

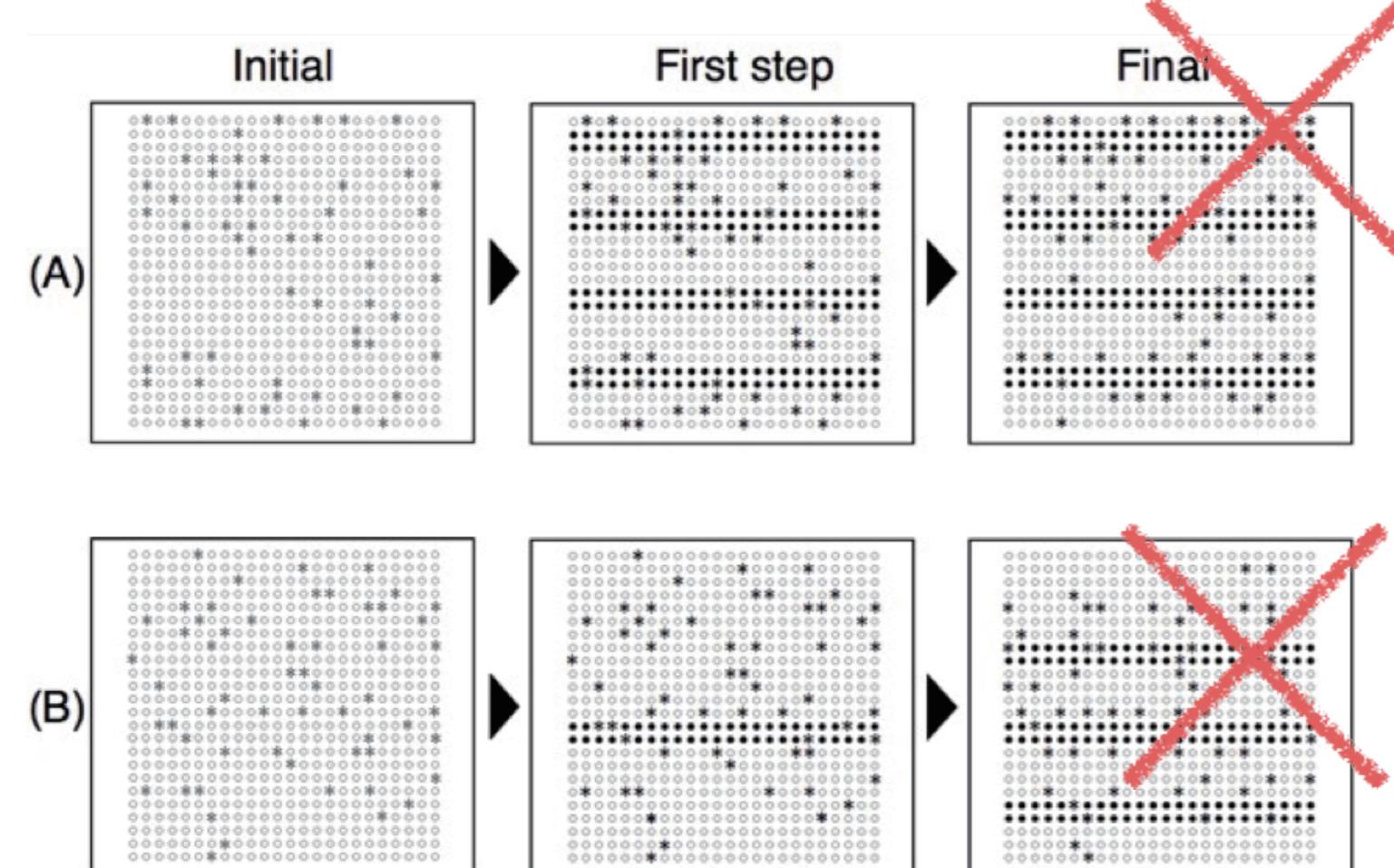
# Energetic assessment between L1<sub>2</sub> and small clusters in Mg-Zn-Y alloy

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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.

