The Kohn-Sham Method –
The Kohn-Sham Equations

- Schrödinger-like equations with local potential

\[
\frac{\hbar^2}{2m} \nabla^2 \psi_i(r) + \psi_i(r) \left[ -\frac{\delta V_{\text{ext}}}{\delta \rho} + \psi_i(r) + \frac{\delta V}{\delta \rho} + V_{\text{xc}}(r) \right] = \epsilon_i \psi_i(r)
\]

- These equations are nonlinear and must be solved iteratively (self-consistently)

DFT: Implementations of the Kohn-Sham Method

- All-electron full potential
- All-electron PAW
- Pseudopotential
- GW (quasi-particles)
- EXX (exact exchange)
- sX-LDA
- Time dependent DFT
- LDA+U

- Semi-relativistic

- Non-relativistic

- Non-periodic

- Periodic

- Non-spin-polarized

- Spin polarized

- Fully numerical (real space)

- Numerical

- Plane waves (FPLAPW)

- Spherical waves (LMTO, ASW)

Kohn–Sham Equations

- Concept of Muffin-Tin Potential
- Linearized Augmented Plane-Wave (LAPW)
- Full-potential version FP-LAPW
- Muffin-Tin Orbital Method (& LMTO)

DFT: Implementations of the Kohn-Sham Method

- Fully relativistic

- Semi-relativistic

- Non-relativistic

- Non-periodic

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- Fully numerical (real space)

- Numerical

- Plane waves (FPLAPW)

- Spherical waves (LMTO, ASW)
**Plane Waves and Pseudopotentials**

The basic idea of the pseudopotential theory:

- Core electrons are localized and therefore chemically inactive (inert)
- Valence electrons determine chemical properties of atoms and SOLIDS

→ Describe valence states by smooth wavefunctions

**Features of the Pseudopotential Method**

- **Pseudopotential is approximation to all-electron case, but…**
  - **Very accurate**
    - Comparable accuracy to AE in most cases
    - Simpler formalism
  
- **Low computational cost**
  - Perform calculations on ‘real-life’ materials

**Allows full advantage of plane-wave basis sets**
- Systematic convergence
- Easy to perform dynamics

**Basis Expansion around atom**

- Previous lectures - delocalized basis set (*plane waves*)
- **Muffin tin approaches**
  - Spherical potentials around each atom
  - Wavefunction expanded in spherical waves (s, p, d, f character)
  - Potential is zero in space between atoms
  - Solution of different sites connected together (multiple scattering, cancellation of orbital tails)

**Muffin tin approaches**

Every day life

Physical model
The original Augmented Plane Wave (APW) method (1)

- All APW descendent methods divide space into atomic centered spheres surrounded by an interstitial region
- The APW basis functions consist of plane waves in the interstitial region augmented into radial solutions of the Schrödinger equation inside the MT-spheres
- For a system with one atom per unit cell

$$\psi_{G}^{APW}(r, \mathbf{k}) = \sum_{L} a_{L}^{G} u_{L}(r, E) Y_{L}(\mathbf{k})$$

$$\mathbf{k}_{G} = \mathbf{k} + \mathbf{G}$$

$\mathbf{k}_{G}$ = wave vector from BZ  
$\mathbf{G}$ = reciprocal lattice vector  
$L$ = set of $l, m$

The original Augmented Planewave (APW) method (2)

Radial parts of an APW basis function for Ce

$\mathbf{k} = \frac{2\pi}{a} (0.101, 0.208, 0.107)$
$\mathbf{G} = \frac{2\pi}{a} (1, 1, 1)$

Energies: for s-states 0.3 Ry  
all other 0.5 Ry

Muffin Tin Orbitals

Two sets of solutions
- Solve Schr. Eq. in sphere
- Solve Laplace Eq. in interstitial for a given energy $E$

Orbitals based on angular momentum character – s, p, d, f

Small basis set!

Main challenges
- Matching conditions at sphere boundary requires orbitals and first derivative to match at sphere boundary
- Needed - secular equation that is linear in energy
The original Augmented Planewave (APW) method (3)

- The coefficients $a^k_{L}$ are found by expanding each planewave into Bessel functions $j_l(k_G r)$ at the MT-spheres, $r = r_{MT}$, requiring the basis functions to be continuous at the sphere boundaries.

