

	Lattice constant (Å)
Experiment	2.873
VASP + SQS	2.821
MuST (KKR-CPA)	2.861

Calculated by *Amish Chovatiya* and *Zachary W. Ulissi*

This is part of a ECSS project

atom 1: atom 2: CPA medium:

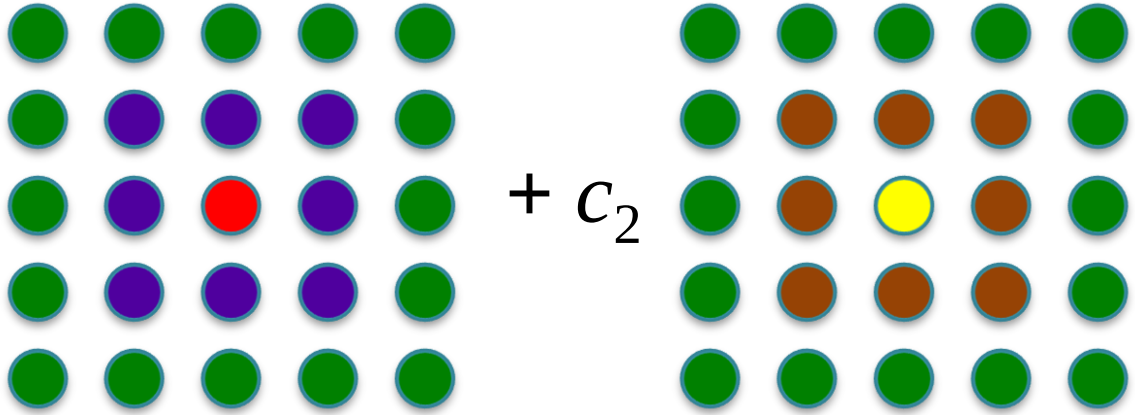


Averaged neighbor:

Embedded cluster:

- The neighboring sites are the averaged "atom."
- The averaging is performed according to the SRO parameters associated with the central atom.

$$\approx c_1 + c_2$$



$$\rho_\alpha(\mathbf{r}) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_F} G_\alpha(\mathbf{r},\mathbf{r};\varepsilon)\,d\varepsilon$$

The average "atom" on the neighboring sites is obtained by averaging the *t*-matrix of the actual atoms, given the species on the central site.

A user community engagement effort

Beyond the conventional KKR-CPA:

