

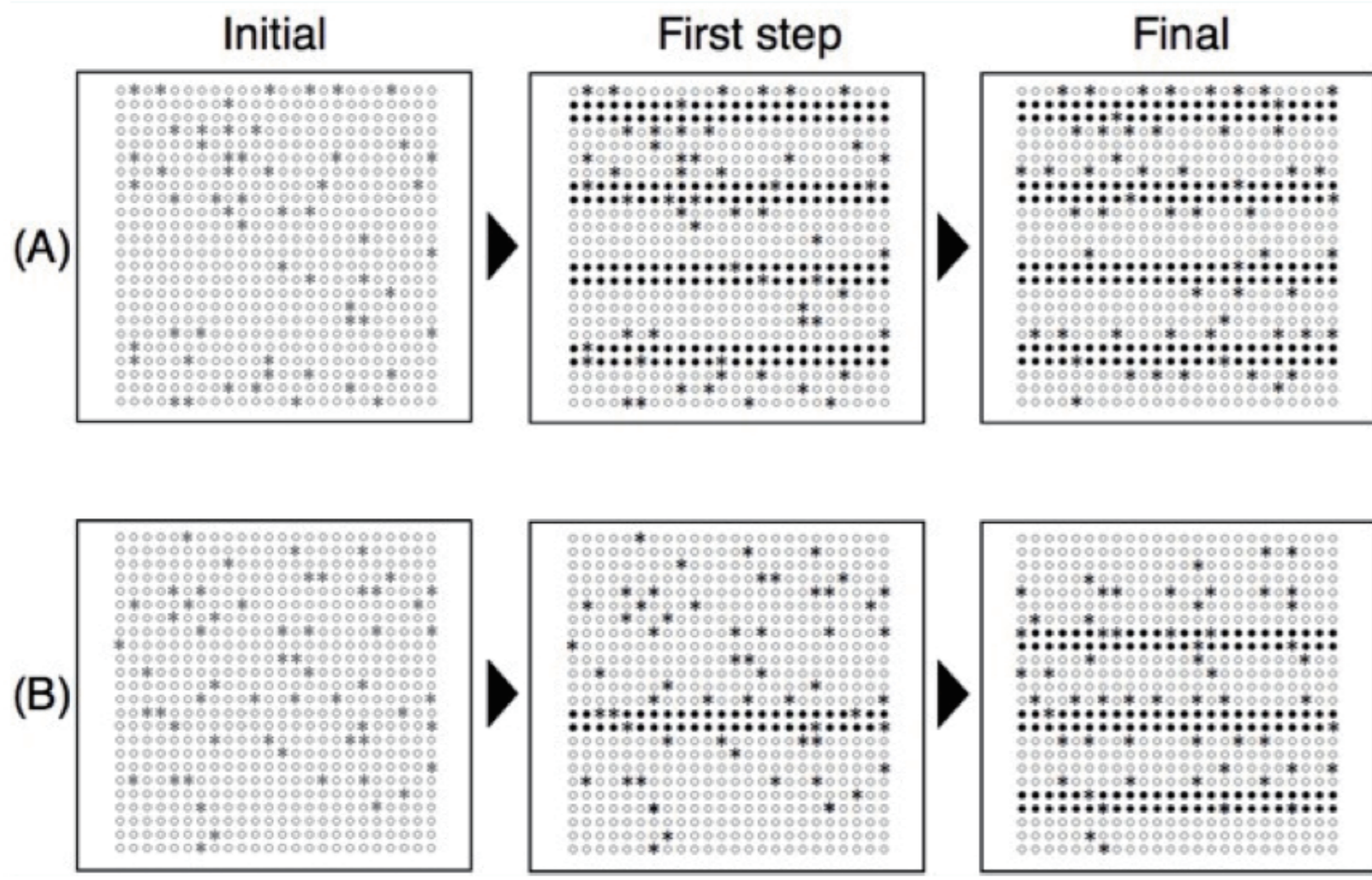
クラスターと溶質原子の相互作用の第一原理計算

科学研究費補助金・新学術領域研究
シンクロ型LPSO構造の材料科学 一次世代軽量構造材料への革新的展開—
平成26年度研究成果報告会(2015・3・8 軽井沢プリンスホテル)