  This yields

  $$a^k_{L} = 4\pi i^L Y_L^*(k_G) j_l(k_G r_{MT}) u_l(r_{MT}, E).$$

- The planewaves are energy independent.
- The radial solutions $u_l$ depend on the energy at which the radial Schrödinger equation is evaluated.

The original Augmented Planewave (APW) method (4)

- An eigenfunction

  $$\Phi_i(r) = \sum_G C_{iG} \chi_G (r, k)$$

  can only be efficiently described by orbital solutions $u_l$ evaluated at the eigenenergy $E_i$ of $\Phi_i$.

- A new set of APW basis functions must therefore be evaluated for each new energy treated.
- As the matrix elements representing operators depend on the choice of basis set the secular equation is non-linear in energy.

$$\det[T_{GG'}(E) + V_{GG'}(E) - E\mathcal{O}_{GG'}(E)] = 0,$$

The original Augmented Planewave (APW) method (5) – Finding the APW Eigenvalues

- The task of finding the APW eigenvalues becomes somewhat more troublesome, due to the asymptote problem.

- When going through a large number of energies, one might hit an energy for which $u_l(r_{MT}, E)$ is very small or even equals zero.

- This yields very large or infinite coefficients $a^k_{L}$.

- The determinant, involving matrix elements with summations over the coefficients will then go to infinity,

  $$\det(E) \to \infty.$$

- Any routine used to find the eigenvalues must therefore be adjusted to handle the asymptotic behavior of the determinant at such energies.

The original Augmented Planewave (APW) method (6) – An asymptote problem

- The APW determinant must be evaluated for a number of energies in order to find the energies corresponding to eigenvalues.

kinetic energy operator

Potential

Overlap
The original Augmented Planewave (APW) method (7)

\[ \det[T_{GG'}(E) + V_{GG'}(E) - E\mathcal{O}_{GG'}(E)] = 0, \]

- The procedure of evaluating the determinant for a number of different energies in order to find the energy eigenvalues makes the APW method very time consuming.
- If the basis functions, and thereby the matrix elements were independent on energy, the secular equation would turn into a \textit{general eigenvalue problem}

**Linearization procedure**

The Linearized Augmented Plane Wave (LAPW) method

- An energy independent basis set must be able to describe all eigen-functions of the different eigenenergies
- By introducing the energy derivatives \( \hat{u}_l = \frac{\partial u_l}{\partial E} \) of the radial solutions \( u_l \)

Andersen constructed an \textit{energy independent LAPW basis set}

\[ \chi^l_{\text{LAPW}}(r, k) = \left\{ \frac{e^{\mathbf{i}kr}}{\sum_{L} R^L_{\text{LAPW}}(r) Y_L(\hat{r})} \right\}_{r \in \mathbb{I}} R^L_{\text{LAPW}}(r) = a^L_k u_l(r, \xi_1) + b^L_k \hat{u}_l(r, \xi_1) \]

The Linearized Augmented Planewave (LAPW) method

- \( \chi^l_{\text{LAPW}} \) provides a sufficient basis for eigenfunctions in an energy range around the linearization energy \( \xi_1 \)
- The two coefficients \( a^L_k \) and \( b^L_k \) are determined by forcing each basis function to be continuously differentiable, i.e., continuous with continuous first derivative, at the surfaces of the MT-spheres.

The Linearized Augmented Plane Wave (LAPW) method

**Radial parts of an LAPW basis function for Ce**

The k and G as for APW basis functions

Reference energies: 0.3 Ry for s-states, 0.5 Ry for other
The Linearized Augmented Plane-wave (LAPW) method

Radial parts of an LAPW basis function for Ce

- The linear combinations of $u(r, E_1)$ and $\hat{u}(r, E_1)$ smoothly connected to the Bessel expansion at $r = r_{MT}$ differ considerably from the original APW solutions $u(r, E_1)$ [2nd, or 3rd order expansion of $u(r, E)$ ?]

Thereby the LAPW basis functions, although more flexible in describing eigenfunctions far from $E_1$, provide a poorer basis set close to $E_1$.

There is no free lunch!
- The poorer basis set requires a larger number of planewaves
- It is easier to solve larger general eigen-equation than to deal with smaller determinant

\[
\text{det}\left(\hat{T} + \hat{V} - E \hat{I}\right)\hat{O} = 0
\]

The matrix is diagonalized, giving all LAPW eigenenergies at one time.