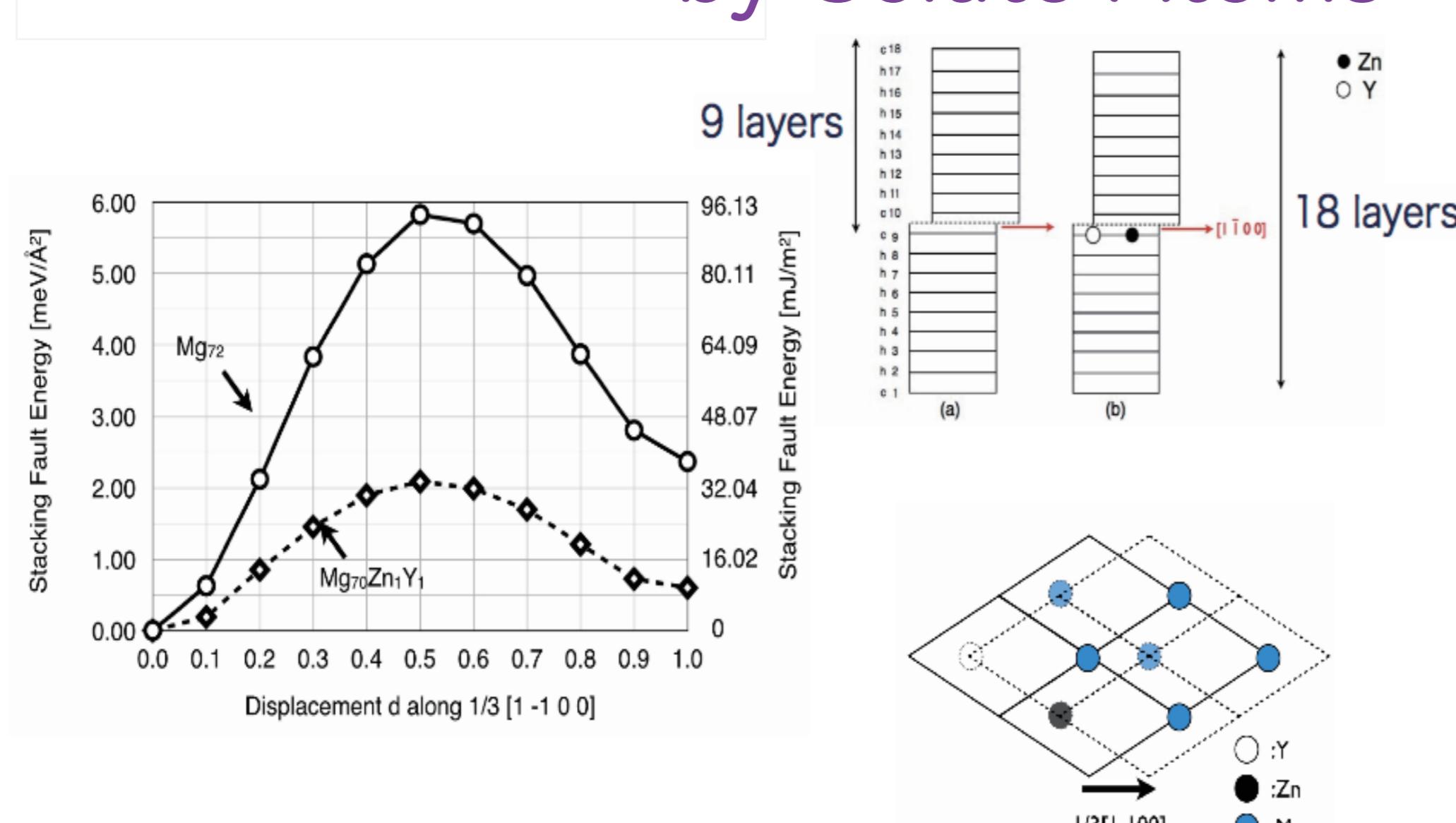
### Assessment by VASP calculation

- 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?