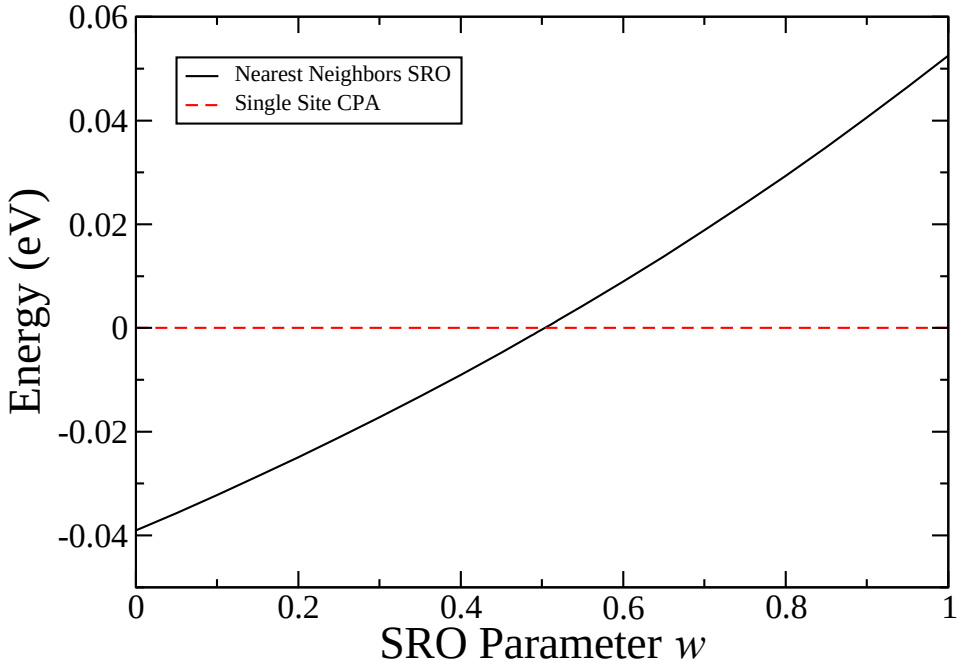
CA-KKR-CPA Method

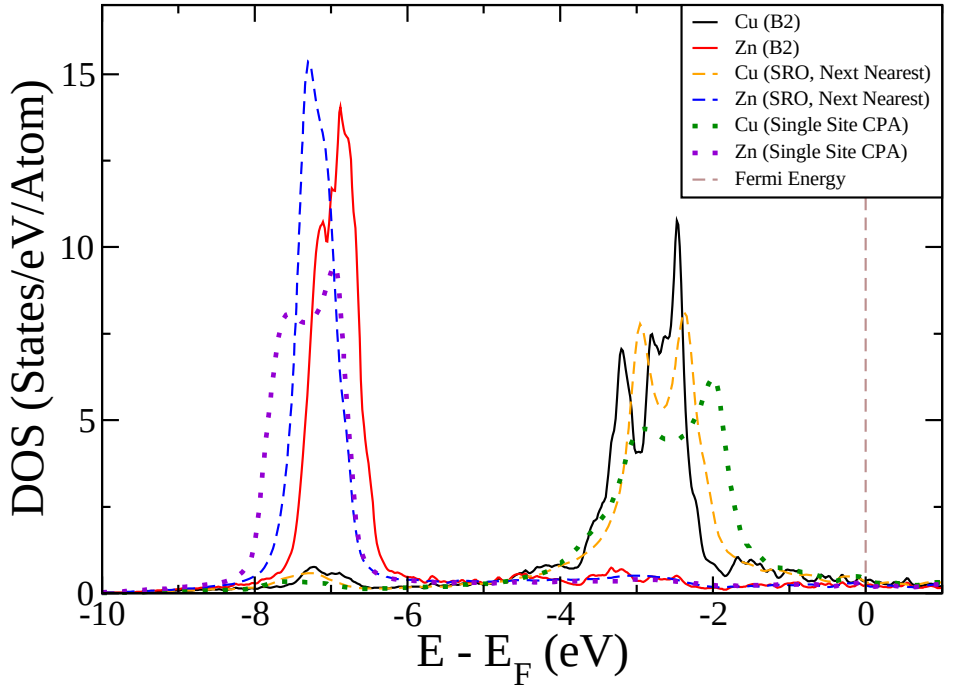
This cluster averaged (CA) embedding method allows to include the short range order effects in the conventional KKR-CPA, where the single site approximation is applied.

Raghuraman, Wang, Widom, Phys. Rev. B **102**, 054207 (2020)

Short Range Order in β-CuZn

- w = 0 refers to the B2 structure (complete short-range ordering) while w = 1 refers to the case of short-range clustering.
- w = 0.5 corresponds to the disordered structure.
- The cluster averaged CPA method demonstrates that CuZn shows short range ordering at low temperatures, which is expected.
- The solid lines are the DOS of Cu and Zn in B2 structure (β' phase)
- The dotted lines are the DOS of Cu and Zn in random structure (β phase)
- the dashed lines are the DOS of Cu and Zn in random structure with short range order
- Disorder is known to produce broadened density of states (DOS), in comparison with the ordered structure
- The broadening of the DOS has reduced due to the addition of short range order in the system.





Raghuraman, Wang, Widom, Phys. Rev. B **102**, 054207 (2020)

Running MuST on Jetstream via Jupyter Hub

A short YouTube video on running the CuZn examples has been prepared by XSEDE Campus Champion, Dr. Helen Kershaw @ Brown University

