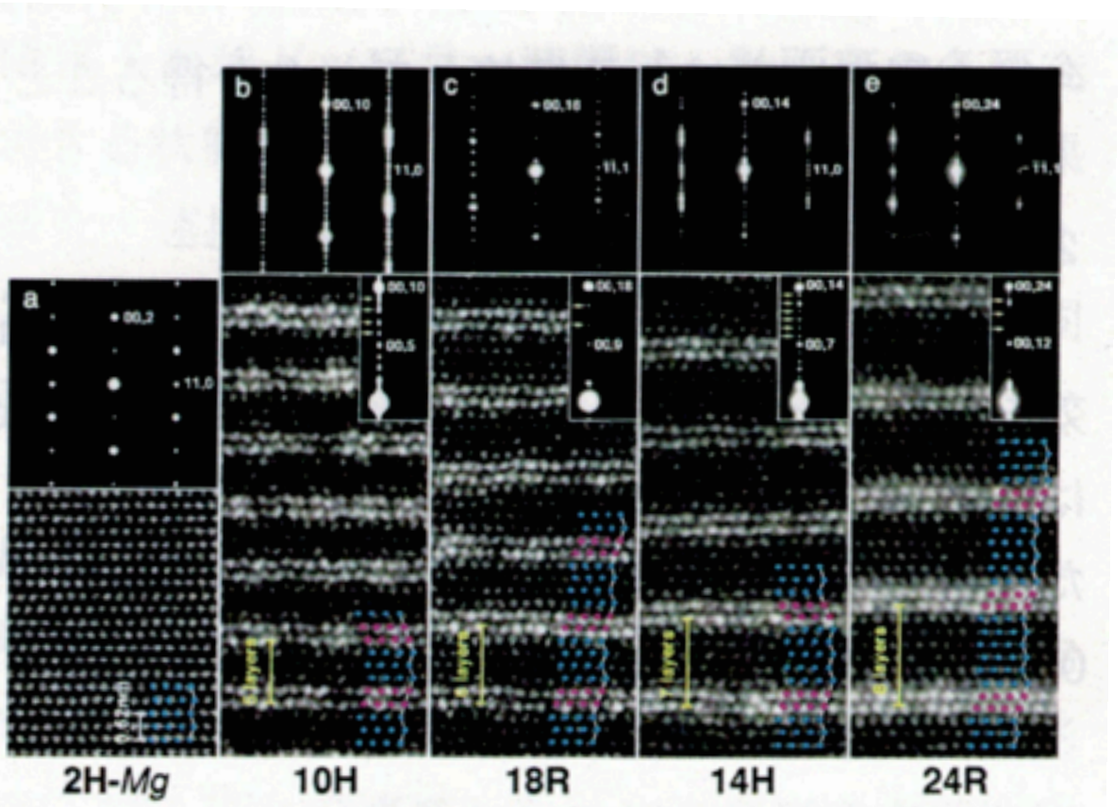
LPSO 2012, (Oct./1-3, Sapporo, Japan)

Solute configuration energies of Mg-Zn-Y alloys

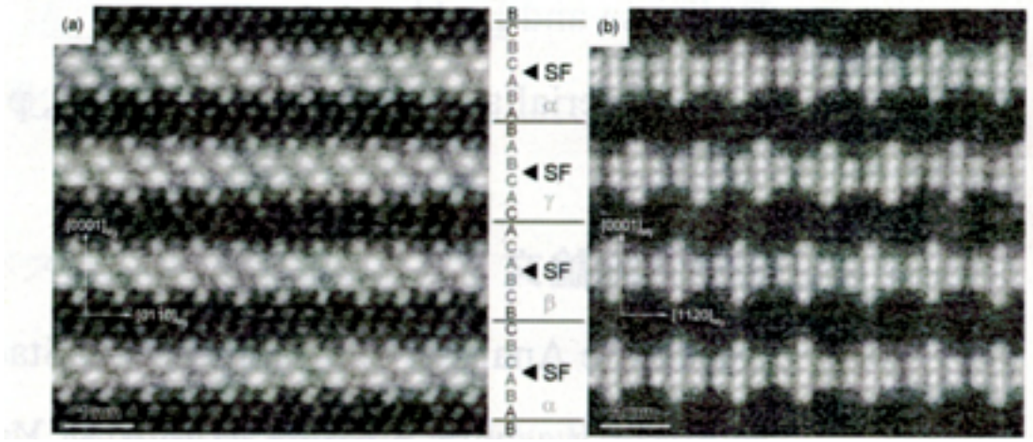
- S. R. Nishitani, Y. Yamamoto, Y. Masaki, and Y.Sakamoto
  Kwansei Gakuin Univ., Sanda, Japan.

Synchronized LPSO Structure

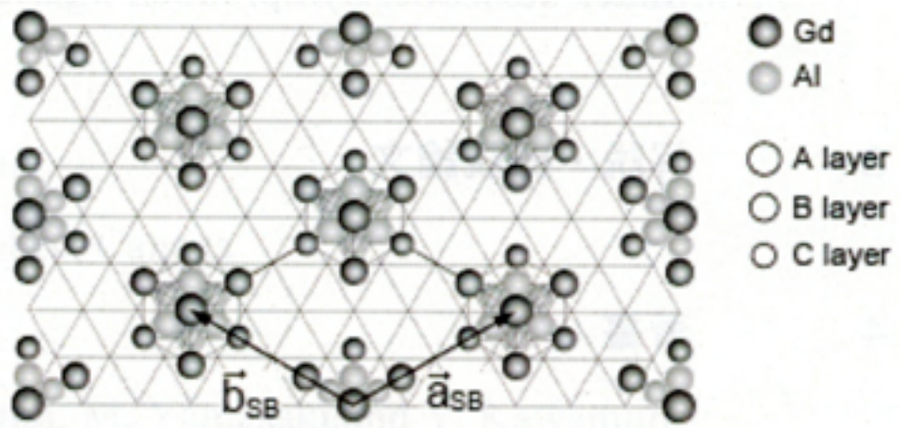
Grant-in-Aid for Scientific Research on Innovative Areas
(Research in a proposed research area) FY2011-2015