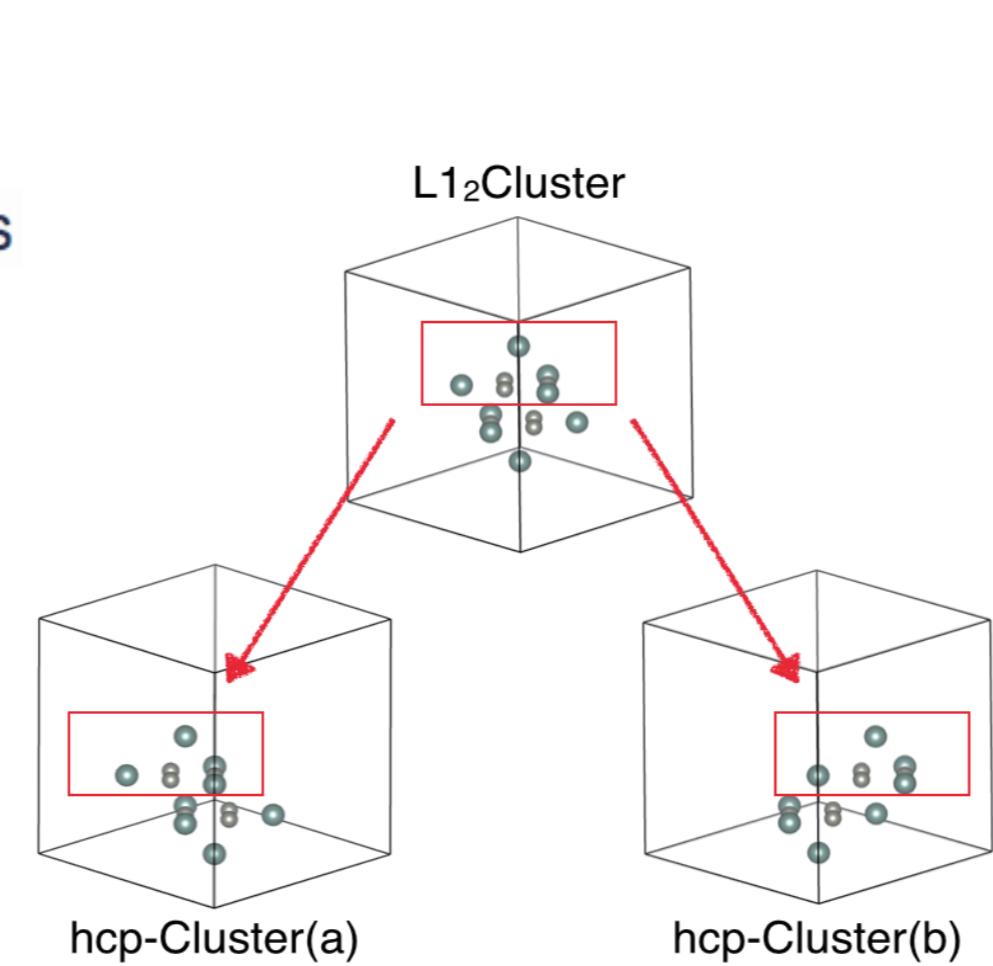
## Inspection of Cluster

- Cluster Stability in various type of lattice.
- Cluster in Stacking Fault.
- Interaction btw Clusters.
- Interaction btw Cluster and Solute Atom.

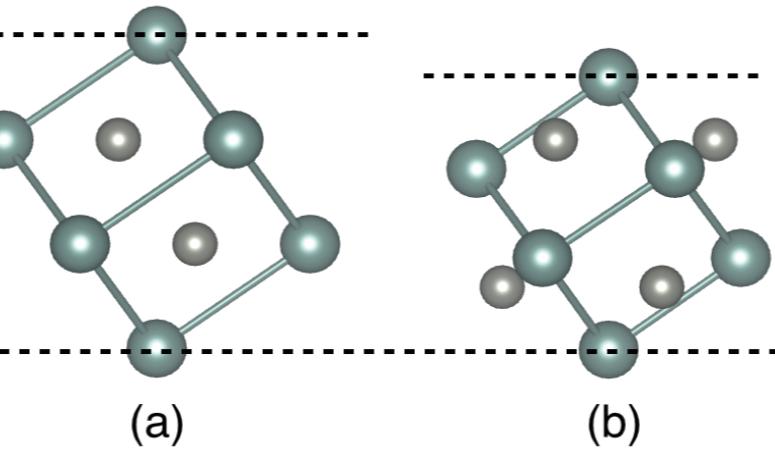
## Introduction of Stacking Fault by Solute Atoms



