

Cluster ordering of Mg-LPSO

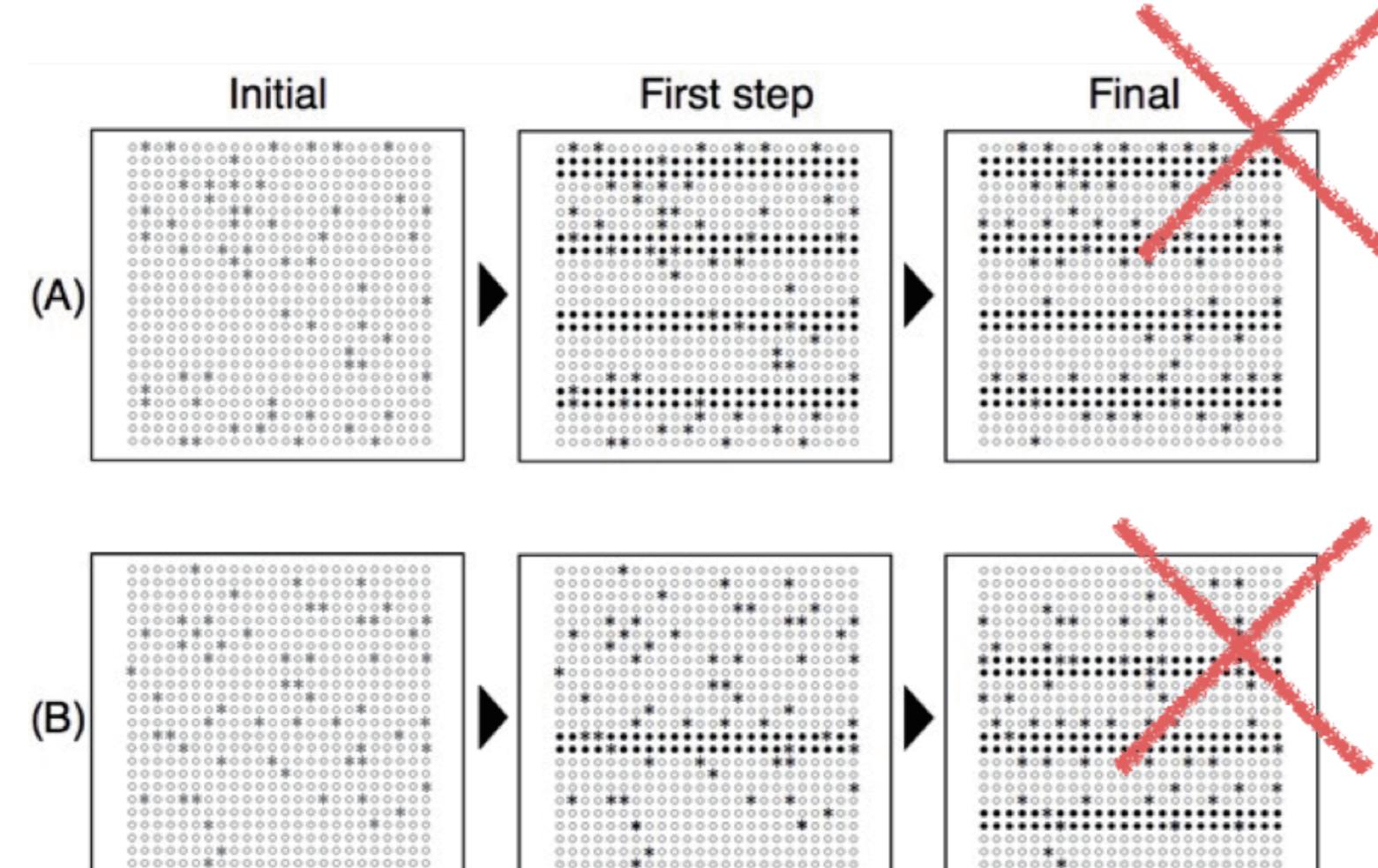
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Expected Formation Mechanism of LPSO structure



Formation scenario of LPSO Structure

- Stacking Fault initiation
 - Stacking Fault is introduced periodically in hcp lattice.
 - Solute Atoms trapped by SF.
- Solute Atoms initiation
 - SF traps Solute Atoms.
 - Solute Atoms condense 4-5 layers from SF layer.
 - Condensed Zn and Y induces New Stacking Fault.