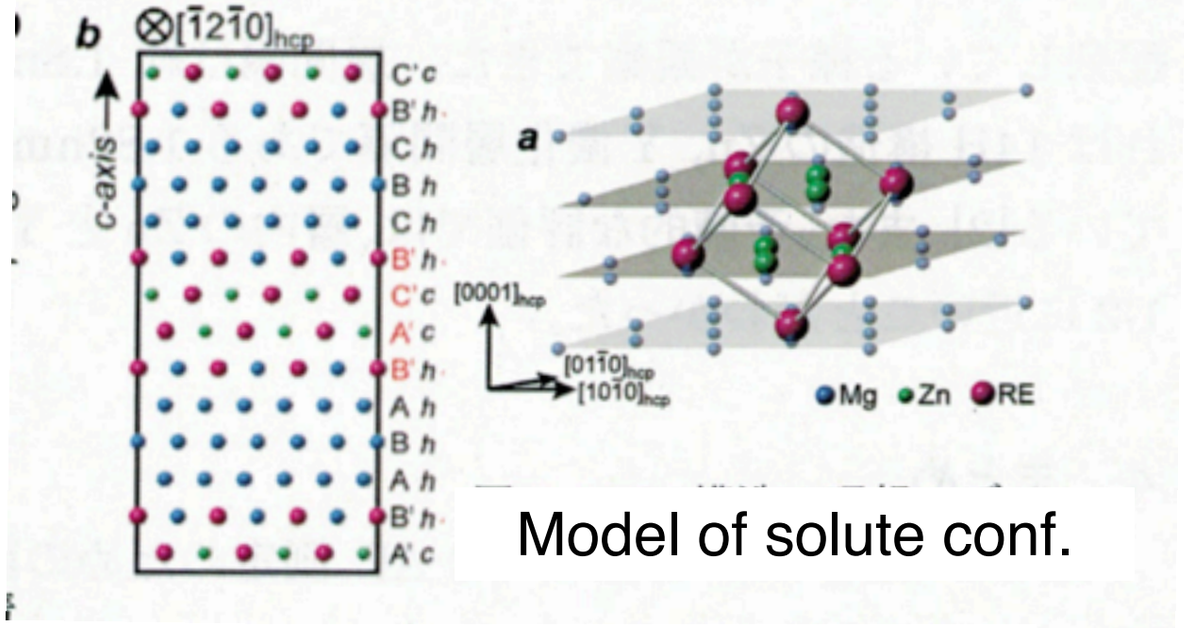
HR-STEM images of LPSOs



HAADF-STEM image of Mg-Al-Gd LPSO

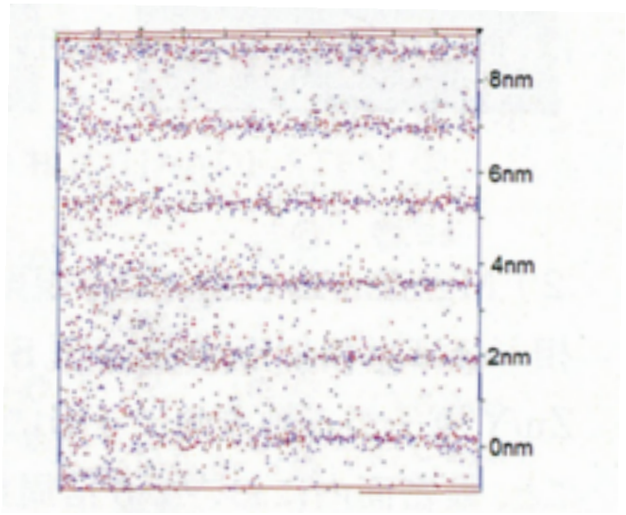


Prof. Kishida and Prof. Inui at Kyoto



Model of solute conf.

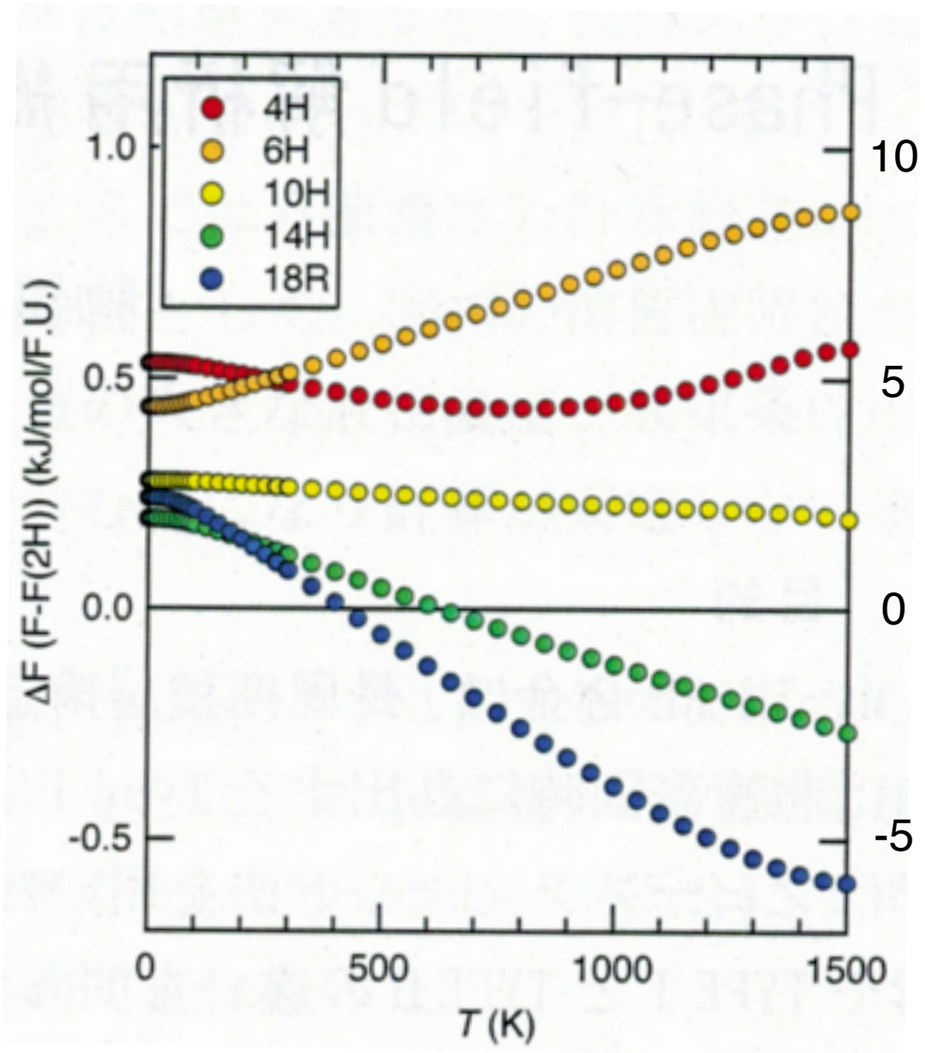
Prof. Abe at Tokyo.