- https://www.youtube.com/watch?v=ev3nHISrs5Q

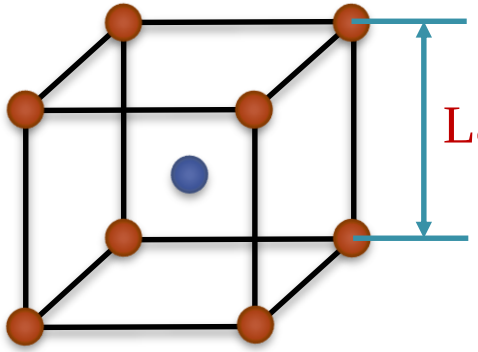
Steps to run the tutorial example under "`MuST/Tutorials/CuZn/B2`"

- Go to webpage: https://must-tutorial.com (created by Dr. Helen Kershaw)
- Click Hub shown on the top banner of the webpage
- Enter your username (`student1`, `student2`, …, or `student40`) and password
- Pull down the menu under New on the upper-right corner and click Terminal
- At the prompt in the new terminal, enter the following commands to run CuZn in the B2 structure:

```
$ cp -r /srv/Tutorials ~/
$ cd Tutorials/CuZn/B2
$ mpirun -n 4 mst2 < i_new
```

Similarly, you can run examples under `Tutorials/CuZn/BCC` and `Tutorials/CuZn/SuperCell`

The total energy of three different CuZn alloy structures



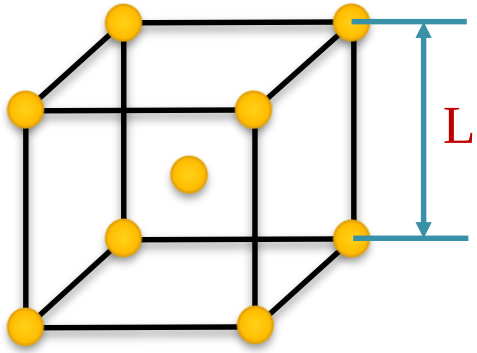
Lattice constant = 5.53 a.u.

Cu:

Zn:

Total energy per atom =−3414.468452 Ryd.

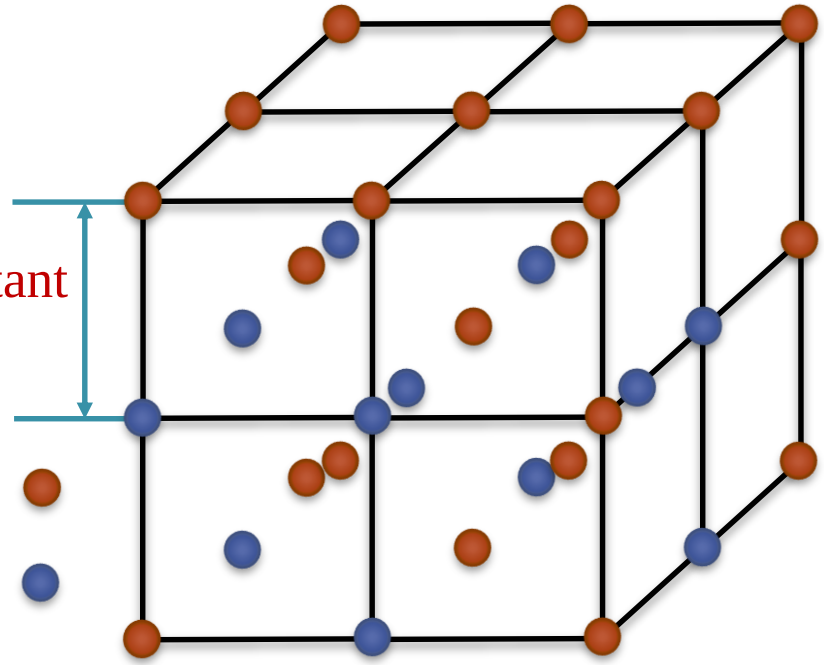
Using this energy difference (ΔE = 0.0058 Ryd = 0.0789 eV), we may estimate the transition temperature in a naive way as follows:
$T_C = \Delta E / k_B \approx \Delta E \cdot 300\ \text{K}/(0.025\ \text{eV}) = 946.6\ \text{K}$



Lattice constant = 5.53 a.u.

Cu/Zn:

Total energy per atom =−3414.462692 Ryd.



Lattice constant
= 5.53 a.u.

8 Cu:

8 Zn:

Total energy per atom =−3414.463548 Ryd.