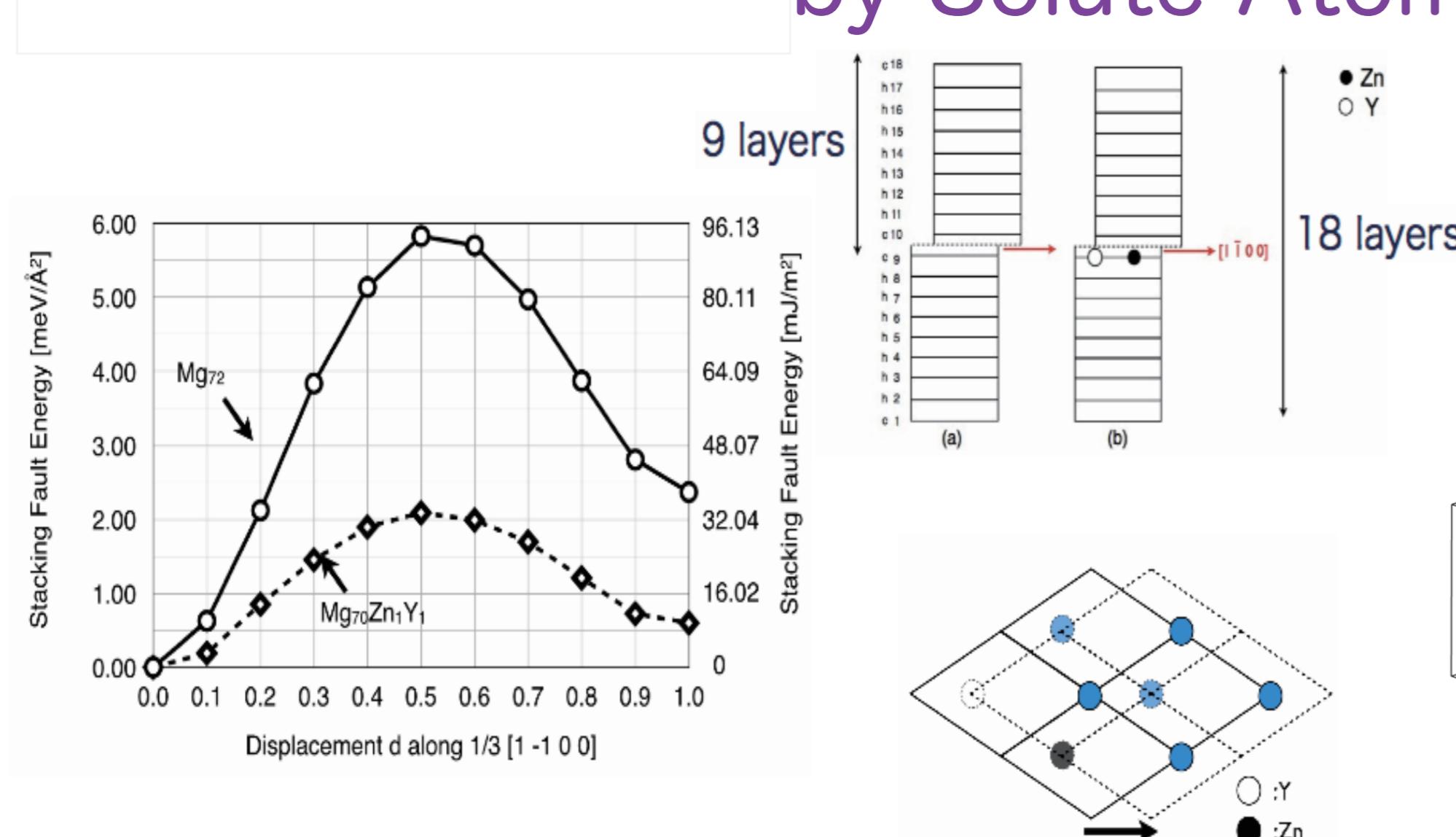
Assessment by VASP calculation

- Stacking Fault initiation
 - Is Stacking Fault in Mg Stable?
 - Is Solute Atoms in Stacking Fault S.
- Solute Atoms initiation
 - Does Stacking Fault trap Solute Atoms?
 - Are Solute Atoms stable in middle distance from SF layer?
 - Do condensed Solute Atoms induce Stacking fault?