関西学院大学工学部 西谷滋人



Illustrations of LPSO formation scenarios



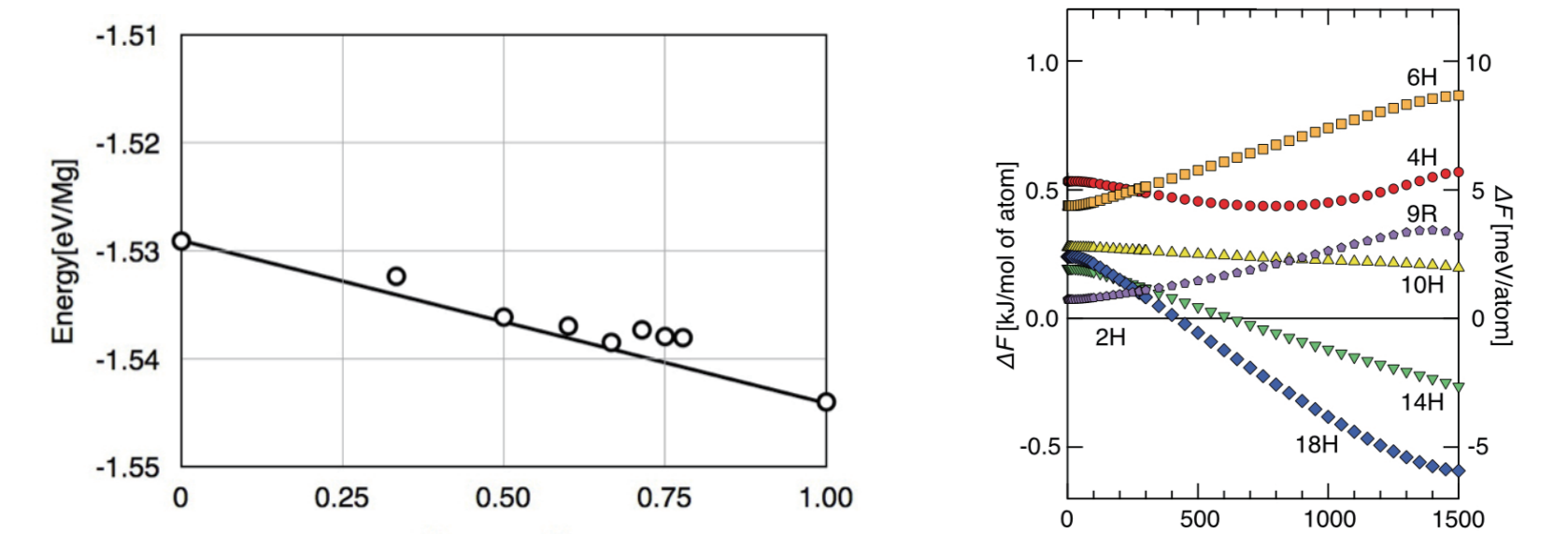
LPSO form scenarios

- Stacking Fault initiate
 - Stacking faults are introduced periodically in hcp-Mg.
 - Solute atoms are then trapped.
- Solute Ordering initiate
 - A SF traps the solution atoms.

First principles calcs.

- Stacking Fault initiate
 - Long period stackings are stable in Mg?
 - Solute atoms are stable in SF?
 - Solute Ordering initiate
 - Really does SF trap the solutions?
- Does a SF with solutions stabilize the middle range ordering of solutions?
- Does condensed solutions really initiate the stacking fault?