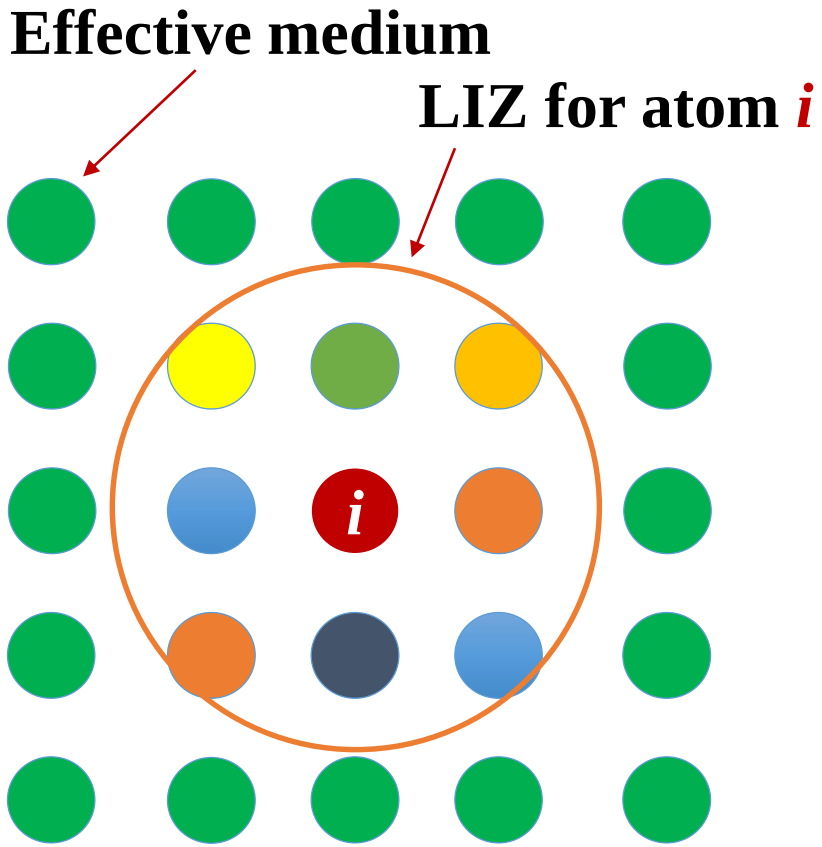
At T = 0, CuZn prefers an ordered structure

- The ordered B2 compound has the lowest energy
- The completely random structure (A2) has the highest energy among the 3 given structures

LSMS with embedding

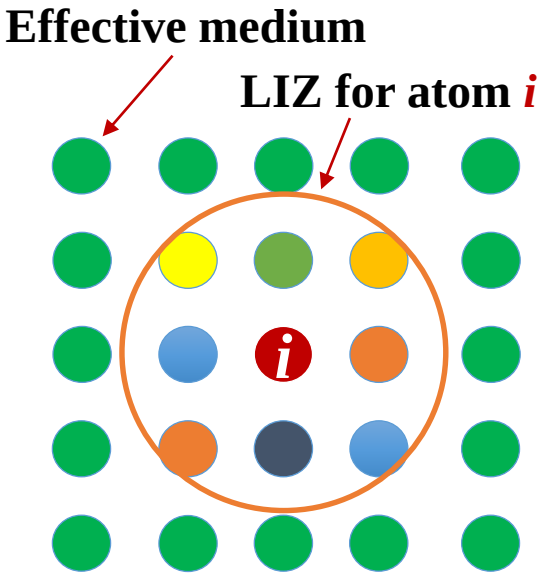
Allows to treat both disorder and strong electron-electron correlation effects

- The LIZ cluster with *M* atoms is embedded in an effective medium
- It is tested in a tight-binding basis and applied to the single band Anderson model by computing the local Green's function of a supercell embedded into a local typical medium.
- It captures the Anderson localization transition and accurately predicts the critical disorder strength.



Zhang *et al*, "Locally self−consistent embedding approach for disordered electronic systems," Phys. Rev. B **100**, 054205 (2019).