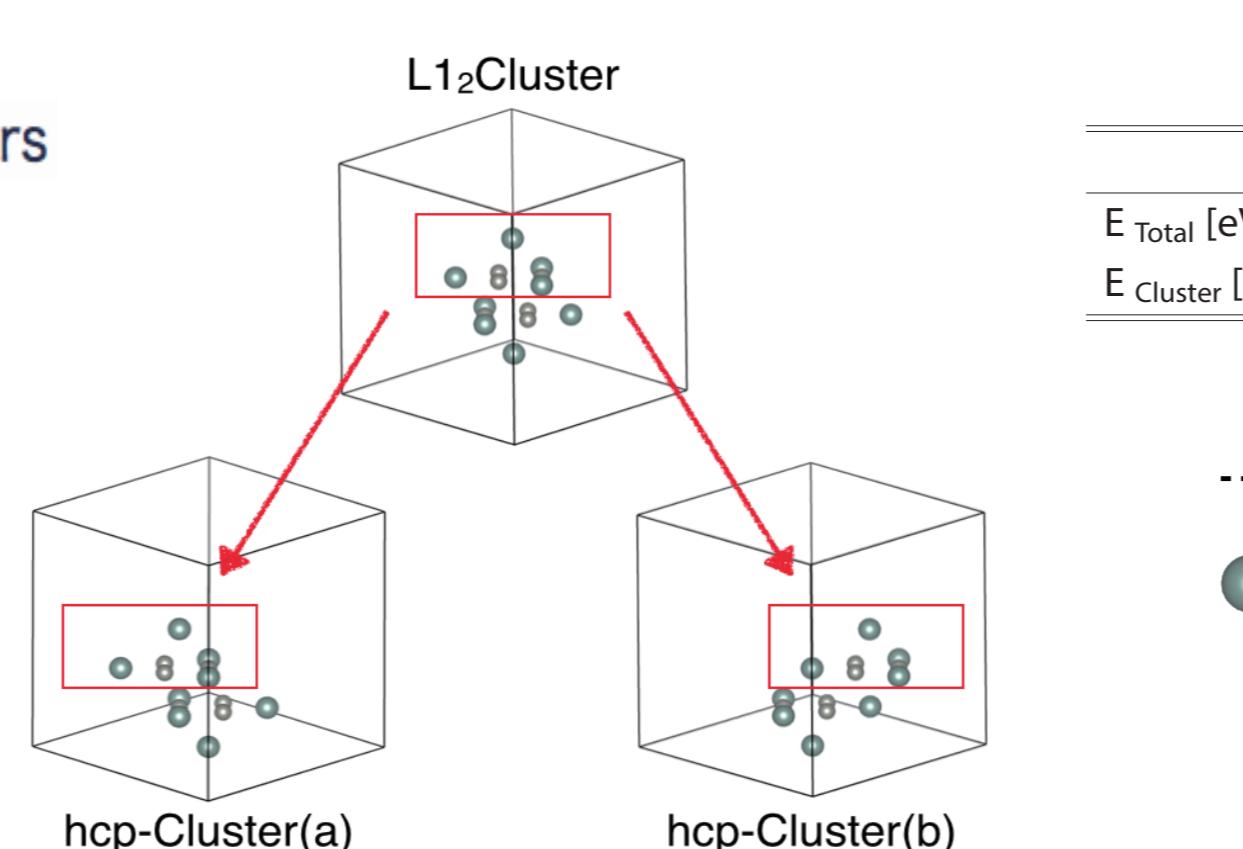
Inspection by First Principle Calculation

- Cluster Stability in various type of lattice.
- Interaction btw solutions.
- Interaction btw Cluster and small cluster.
- Possibility of vacancy diffusion.