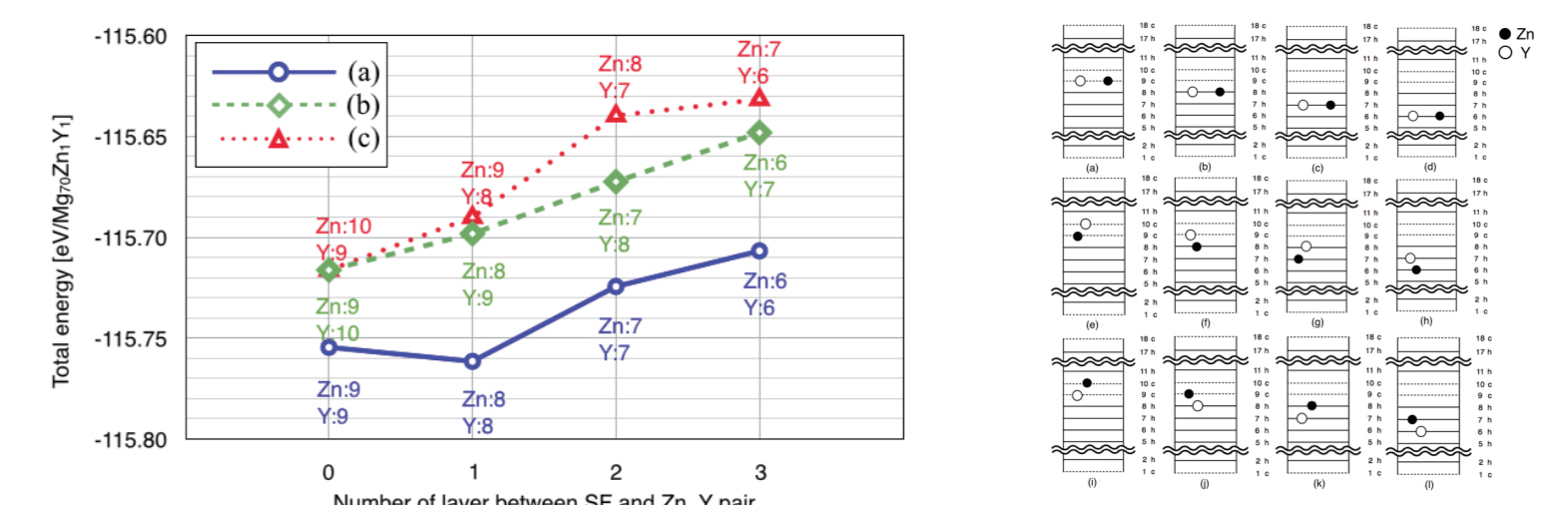
Periodic Stacking Fault ?



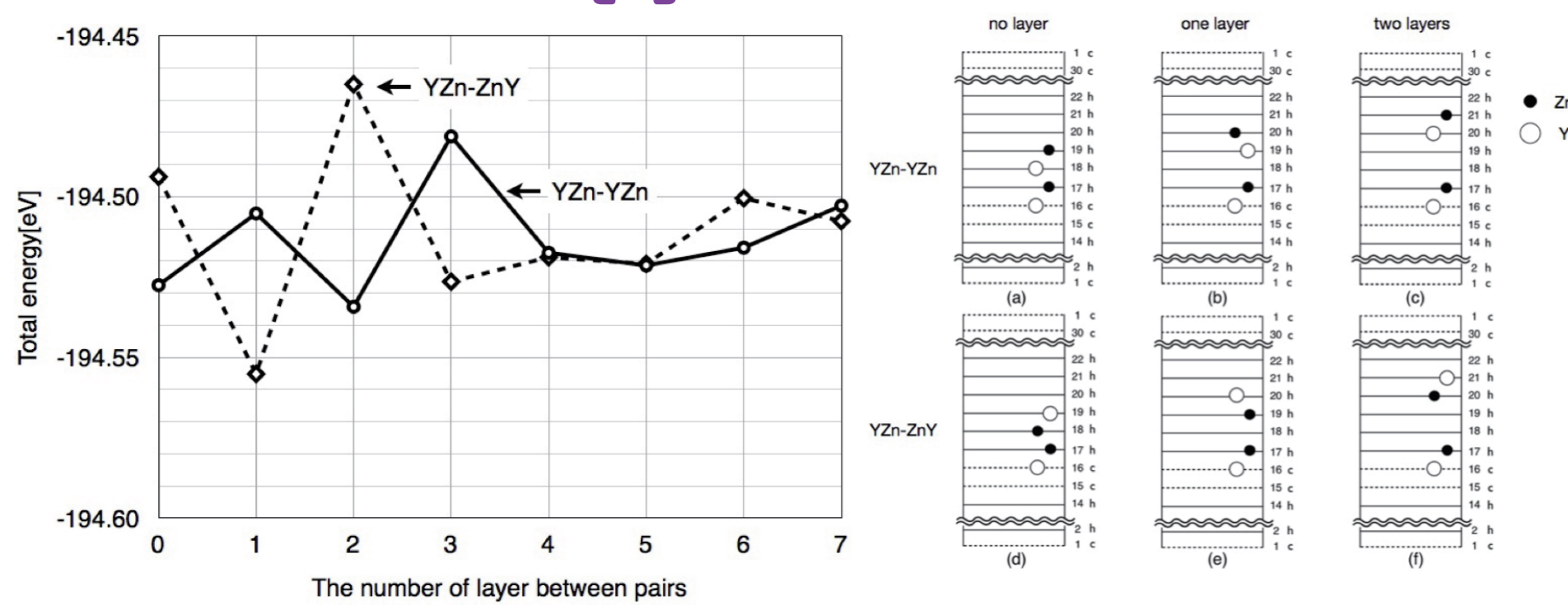
Stability at elevated temps. calc. by Phonon.