The APW (LAPW) + localized orbitals
- The variational freedom can be improved by using a complementary basis set consisting of local orbitals.
- They are local in the sense that they are completely confined within the MT-spheres

\[
\chi_{M}^{L}(r, k) = \begin{cases} 0 & r \in I \\ \hat{K}_{M}^{L}(r) Y_{L}(f) & r \in MT \end{cases}.
\]

\[
\hat{K}_{M}^{L}(r) = a_{M}^{L} u(r, E_1) + b_{M}^{L} \hat{u}(r, E_1)
\]

is determined using the condition that localized orbital should vanish at $r = r_{MT}$

- Localized orbitals can be generated for another reference energy

LAPW vs. LAPW+lo

Convergence of total energy for cerium (Z = 58)

Multiplied by 100
Full potential LAPW (FP-LAPW)

- In its general form the LAPW (LAPW+lo) method expands the potential in the following form

\[ V(r) = \sum_{LM} \sum_{\mathbf{K}} V_{LM}(r) Y_{LM}(\mathbf{r}) + \sum_{\mathbf{K}} \psi_{\mathbf{K}}(\mathbf{r}) \]

and the charge densities analogously.

- Thus no shape approximations are made, a procedure frequently called a "full-potential" method.

- The "muffin-tin" approximation used in early band calculations corresponds to retaining only the \( i = 0 \) component in the first expression and only the \( \mathbf{K} = 0 \) component of the second.

- This (much older) procedure corresponds to taking the spherical average inside the spheres and the volume average in the interstitial region.

FP LAPW method - Summary

- The LAPW method is a variational expansion approach which solves the equations of DFT by approximating solutions as a finite linear combination of basis functions.

- What distinguishes the LAPW method from others is the choice of basis.

- The LAPW basis is constructed to be particularly accurate and efficient for the solution of the all-electron ab initio electronic-structure problem, where solutions are rapidly varying and atomic-like (like isolated-atom solutions) near the atoms but more smoothly varying and not atomic-like throughout the rest of the cell.

FP LAPW method - References


FP LAPW method - Codes

WIEN2k
http://www.wien2k.at

Peter Blaha, Karlheinz Schwarz & coworkers
Inst. f. Materials Chemistry, TU Vienna

The EXCITING FP-LAPW Code (GNU – licence)
EXCITING is still in its beta state so check the consistency of your results carefully!
http://exciting.sourceforge.net
Claudia Ambrosch-Draxl
Karl-Franzes Universität Graz, Austria

FP LAPW method - Applications

Theoretical Mineral Physics
Ronald Cohen, Geophysical Laboratory, Carnegie Institution of Washington

The state-of-the-art in theoretical mineral physics uses first-principles methods.

- In 1992, a phase transition in stishovite (SiO₂) from the rutile structure to the CaCl₂ structure at 45 GPa was predicted using the LAPW method.
- New Raman experiments found exactly what was predicted theoretically, with a best estimate of the phase transition pressure of 50 GPa.

FP LAPW method – Applications SiO₂
Raman frequency vs. hydrostatic pressure

transition solid lines – predicted Raman frequencies
points – experimental data

FP LAPW method – Applications SiO₂
Valence charge density computed for SiO₂ stishovite.

Insight into the nature of bonding

The oxygen ions are elongated towards the three surrounding silicon atoms.
Theoretical mineral physics

One of the most active areas in first-principles mineral physics is for properties of the Earth’s core.

- Temperature of the core?
- Composition?

Muffin Tin Orbital Method

Temperature of the core?
Composition?

Solutions in the Interstitial Region

\[-\nabla^2 \psi(r, E) + \left[ V_{\text{ext}}(r) - E \right] \psi(r, E) = 0\]

- Potential in interstitial region is zero
  Interstitial region has no space, electron kinetic energy in region is zero as well

\[ \nabla^2 \psi(r, E) = 0 \quad \Rightarrow \quad \psi(r) = R(r) Y_l^m(\hat{\mathbf{r}}) \quad L = 0, 1, 2, \ldots |m| < l \]