Introduction of Stacking Fault by Solute Atoms



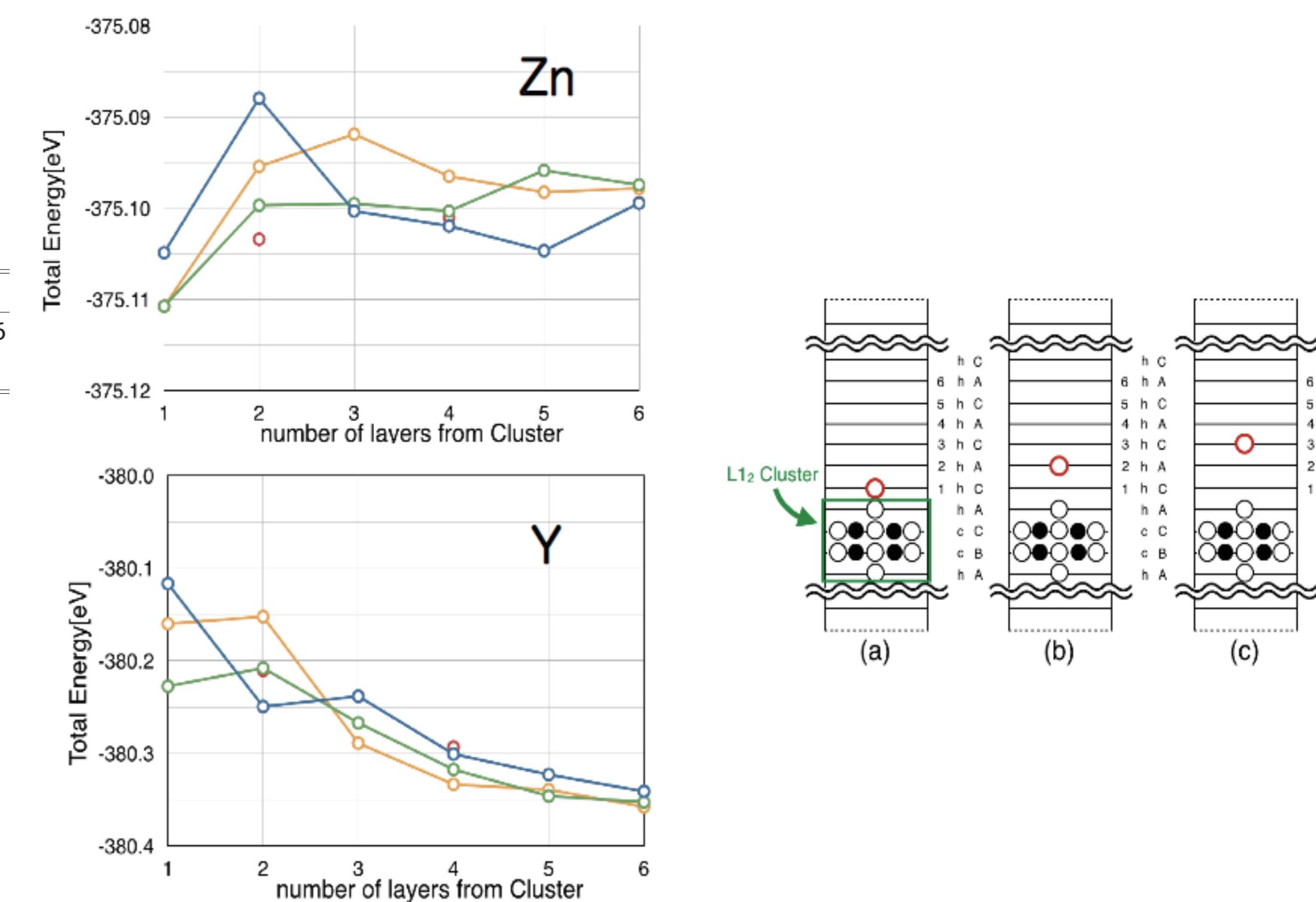
Cluster Stability



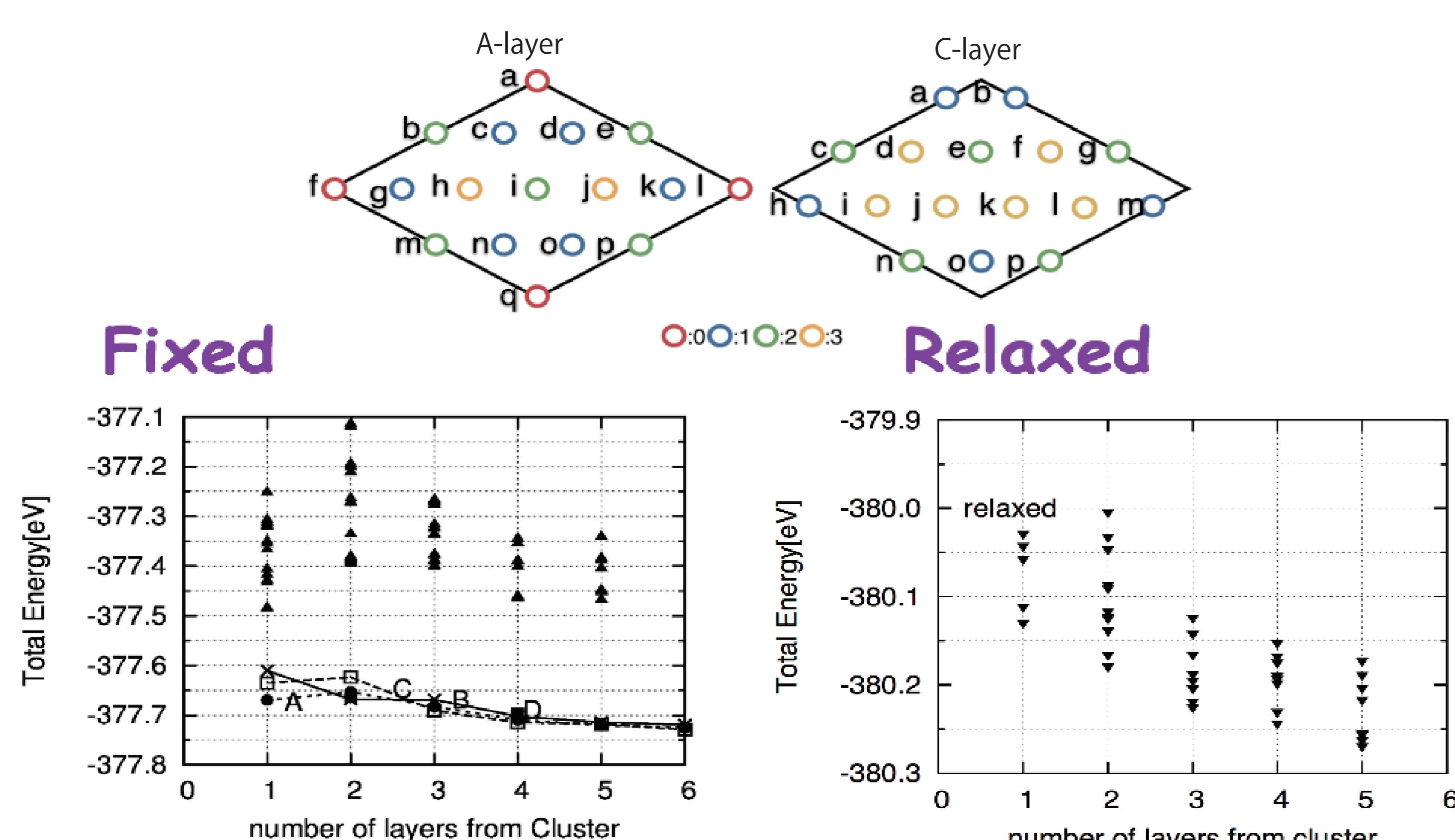
Cluster energies in different stacking sequences.