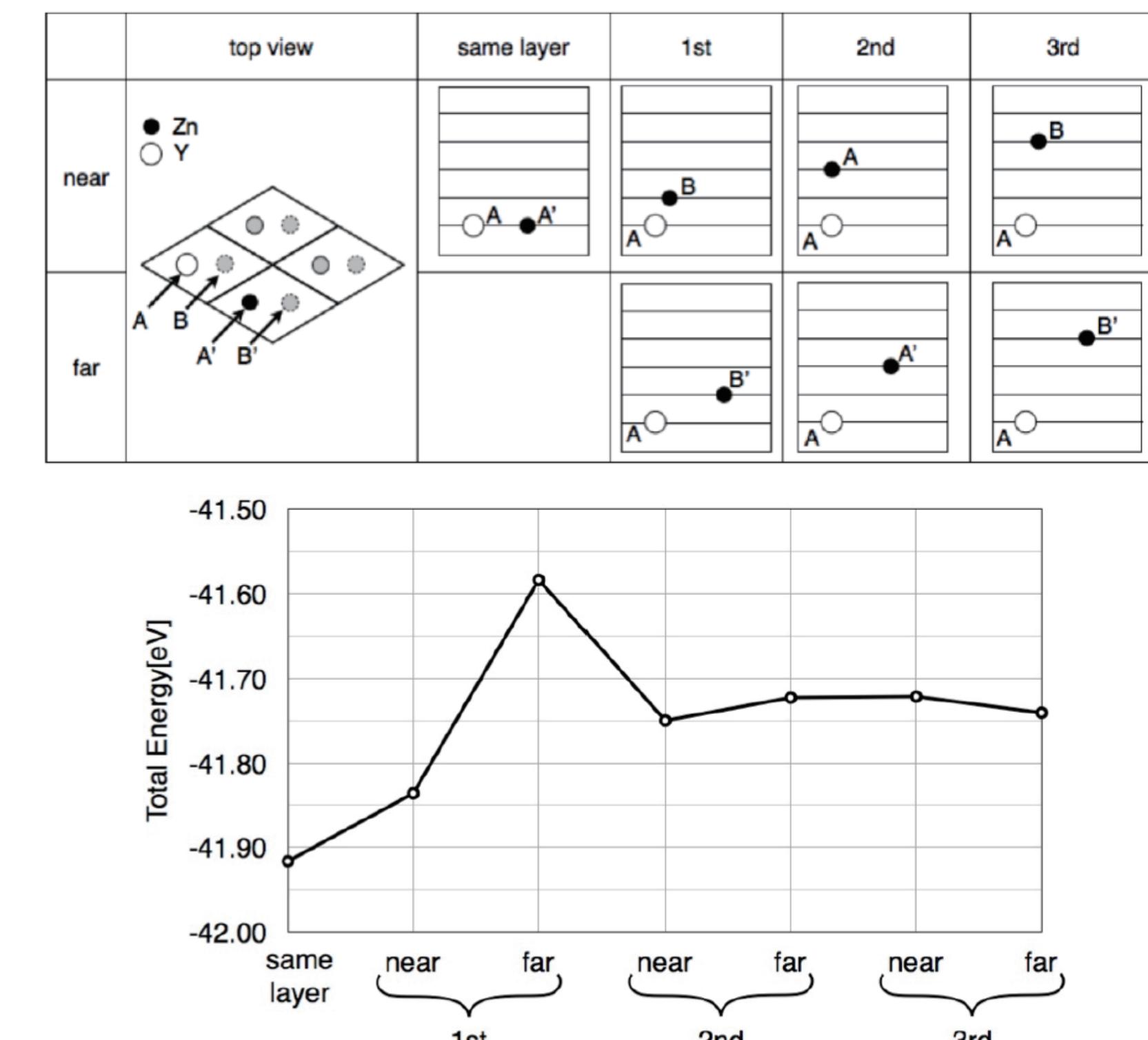
## Cluster Stability



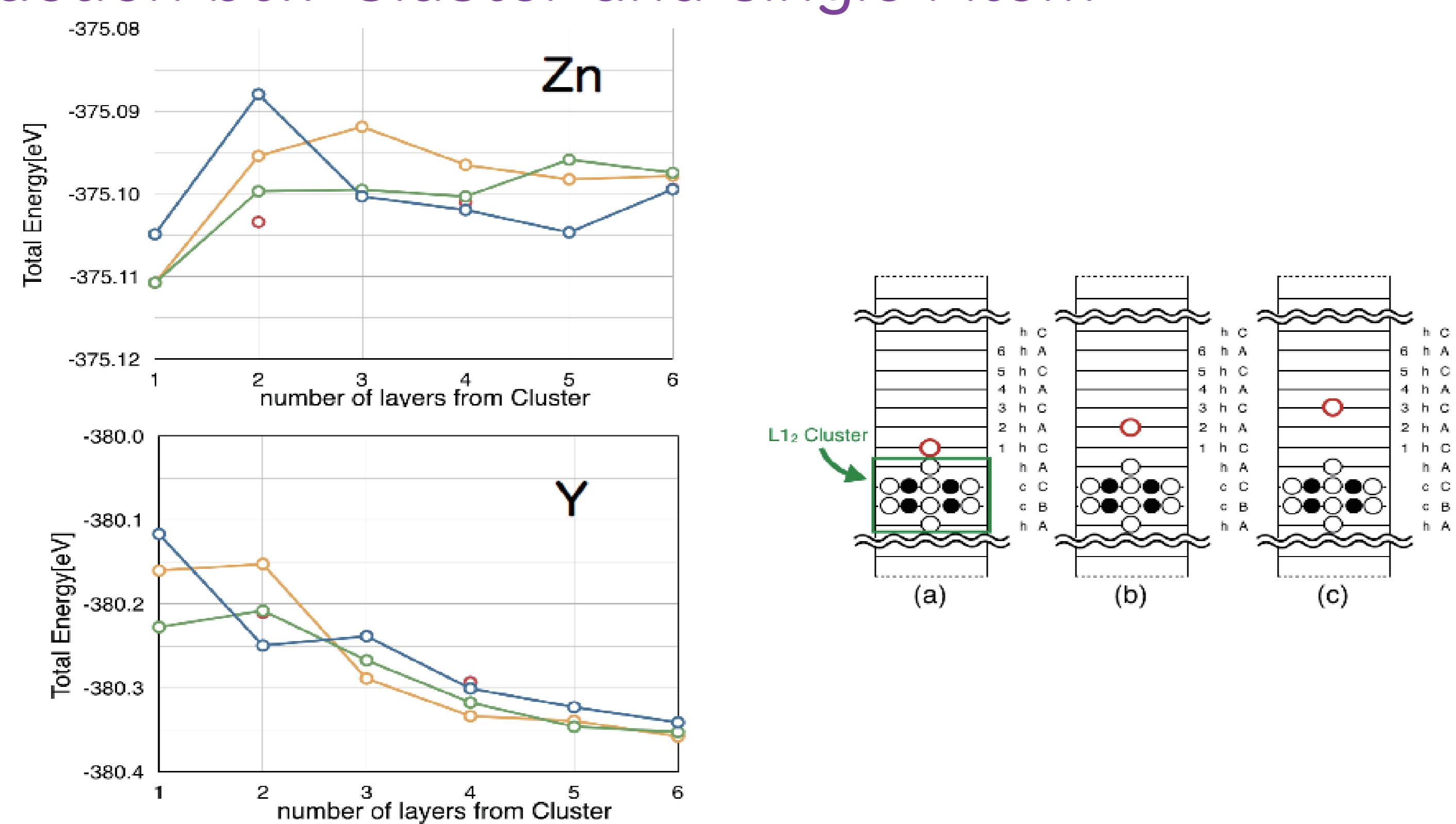
Cluster energies in different stacking sequences.					
E Total [eV]	hcp(a)	hcp(b)	fcc	6H	14H
E Cluster [eV]	-3.040	-4.418	-3.796	-4.043	-4.046