- Take advantage of spherical symmetry – express wavefunction in terms of spherical harmonics and radial portion

\[ J_l(r) = J_l(r) Y_l^m(\hat{\mathbf{r}}), \quad J_l(r) = \frac{1}{2l+1} \left( \frac{r}{w} \right)^l \]
\[ K_l(r) = K_l(r) Y_l^m(\hat{\mathbf{r}}), \quad K_l(r) = \frac{w}{r} \left( \frac{r}{w} \right)^l \]

- We get two solutions for Laplace’s equation
  - regular one, \( J_l(r) \) (goes to zero at \( r=0 \)) and
  - irregular one, \( K_l(r) \) (blows up at \( r=0 \))

Making Life Easier with ASA

Atomic Sphere Approximation

- Many crystals are close-packed systems (fcc, bcc, and hcp)
- Most of the space is filled by atomic spheres
- What if we cheat a little…and have the spheres overlap??
- Doing this, we remove the interstitial region and our integration over space becomes an integration of atomic spheres.
- This approach works best when the system is close packed, otherwise we have to pack the system with empty spheres to fill space
- How to choose radius of spheres?

\[ V_{\text{ext}}(r) = \sum \frac{e^2}{4\pi \epsilon_0 \epsilon_r} \frac{Q_a}{r} \]

Many spherical systems (fcc, bcc, and hcp)
Solutions within the Atomic Spheres

\[ \varphi(r, E) = \varphi(r, E)Y_L(\hat{r}) \]

\[ -\nabla^2 \varphi(r, E) + [V(r) - E] \varphi(r, E) = 0 \]

We need to match radial amplitude up with interstitial solutions, \( J \) and \( K \), at \( r_s \)

\[ \varphi(r, E) = \frac{1}{N_p(E)} [K(r) - P_p(E)J(r)] \]

Normalization function

Potential function obtained from matching conditions

Muffin Tin Orbitals

- We can define the total wavefunction as a superposition of muffin tin orbitals as

\[ \psi(r) = \sum_{RL} \psi_{RL}(r, E) \]

- Where the muffin tin orbitals are given by:

\[ \Psi(r, E) = N_{RL}(E) \psi_{RL}(r, E) + P_p(E)J(r) \]

Muffin-tin Head

Muffin-tin Tail

\[ = K_s(r) \]

for \( r_s < r_s \)

\[ = -\sum_{l} S_{RL,R'L'}J_l'(r_s) \]

Structure constants – lattice info

Canceling Muffin Tin Tails

Tail Cancellation needed

\[ \sum_{RL} a_{RL} [P_{RL}(E) \delta_{RL,R'LL'} - S_{RL,R'L'}] = 0 \]

\[ \det [P_{RL}(E) \delta_{RL,R'LL'} - S_{RL,R'L'}] = 0 \]

For periodic systems, we can write this in k-space and get the band structure!
This allows us to express the system in terms of linear muffin tin orbitals that depend on $r$ and $E_v$.

The Linearization of the problem

- Taylor expansion of the orbital...
  \[ \varphi_{RL}(r,E) = \varphi_{RL}(r,E_v) + (E - E_v) \varphi_{RL}(r,E_v) \]
  with $E_v$ being a reference energy for the problem

- This allows us to express the system in terms of linear muffin tin orbitals that depend on $\varphi$ and $\varphi_{RL}$
  \[ \psi_{RL}(r) = \varphi_{RL}(r) + \sum_{R'L} \varphi_{RL}(r) \psi_{R'L,RL} \]
  \[ \text{chosen in such a way that the linear muffin tin orbitals and its derivatives match continuously to tail functions at muffin-tin sphere radius} \]

\[ \Rightarrow \text{ LMTO method} \]

Advantages of the LMTO over MTO

- **Speed Improvement**: Removal of non-linearity in determinant equation, accelerates calculations.
- **Accuracy**: Eigenvalues correct up to third order in $(E-E_v)$
- **Limitations**: Can run into problems with semi-core d-states outside of the effective energy window.
  - Two reference energies often required

Full Potential Linear Muffin-Tin Orbital (FP-LMTO) method

- In a full potential method the idea is to describe the potentials and charge densities in the crystal without the approximation of regarding them as necessarily spherical.
- In FP-LMTO the unit cell is divided into non-overlapping muffin-tin spheres around the atoms and an interstitial region outside these spheres.