	hcp(a)	hcp(b)	fcc	6H	14H
E Total [eV]	-152.543	-153.920	-153.057	-153.441	-157.406
E Cluster [eV]	-3.040	-4.418	-3.796	-4.043	-4.046

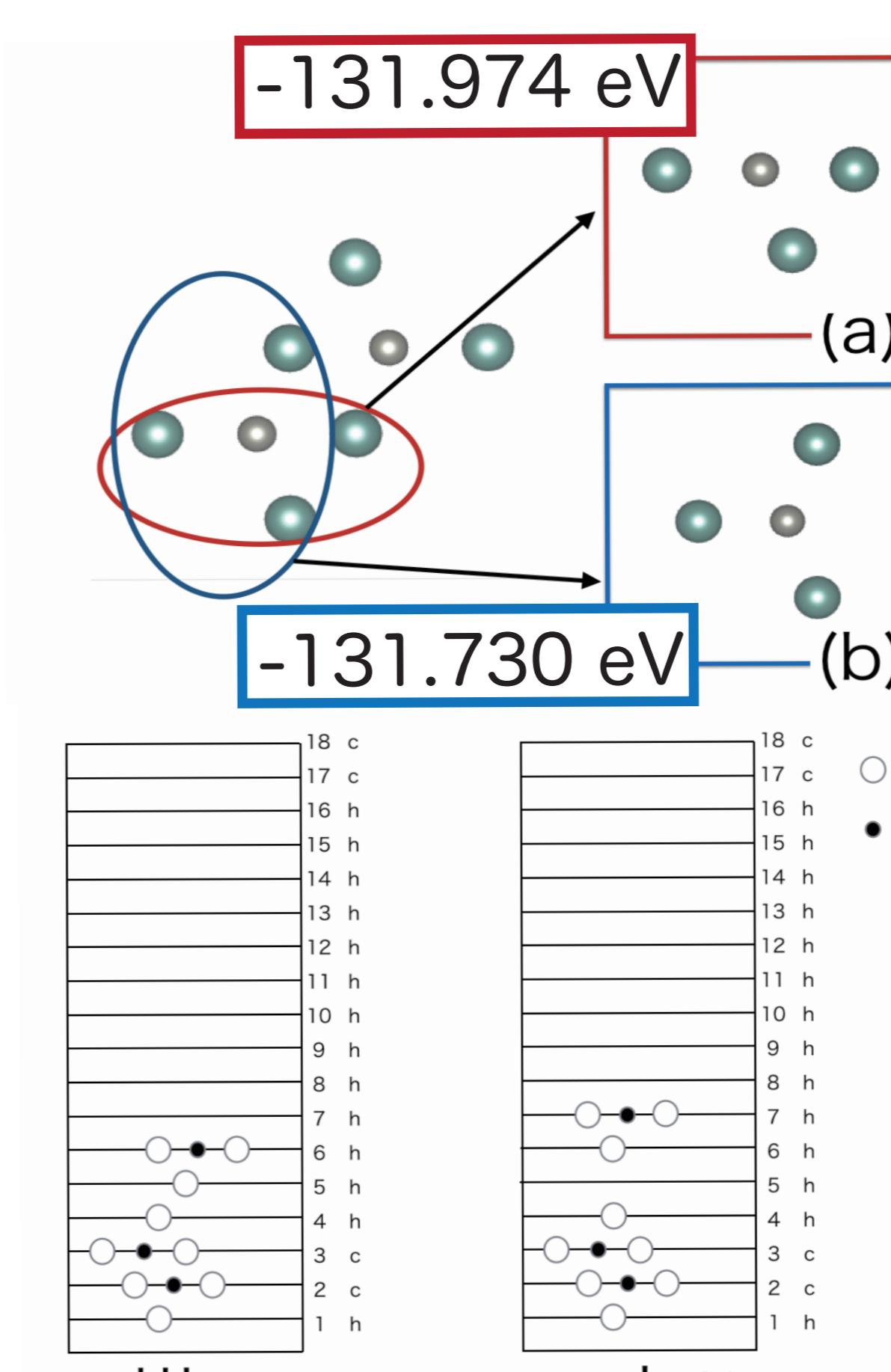
Interaction btw cluster and solution



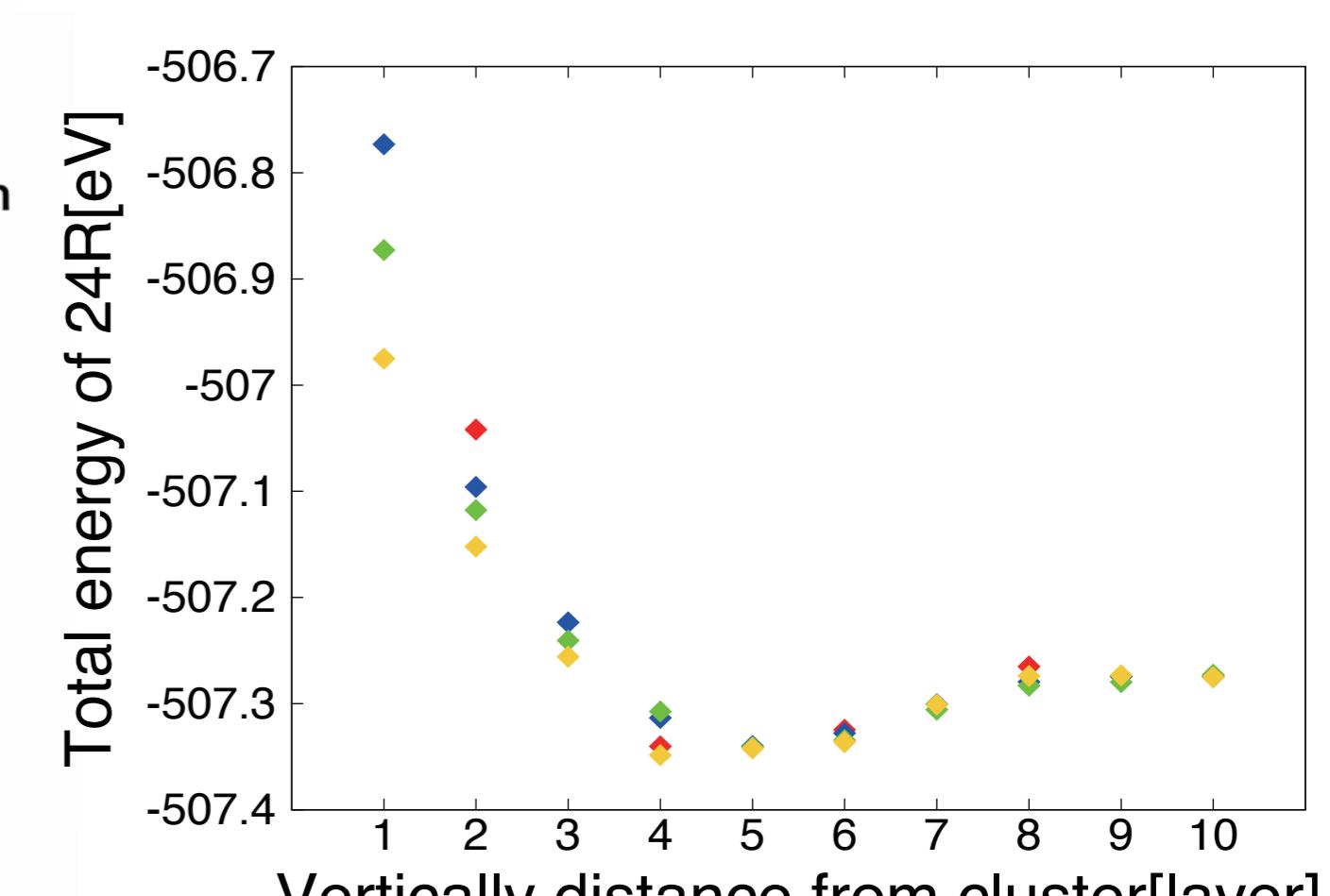
Interaction btw Cluster and Zn-Y pair