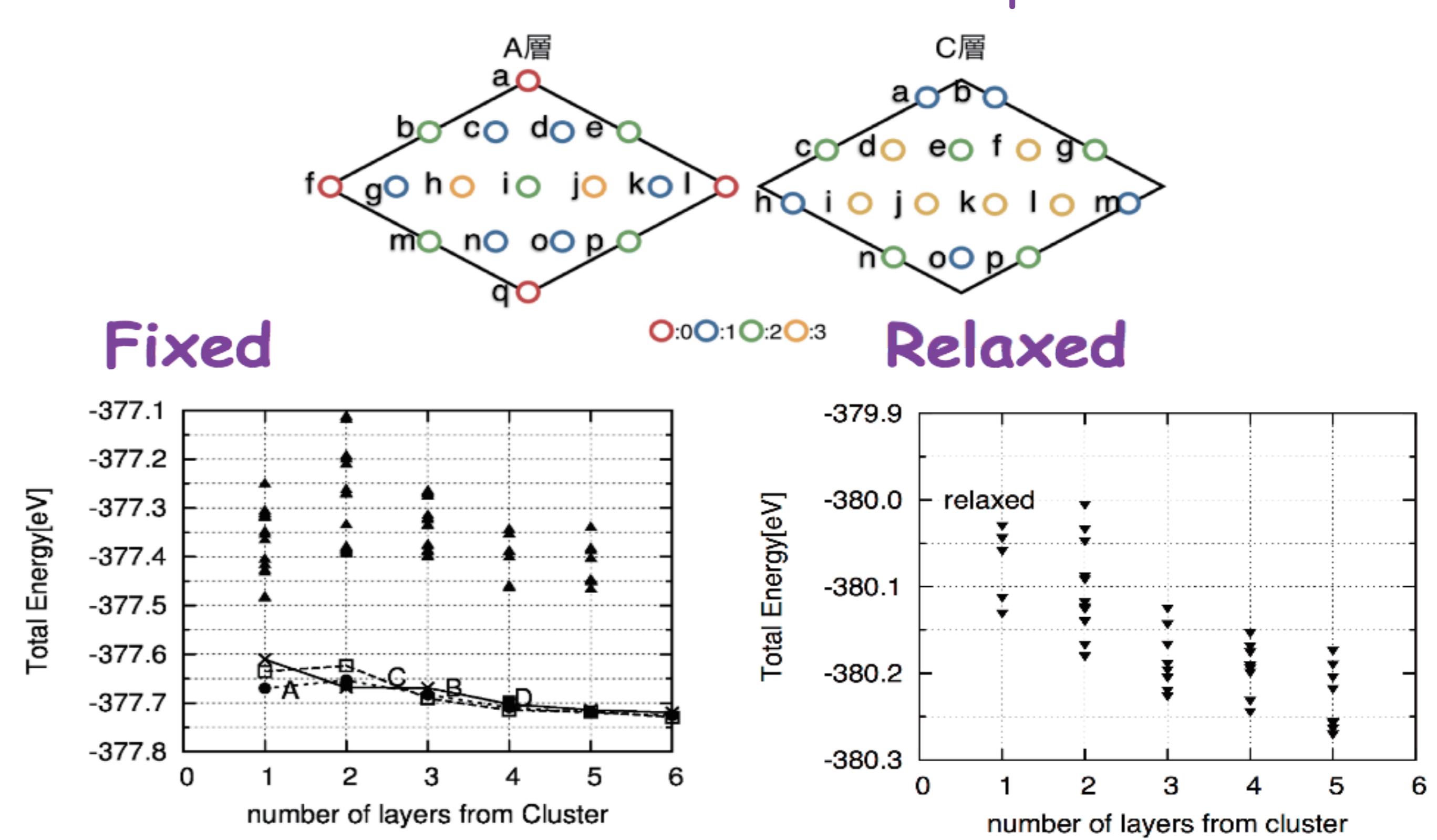
## Interaction btw solute atoms



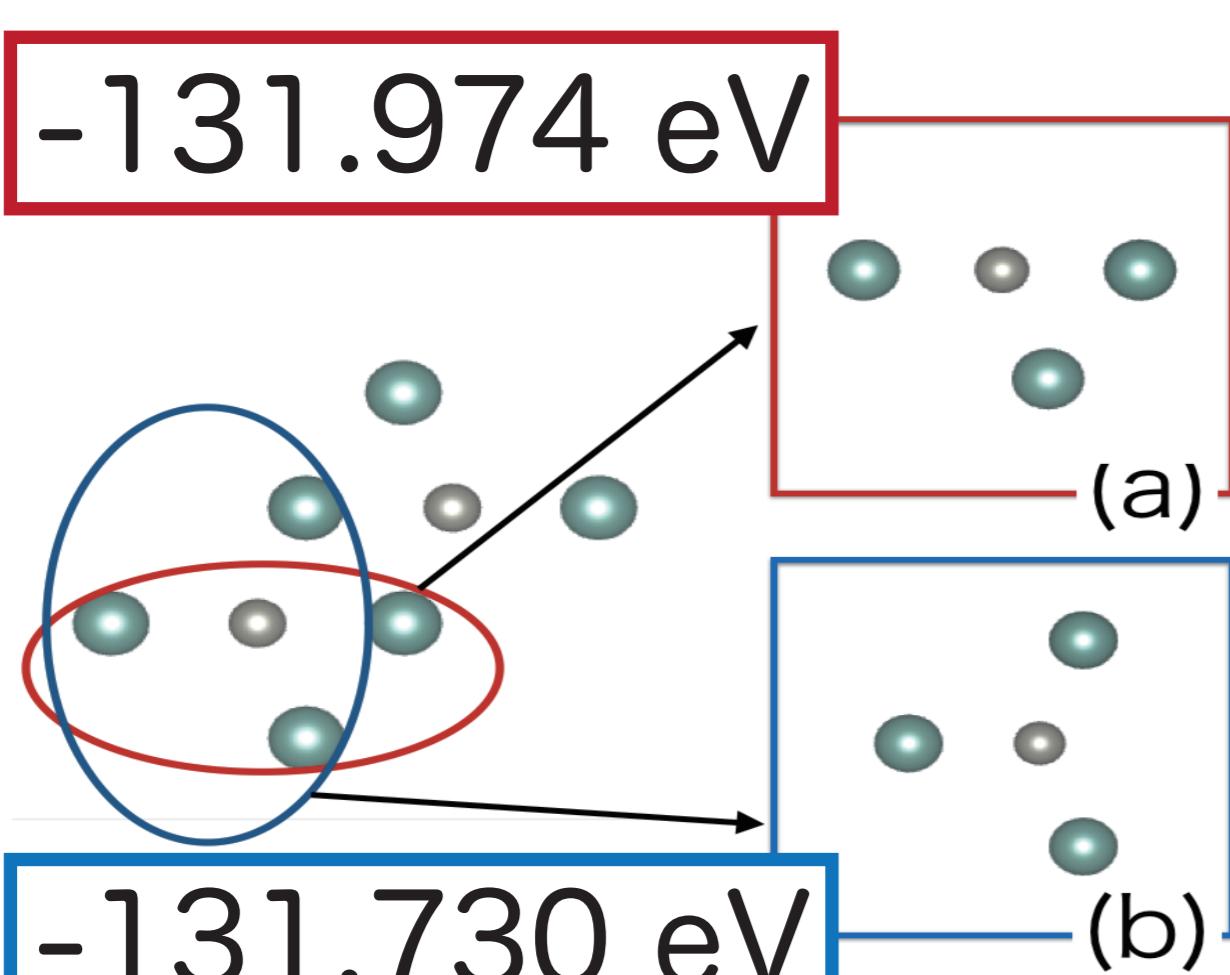
## Interaction btw Cluster and single Atom



## Interaction btw Cluster and Zn-Y pair



## Interaction btw L1<sub>2</sub> Cluster and Small\_Cluster



For making smaller clusters, we divide an L1<sub>2</sub> cluster vertically or horizontally like (a) or (b). Then we insert the small cluster in hcp Mg with the 6 layers. The first principle calculations show that (a) type cluster shows 0.2 eV lower energy than (b) type cluster.

## 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 in 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.