S. Iikubo, K. Matsuda and H. Ohtani: Phys. Rev. B, 86, 054105(2012).

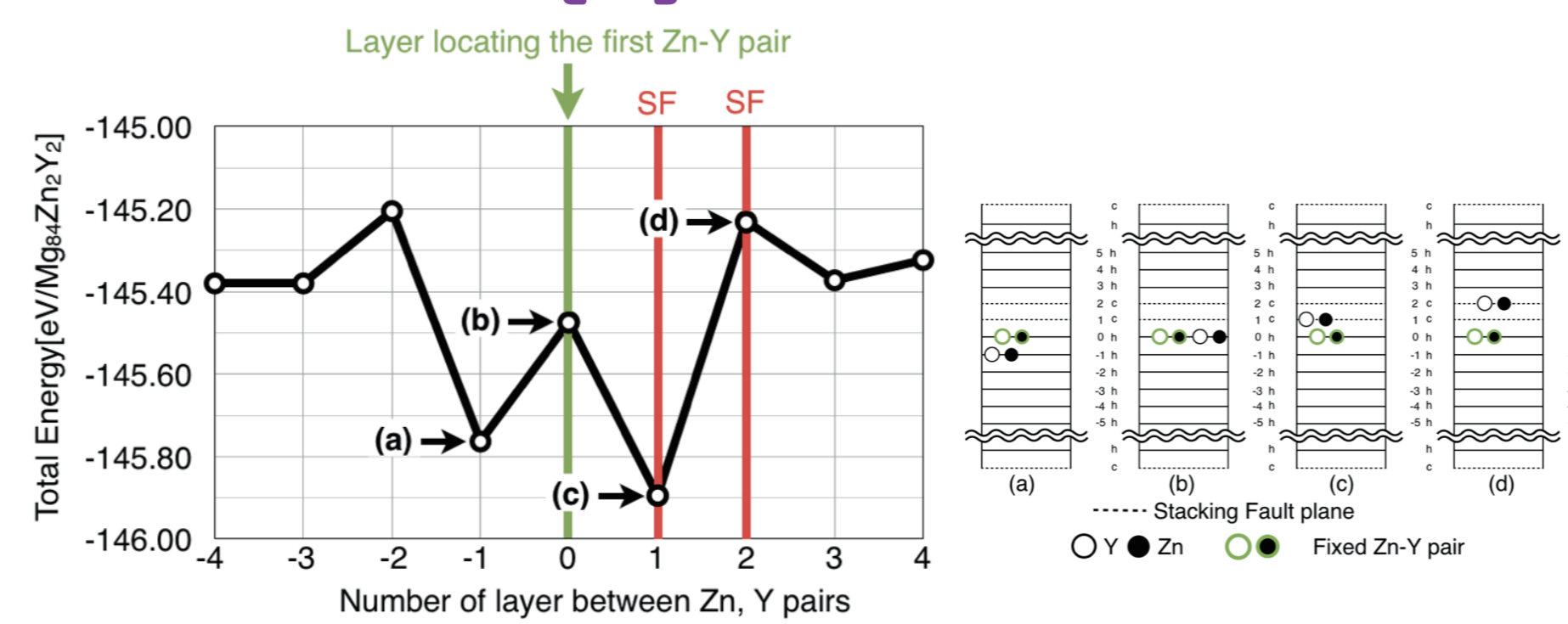
Does SF trap solutions?