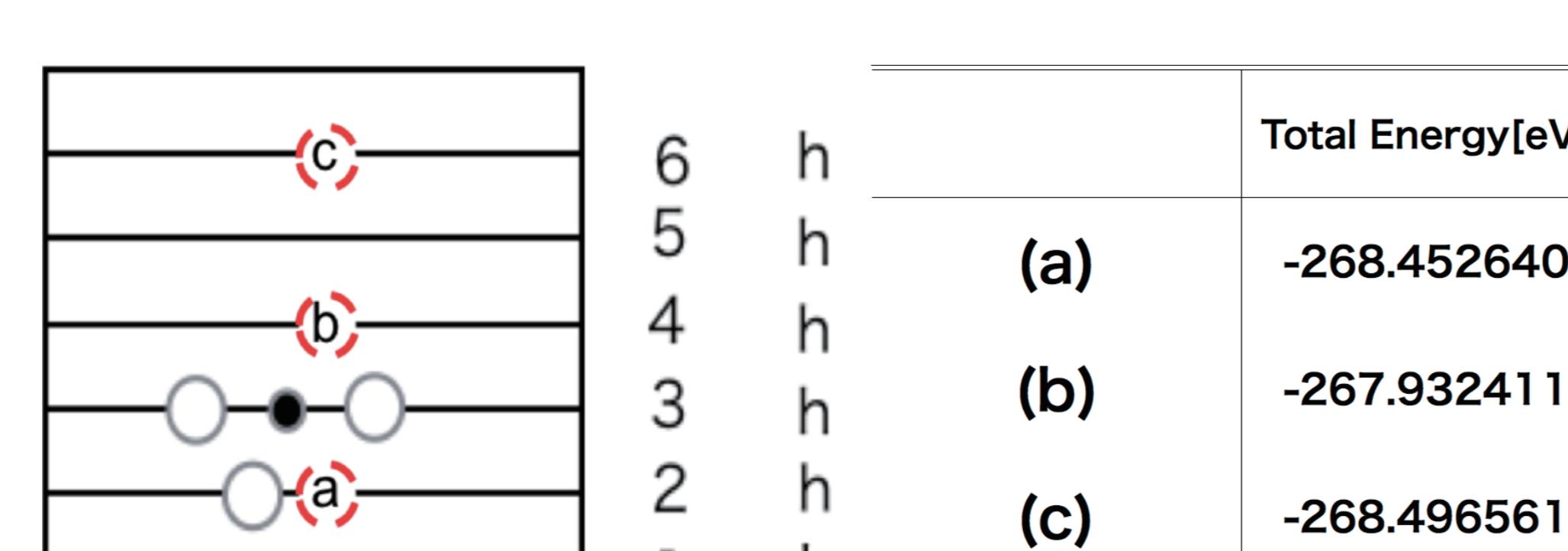
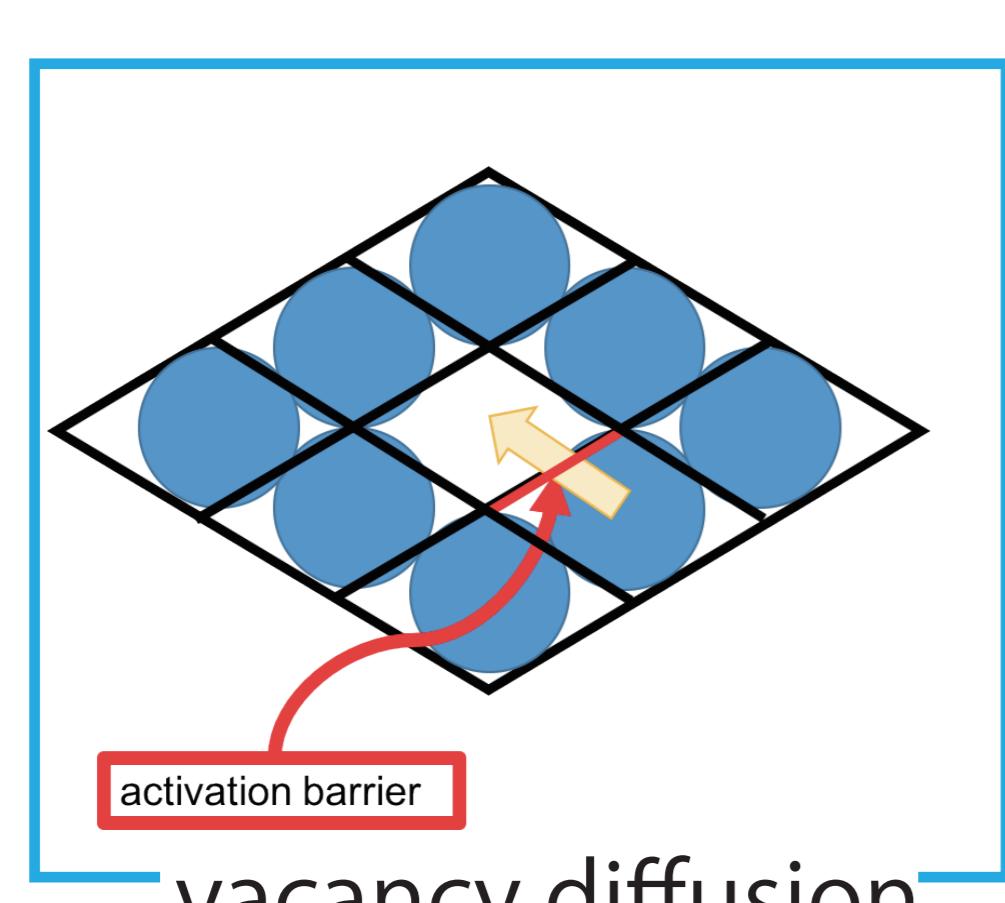
Interaction btw L1₂Cluster and Small_Cluster