3D-AP of Mg-Zn-Y

Prof. Nagai of MRI at Tohoku

- Stacking order
- Quasi-harmonic Free energy shows 18R stability at high temperatures.
- But the energy difference is very small comparing to k_BT.

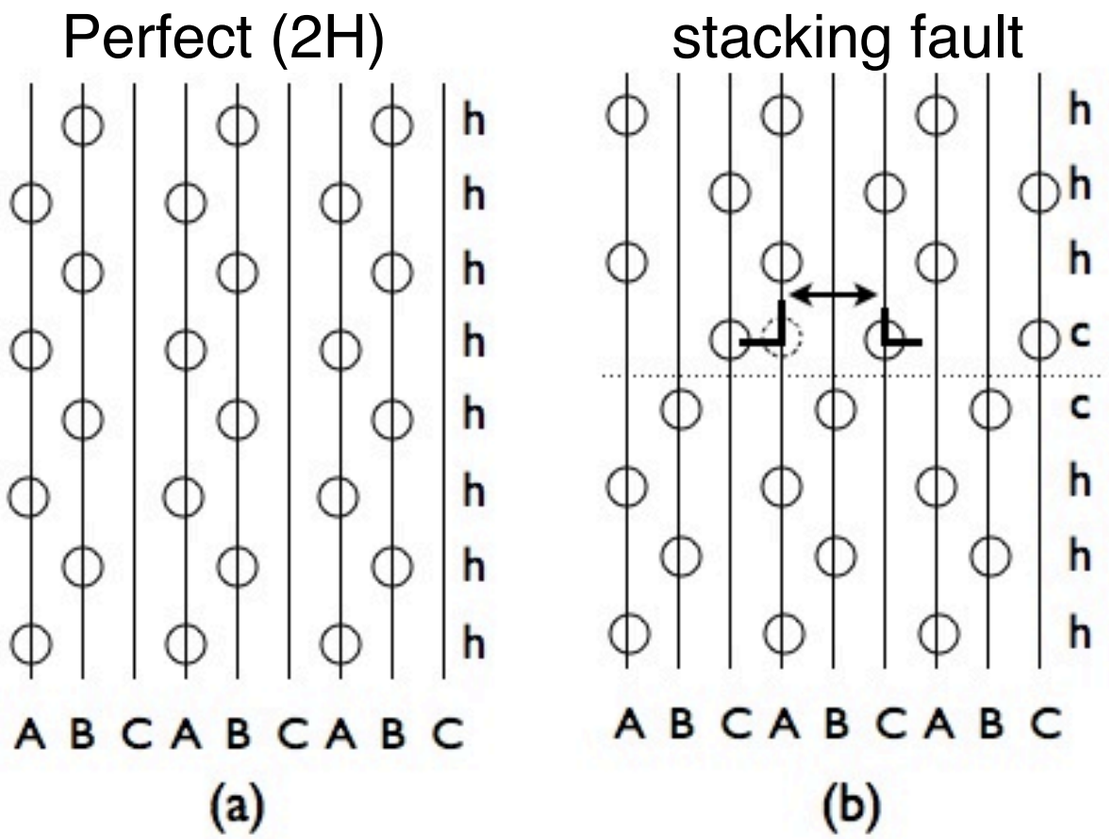


Ilkubo, Tokunaga, and Otani at KyuTech.

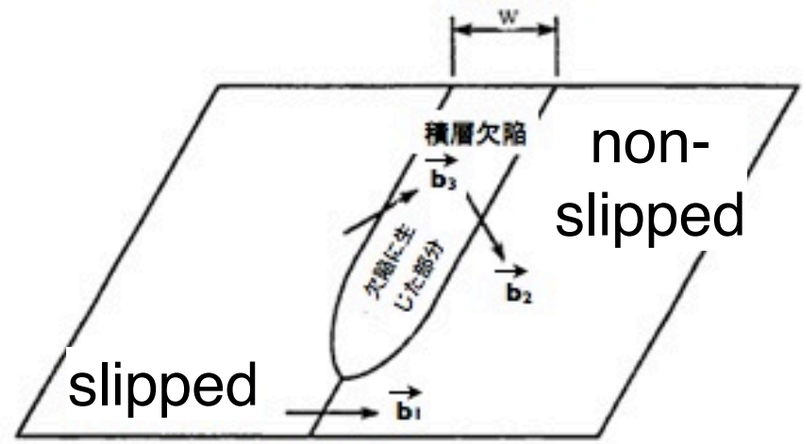
for formation mechanism,
from structure energies...