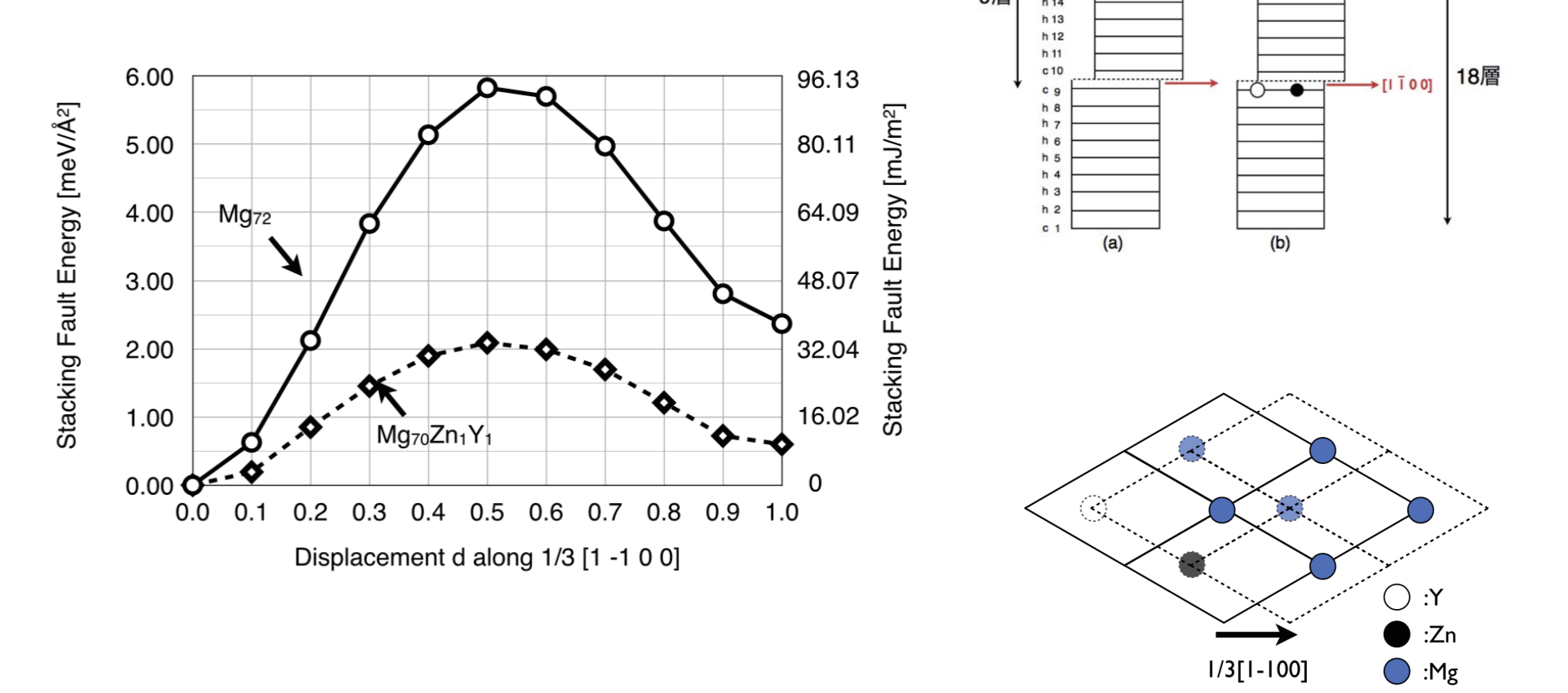
Middle range ordering of solutions [I]



Middle range ordering of solutions [II]



Does condensed solutions initiate SF?



List checked by first principles calcs.

- Stacking Fault initiate
 - Long period stackings are stable in Mg?
 - Solute atoms are stable in or around SF?
- Solute Ordering initiate
 - Really does SF trap the solutions?
 - Does a SF with solutions stabilize the middle range ordering of solutions?
 - Does condensed solutions really initiate the stacking fault?