About Small_cluster,
We divided L1₂ Cluster vertically and horizontally like (a) and (b).
And we insert their Small_Clusters into 6R model of Mg have LPSO structure.
As a result of first principle calculation,
(a) type has 0.2 eV lower energy than (b) type.

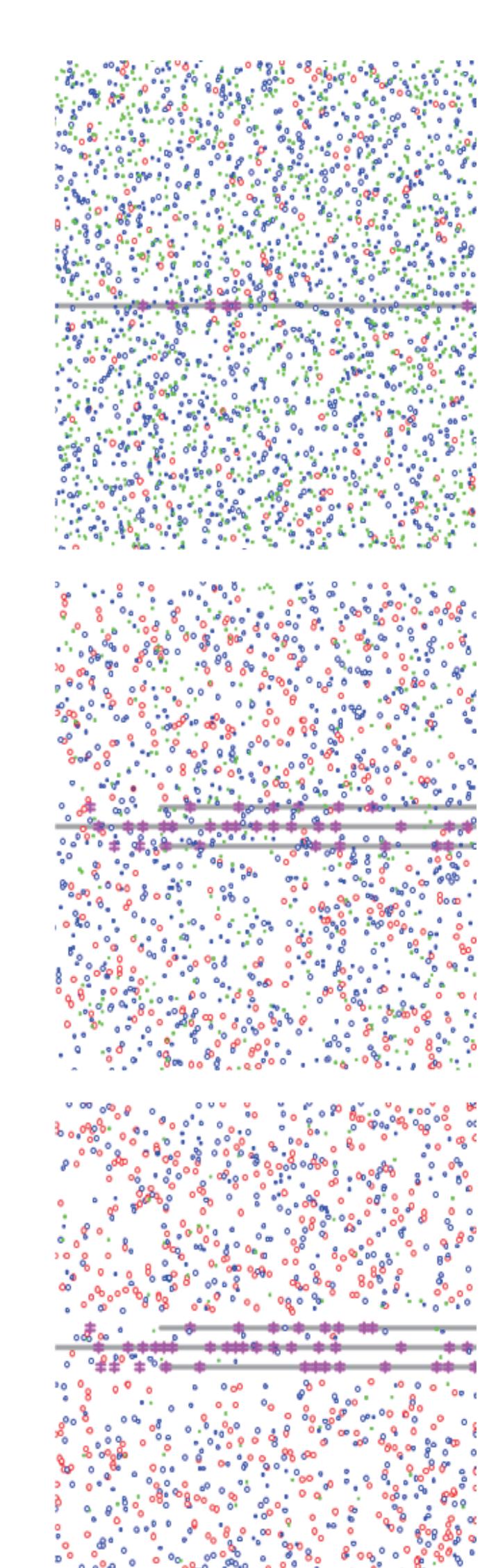


Possibility of vacancy diffusion



modified scenario

1. Zn and Y pair stayed in same stacking layer.
2. Condensed Zn and Y induces Stacking Fault.
3. Stacking Fault traps Zn and Y.
4. Clusters are formed Stacking Fault layer.
5. Small_Clusters are swept out from stacking faults.
6. Solute Atoms condense 4-5 layer from SF layer.
7. repeat 2-6 steps.



For revealing kinetics of the solute movement,
we calculate the stability of the vacancy around the small cluster.
We expect vacancy is stable near small cluster.
But, against expectations, the result of calculation
when vacancy is inserted far position shows low energy.
So, we need to inspect again by calculating about multi-vacancies.