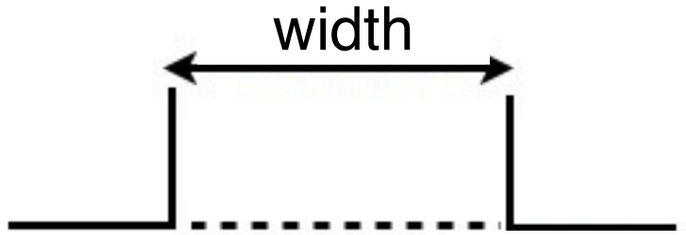
- Stacking order
- Zn, Y in hcp, fcc-Mg
- Zn, Y solute ordering? in hcp-Mg

stacking fault and partial dislocations



extended dislocations





$E_{s.f.}$

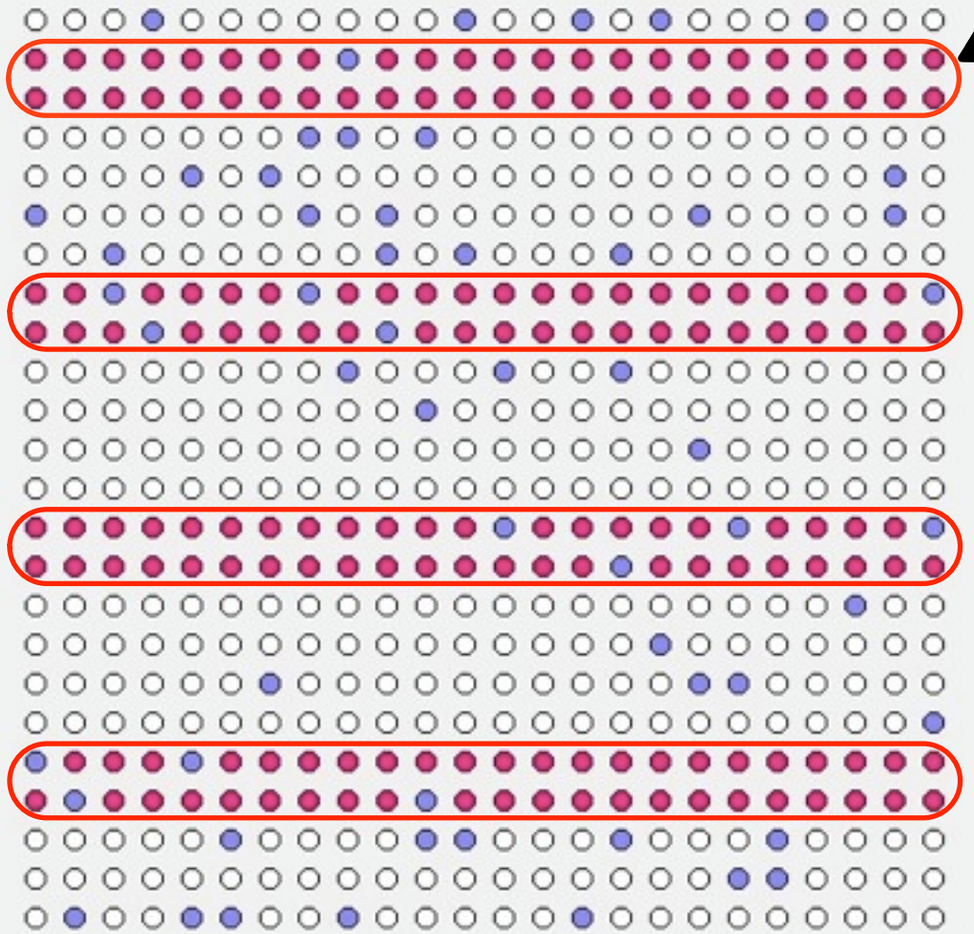
E_{rep} btw partials

for formation mechanism,
from structure energies...

- Stacking order
- Zn, Y in hcp, fcc-Mg
- Zn, Y solute ordering? in hcp-Mg
- before those, in Si (+P,B)

- Two Scenarios

- Controlling process
  - Stacking fault
  - Zn-Y pair diffusion or ordering



Stacking fault

○ : hcp Mg
● : fcc Mg
● : Zn-Y pair

Mg-TM-RE
Mg:1.6A
Zn:1.39A
Y:1.8A

$$\Delta E_{\mathrm{hcp}} = E_{\mathrm{pair}} - E_{\mathrm{isolated}}$$
$$= -0.11(\mathrm{adjacent})$$
$$\sim -0.20(\mathrm{in\,plane})$$
$$[\mathrm{eV/pair}]$$