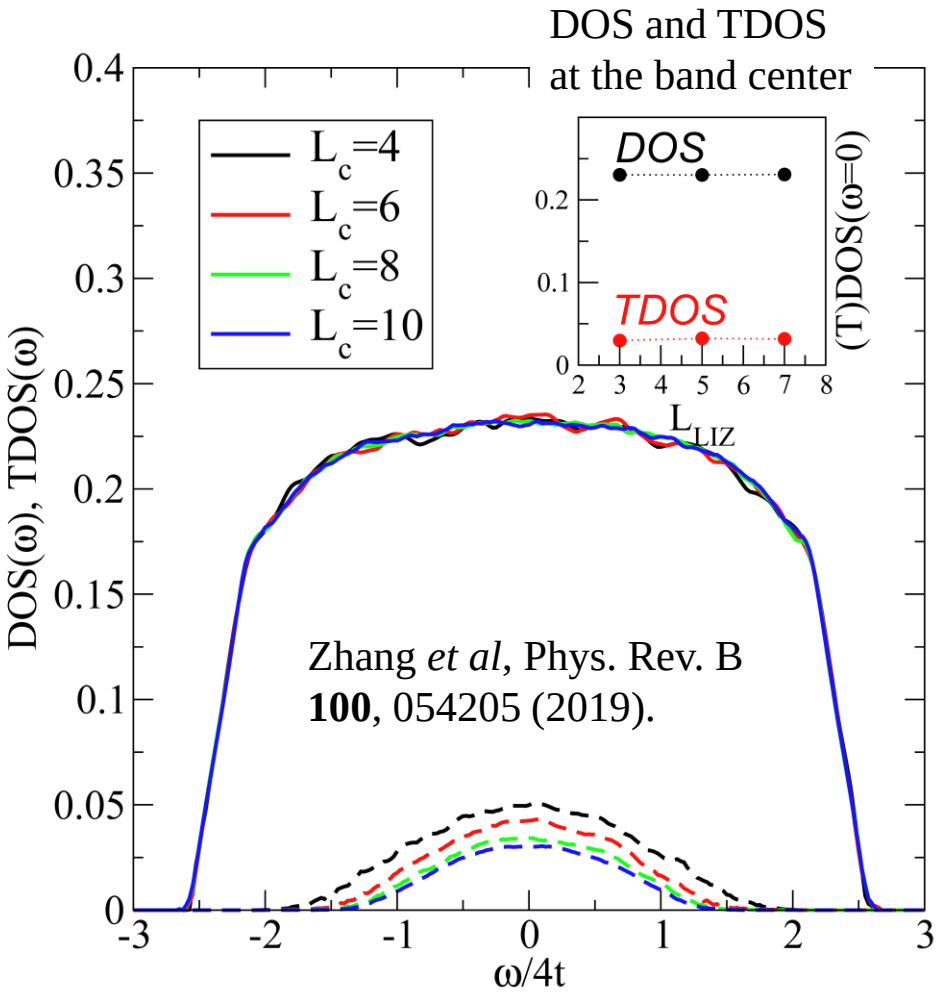
Effective medium approach to disordered materials