LMTO - Comparison with PPs and plane waves

- **Comparison to PPs and plane waves**
  - Very complicated formalism (and codes !)
  - No forces and stresses up to now !
  - Problem to judge convergence of results
  - Relatively small secular matrices
    - (standard diagonalization techniques efficient)
  - All-electron technique
    - (core electrons in spheres)
  - Minimal basis, full analogy to atoms
  - Simple, approximative tight-binding version
- **LMTO is commonly used, specially for metals**
Multiple Scattering Theory &
Basics of the alloy theory

Multiple Scattering Theory (MST)

- **Multiple scattering techniques** determine electronic structure by accounting for the scattering events an electron wavefunction experiences within a solid.
- **This is tougher than it looks**
  - single scatterer, single scattering event – analytic solution
  - two or more scatterers, infinite number of possible scattering events, recursive solutions required for wavefunctions

Short History of MST

- Lord Rayleigh (1892) *On the Influence of Obstacles in Rectangular Order upon the Properties of a Medium* Phil Mag. – Laplace Equation
- N. Kasterin (1897) extends MST to Helmholtz equation (scattering of sound waves by collection of spheres)
- Korringa (Physica, 1947) – first use to find electronic states in solids (computational facilities however not up to the task)
- Kohn and Rostoker – rediscover in 1950’s (Phys. Rev.)
- This leads to the Korringa Kohn Rostoker approach (KKR)
- 1960’s – first serious calculations using the approach – computers begin to catch up with the theory!

Muffin tin approaches (KKR & LMTO)

Every day life

Physical model
Multiple Scattering Theory – Basic Equation

\[ [H_o + V] \psi(\vec{r}) = E \psi(\vec{r}) \]

- \(H_o\) is the free space Hamiltonian
- \(V\) is the perturbing potential
- \(\psi\) is the electron wavefunction

\[ \psi(\vec{r}) = \chi(\vec{r}) + \int G_o(\vec{r}, \vec{r}') N(\vec{r}') \psi(\vec{r}') d^3r' \]

- We can express the wavefunction at some position as a sum of the free space wavefunction, \(\chi\), and contributions from the perturbing potential, \(V\), at different sites.
- In this case, \(G_o\) is the free electron propagator and describes motion in regions where no scattering from the potential occurs.

Letting Green do the expansion

- In analogy to the previous wave function equation, we can do a similar expansion for the system Green function.

\[ G = G_o + G_o VG \]

- We can expand this equation out to infinity...

\[ G = G_o + G_o VG_o + G_o VG_o VG_o + G_o VG_o VG_o VG_o + ... \]

- The total Green function acts as the system propagator.
- This expansion shows the infinite number of scattering events that can occur through potential interactions.
- Electron propagation in free space is described by \(G_o\).

Introducing \(T\)-matrix

- We can rearrange the last equation to isolate the effects of the potential.

\[ G = G_o \left( V + VG_o V + VG_o VG_o V + ... \right) G_o \]

\[ G = G_o + G_o TG_o \]

where

\[ T(V) = V + VG_o V + VG_o VG_o V + ... \]

- The scattering matrix, \(T\), completely describes scattering within the potential assembly. It contains all possible scattering paths.
Assume the potential is made up of a sum of terms due to different cells or atoms.

\[ V = \sum_i V^i \]

The \( T \) matrix in this case becomes:

\[ T = T \left( \sum_i V^i \right) = \sum_i V^i + \sum_i V^i G \sum_j V^j + ... \]

We can separate out the sequences where the scattering always involves the same cell or atom into the cell \( t \) matrix.

\[ t^i = V^i + V^i G_0 V^i + V^i G_0 G_v V^i + ... \]

We can now write the \( T \) matrix in terms of the single site scattering matrices, \( t_i \).

\[ T \left( \sum_i V^i \right) = \sum_i t^i + \sum_j \sum_i t^i G_j t^j + ... \]

This equation shows that the scattering matrix of an scattering assembly is made up of all possible scattering sequences.

Each scattering sequence involves scattering at individual cells with free electron propagation in between.

\[ T = \sum_i T^i \text{ where } T^i = t^i \delta_{ij} + t^i G \sum_j T^j \]

Solve the radial Schrodinger’s equation for an isolated muffin tin potential and determine the regular and irregular solutions, \( Z \) and \( S \).