Scenario No.1:
Stacking fault induced

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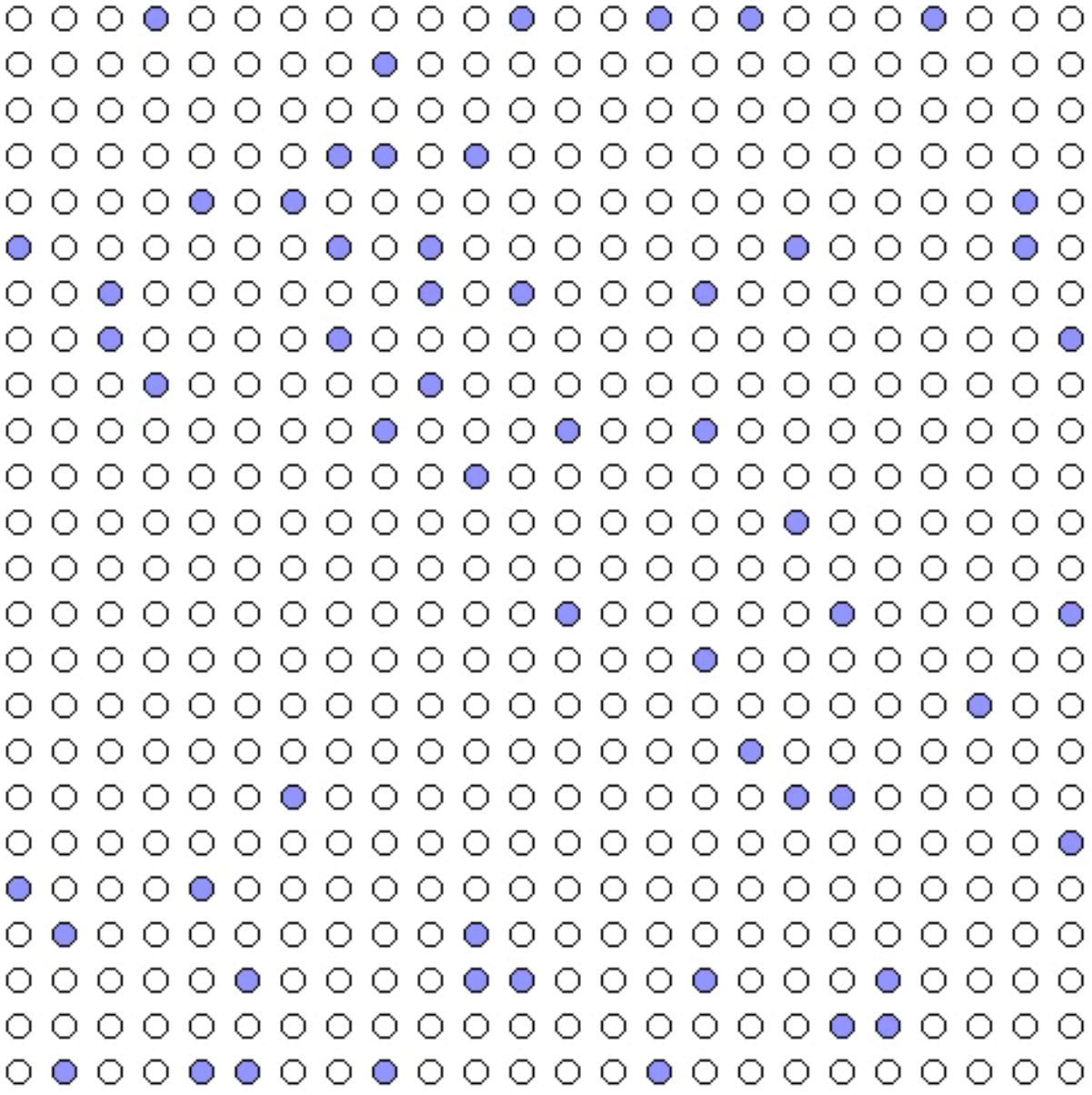
Stacking fault induced