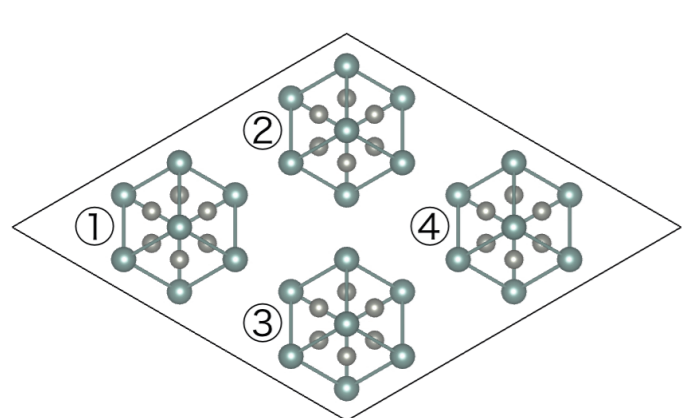
Cluster?

- Cluster stability in hcp, fcc, SF Mg.
- Interactions btw clusters.
- SF in cluster
- Interactions btw cluster and solutions.

Modified scenario

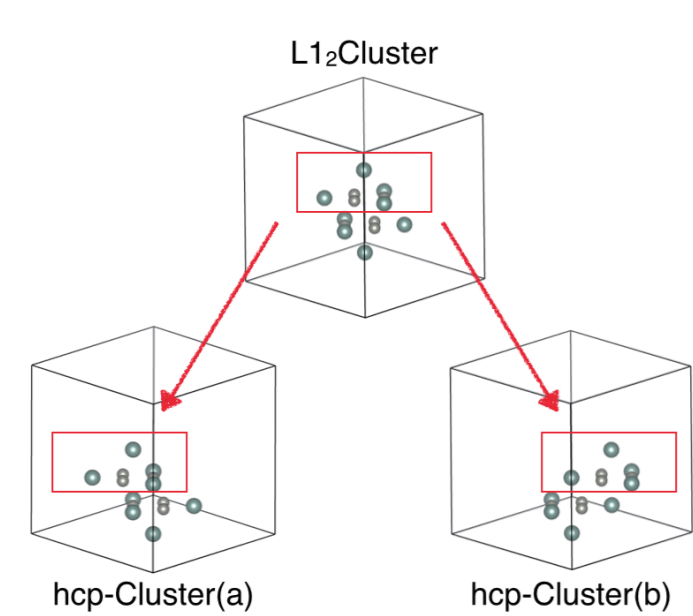
- Zn and Y pairs stayed in the same stacking layer.
- Zn and Y condensed layer induces SF easily.
- SF traps Zn and Y.
- Clusters are formed there.
- Further Zn and Y are swept out or step away from SF with clusters.
- Repeat 2-5 processes.

Cluster stability

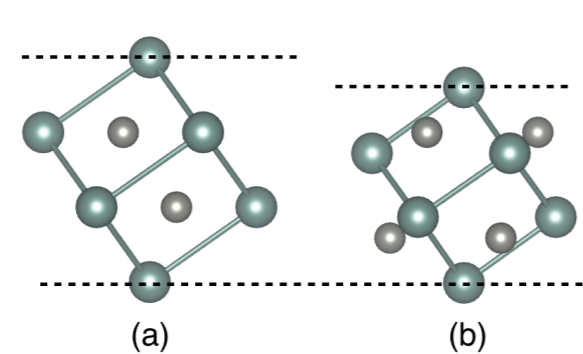


Configurations of 1-4 clusters.				
Number of cluster configurations	1	2	3	4
①	②	③	④	⑤