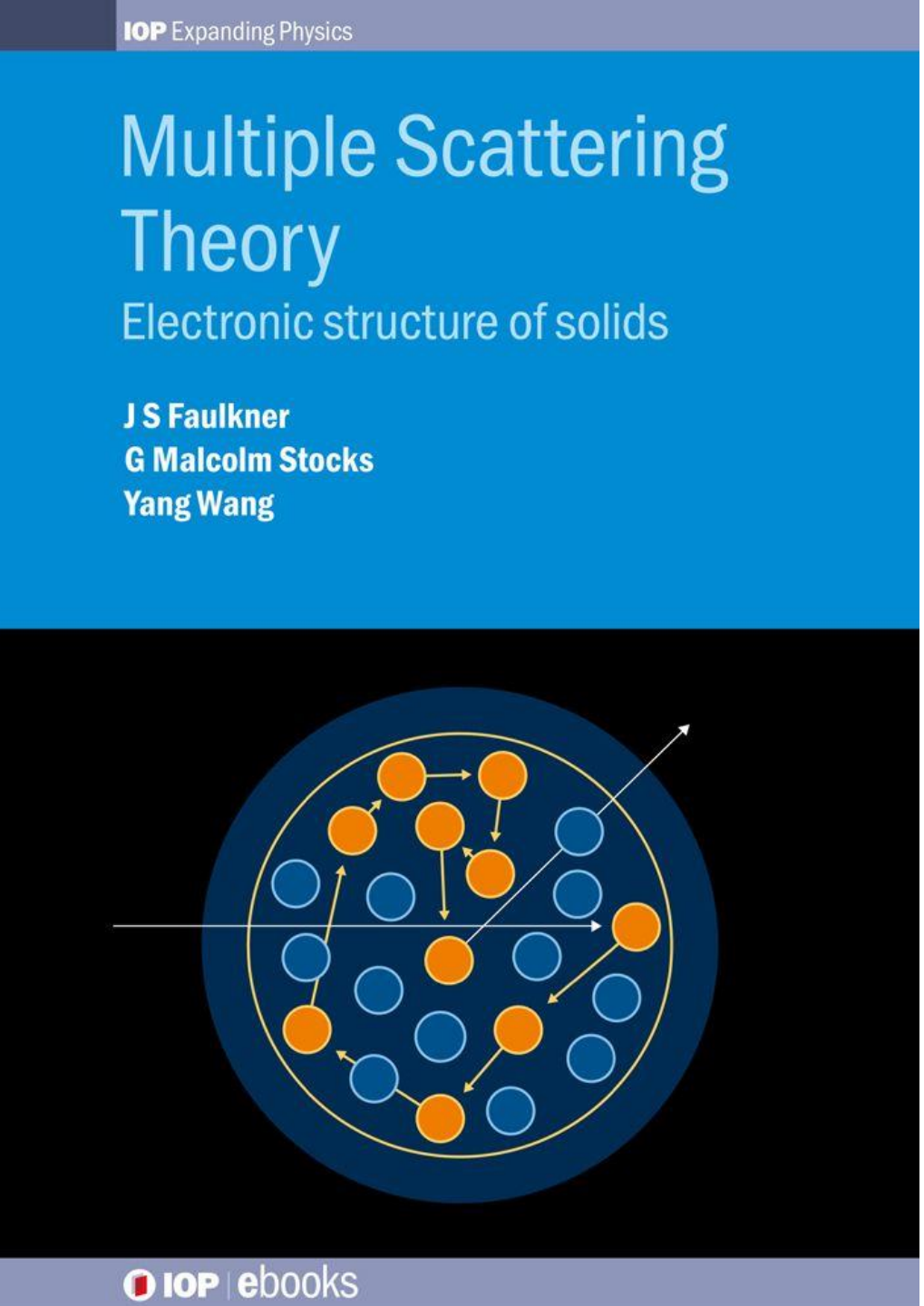
LSMS with LIZ embedding

- The LIZ cluster with *M* atoms is embedded in an effective medium.
- Using typical medium (TM) as the effective medium allows to determine the order parameter to capture the Anderson localization transition, a metal–insulator transition driven by disorder.

- The calculation is performed on a single band Anderson model by computing the local Green's function of a supercell embedded into a local typical medium (TM).
- TM based dynamical cluster approximation (DCA) method, which is an extension of dynamical mean field theory (DMFT), provides a consistent and systematic description of the Anderson localization transition, and obtains the correct critical disorder strengths.



Comparison of the average DOS (solid curves) and the typical TDOS (dashed curves) at different supercell sizes L_c with fixed LIZ size L_{LIZ} = 3. The disorder strength is set to be W = 2.0.



Summary

MuST code has become available since 12/31/2019 at https://github.com/mstsuite/MuST

Obtaining the package

```
$ git clone https://github.com/mstsuite/MuST
```

Current capabilities include

- Muffin-tin/full-potential
- Non-spin-polarized/spin-polarized/spin-canted
- Non-relativistic/scalar-relativistic/fully-relativistic
- LDA/GGA functionals (supported in LibXC library)

Under development

- LSMS with effective medium embedding
- Kubo-Greenwood formula for electronic transport in disordered alloys

We welcome collaborators and users to participate the effort to make MuST an efficient and robust community code!