Scenario No.2:
Diffusion control or
solute ordering induced

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Diffusion control or
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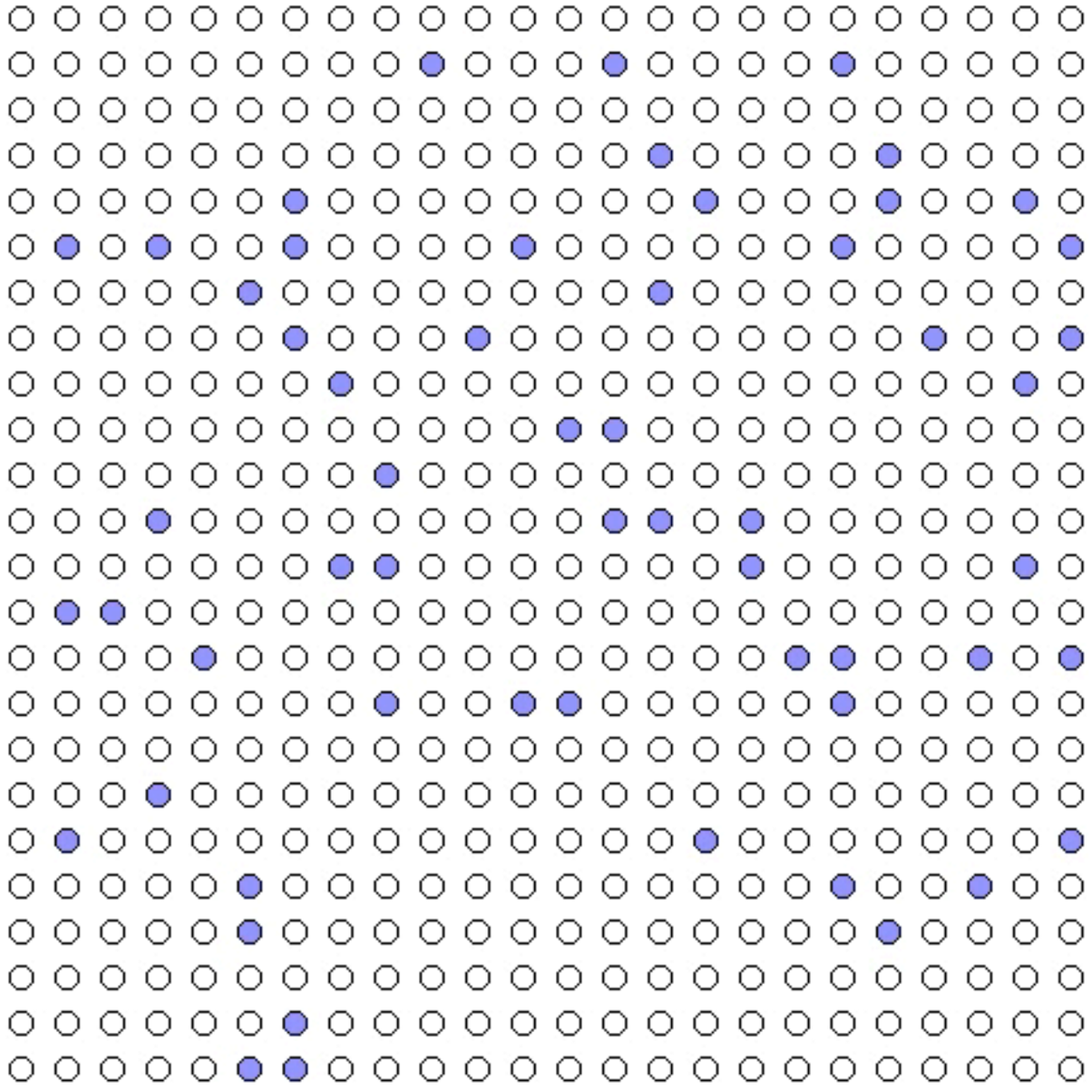
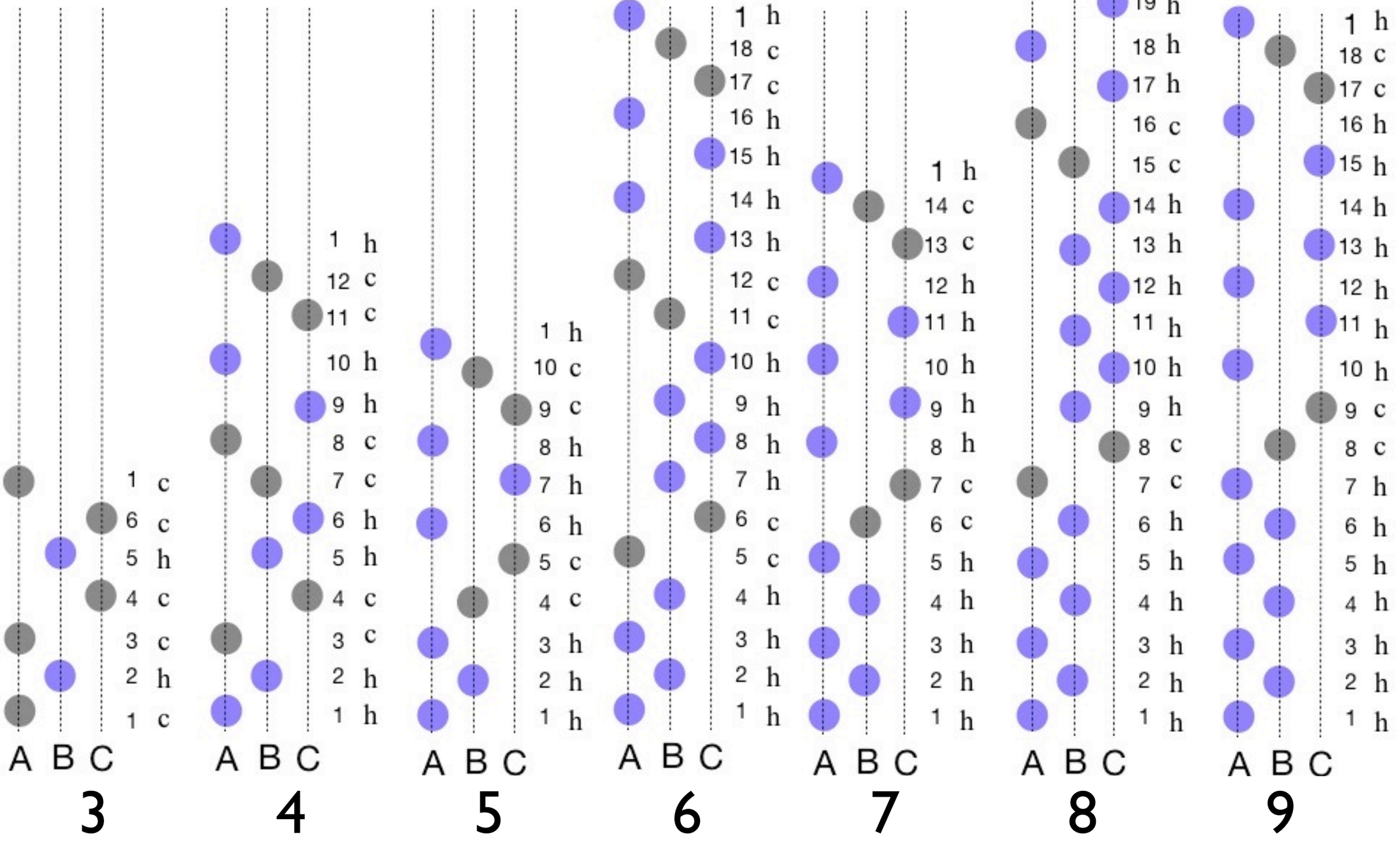
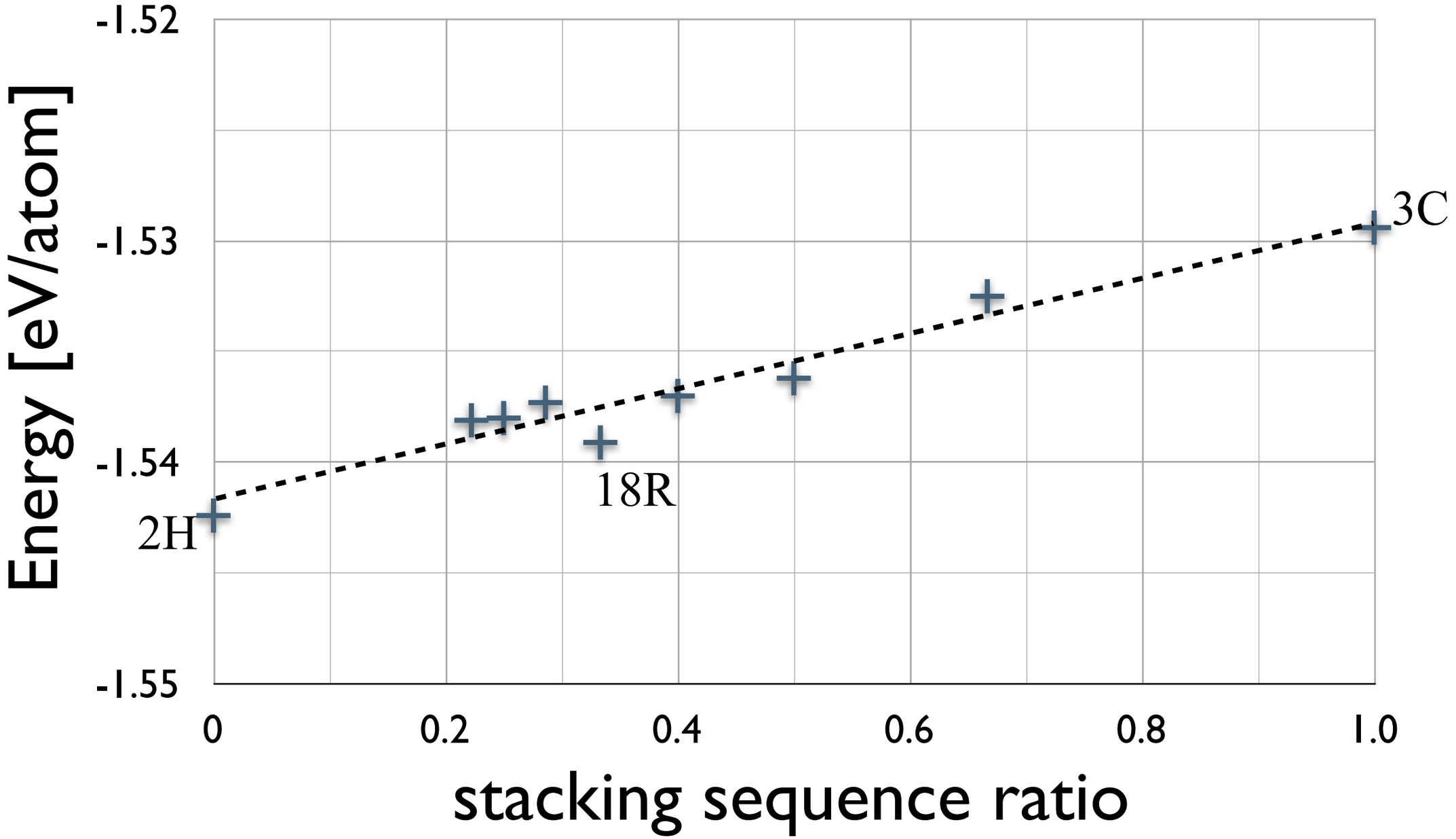