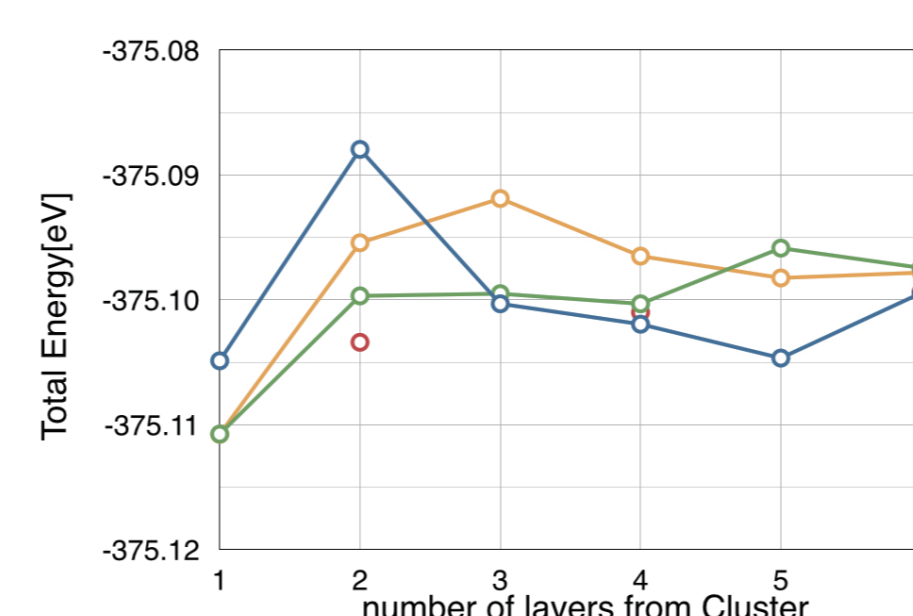
Total Energy and cluster energy.				
number of cluster	1	2	3	4
E_{Total} [eV]	-484.567	-527.695	-570.704	-613.773
$E_{Cluster}$ [eV]	-1.059	-4.080	-4.067	-4.046



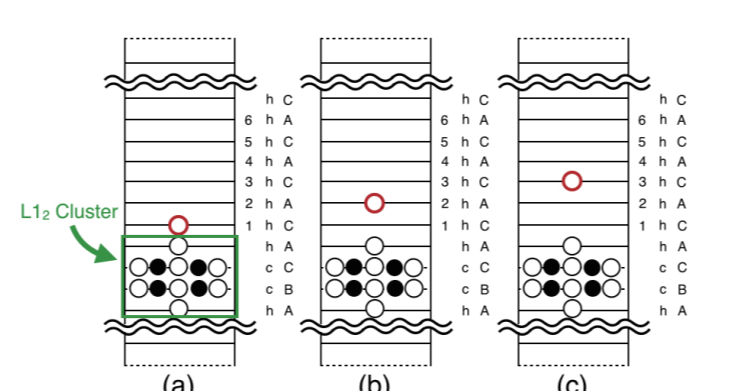
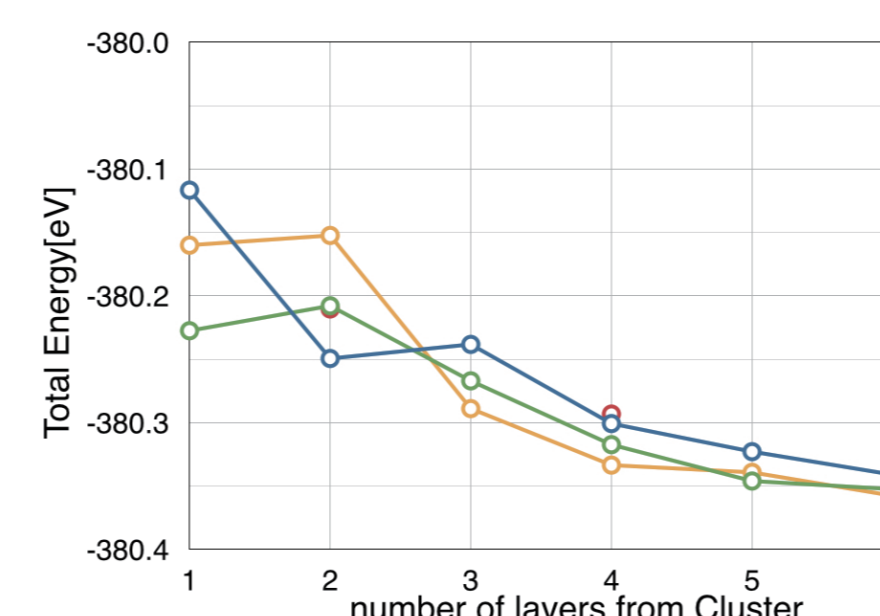
Cluster energies in different stacking sequences.				
	hcp(a)	hcp(b)	fcc	14H
E_{Total} [eV]	-152.543	-153.920	-153.057	-153.441
$E_{Cluster}$ [eV]	-3.040	-4.418	-3.796	-4.043



Interaction btw cluster and solutions



Y



Interaction btw cluster and solution pair