The atomic \( t \) matrix is diagonal in the angular momentum representation.

\[ t_i^o = i \sin \delta e^{i\delta} \]

The phase shift, \( \delta \), can be found from the atomic wavefunction.

In the \( MT \) formalism, the \( T \) matrix becomes:

\[ T^{ij} = t^i \delta_{ij} + t^i \sum_k \widetilde{G}^k T^{kj} \]

There exists a matrix \( M \) such that \( T^{ij} \) are the elements of its inverse.

The matrix \( m \) is just the inverse of the cell \( t \) matrix.

\[ M^{ij} = m^i \delta_{ij} - \widetilde{G}^j \left( 1 - \delta_{ij} \right) \]

The inverse of the \( T \) matrix is cleanly separated into

- potential scattering components, \( m \), and
- structural components, \( G \).
Getting the Band Structure Together

- The poles of $M(E)$ determine the eigenenergies for the system for a given $k$ through the following equation:

$$\text{det}\left[m(E) - \tilde{G}(E, \tilde{k})\right] = 0 \Rightarrow \varepsilon(\tilde{k})$$

- This allows us to calculate the system band structure.

- Possibility to calculate non-periodic systems (clusters)

Problem with the KKR method

- Linking interstitial region ($V=0$) with spherical regions with muffin tin potentials can be difficult

- Determinant used to find band structure is a non-linear function of energy (energy dependence carried in the site $t$ matrices) – this can not be reduced to a standard matrix eigenvalue problem

- The Solution – Linearize the equation – LMTO approach (Andersen, PRB, 1975 – 1370 citations)

Present Applications the KKR method

- Practically only first-principles method for very important class of materials, i.e., random alloys on the market

- Other methods → supercells

- Coherent Potential Approximation (CPA) relatively easily implemented

  - Virtual Crystal Approximation (VCA)
    - Potential of a Random Binary Alloy $A_xB_{1-x}$
      $$V(A_xB_{1-x}) = xV(A) + (1-x)V(B)$$
      $$\Rightarrow$$ Periodicity of the system restored

Random Alloys

$$\langle G \rangle = G_0 + G_0 \Sigma(G) = (G_0^{-1} - \Sigma)^{-1}$$

$$\Sigma = \langle T \rangle (1 + G_0 \langle T \rangle)^{-1}$$

Self-energy

Configurationally averaged Green’s function
Coherent Potential Approximation (CPA)

**Best single-site solution for describing scattering in substitutional alloys**

Atom in binary alloy → Atom in equivalent effective medium

- Scattering properties of alloy can be represented by an effective medium.
- Treat scattering by atom as an impurity in the effective medium.
- Introduction of atom should give no scattering in the correct effective medium (iterative solution).

**Application of KKR-CPA method- FeCr Alloys**

- **Cr magnetic moment**
- **Fe magnetic moment**

**FeCr Alloy**

**Experimental (Aldred et al., 1976)**

**Cluster expansion**

Ortho-normal and complete set of basis functions are introduced.

$s$ is the configuration variable (+/- 1 for binary systems)

Basis for M lattice sites is given as:

$\Phi_{\sigma}(\sigma) = \Theta_{a_1}(\sigma)\Theta_{a_2}(\sigma)\cdots\Theta_{a_M}(\sigma)$.

Energy of the lattice (M sites) is given as:

$E(\sigma) = J_0 + \sum_{K=1}^{M} \sum_{\alpha_k} \sum_{\beta_k} J^{(K)}_{\alpha_k\beta_k}(\sigma)$.

For all cluster sizes $K$ with number of atoms $= K$

$J^{(K)}_{\alpha\beta} = \left\langle E(\sigma) \mid \Phi^{(K)}_{\alpha\beta}(\sigma) \right\rangle$

Average of energies of all configurations projected onto the basis function.

**Cluster expansion**

For binary system

$Z = J_0 + J_1 \sum_{i<j} \hat{S}_i \hat{S}_j + \sum_{i<j<k} J_{ijk} \hat{S}_i \hat{S}_j \hat{S}_k + \ldots$
The cluster expansion is able to represent any function $E(\phi)$ of configuration $\phi$ by an appropriate selection of the values of $J_i$.

- Converges rapidly using relatively compact structures (e.g., short-range pairs or small triplets).
- Unknown parameters of the cluster expansion is determined by fitting first-principles energies as shown.


Thank you!