Stacking order in Mg

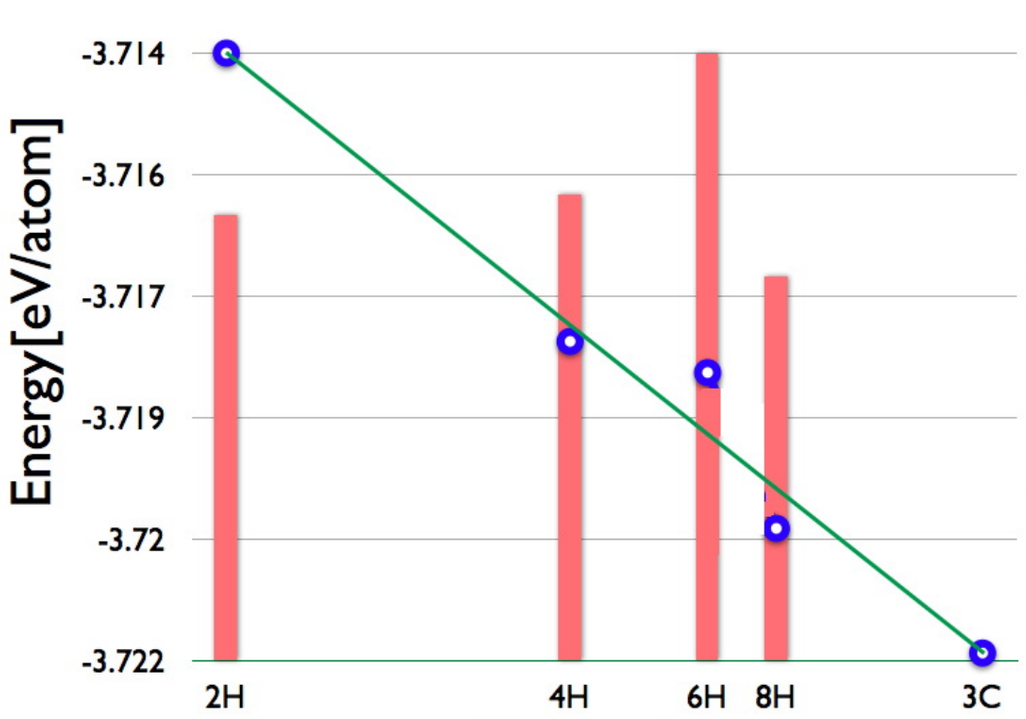
18R



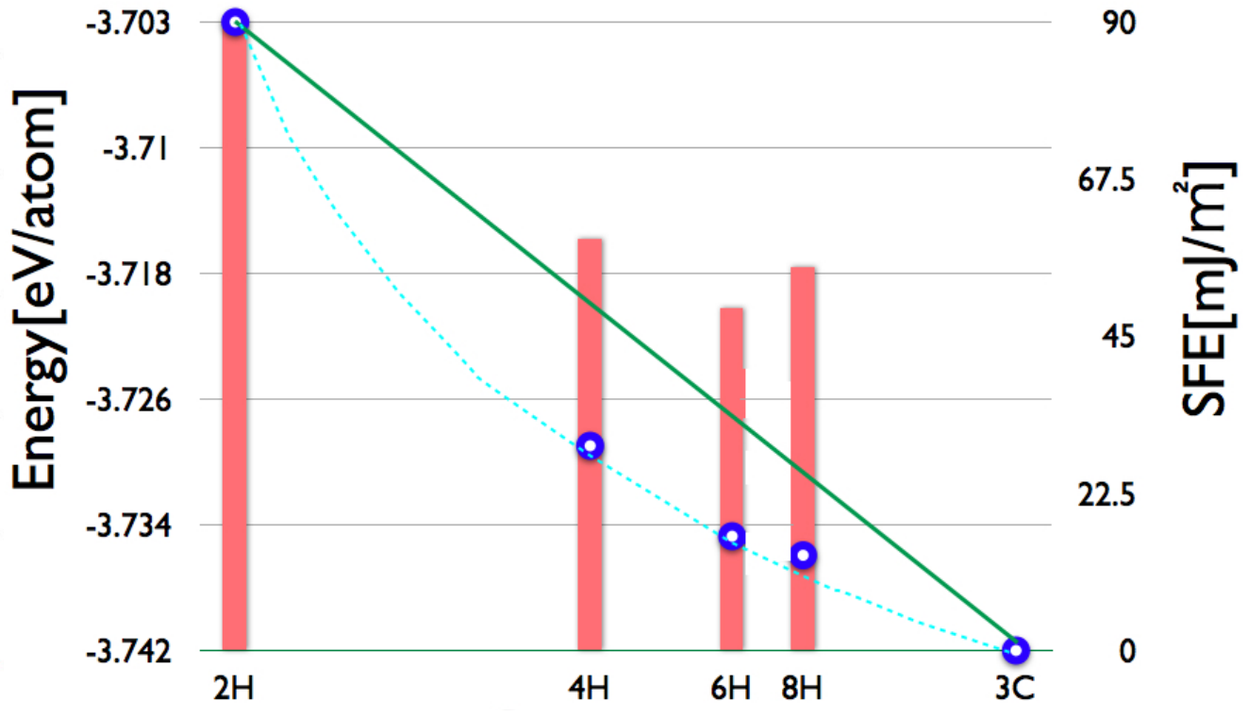
Energy change on stacking sequence ratio

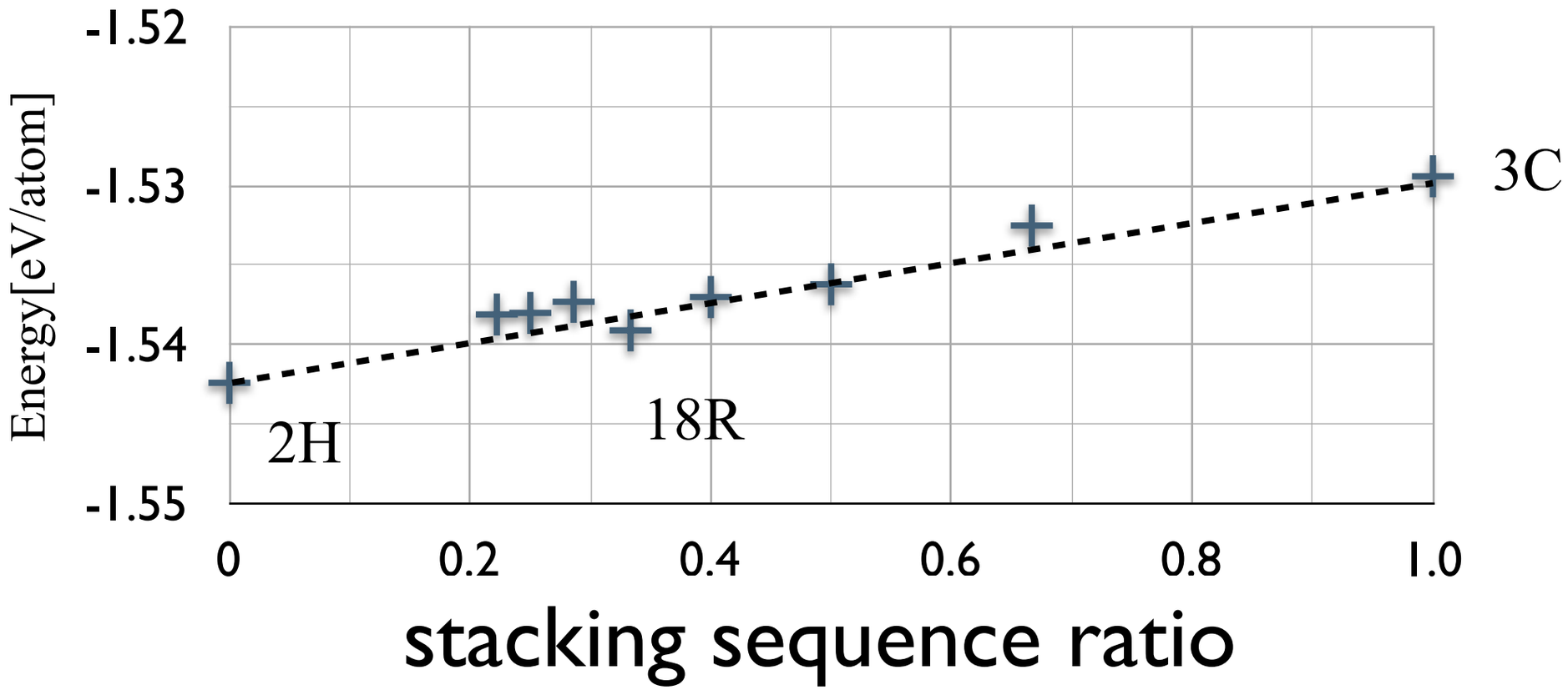


Cu


-3.714
-3.716
-3.717
-3.719
-3.72
-3.722
Energy[eV/atom]
2H
4H
6H
8H
3C
stacking sequence ratio

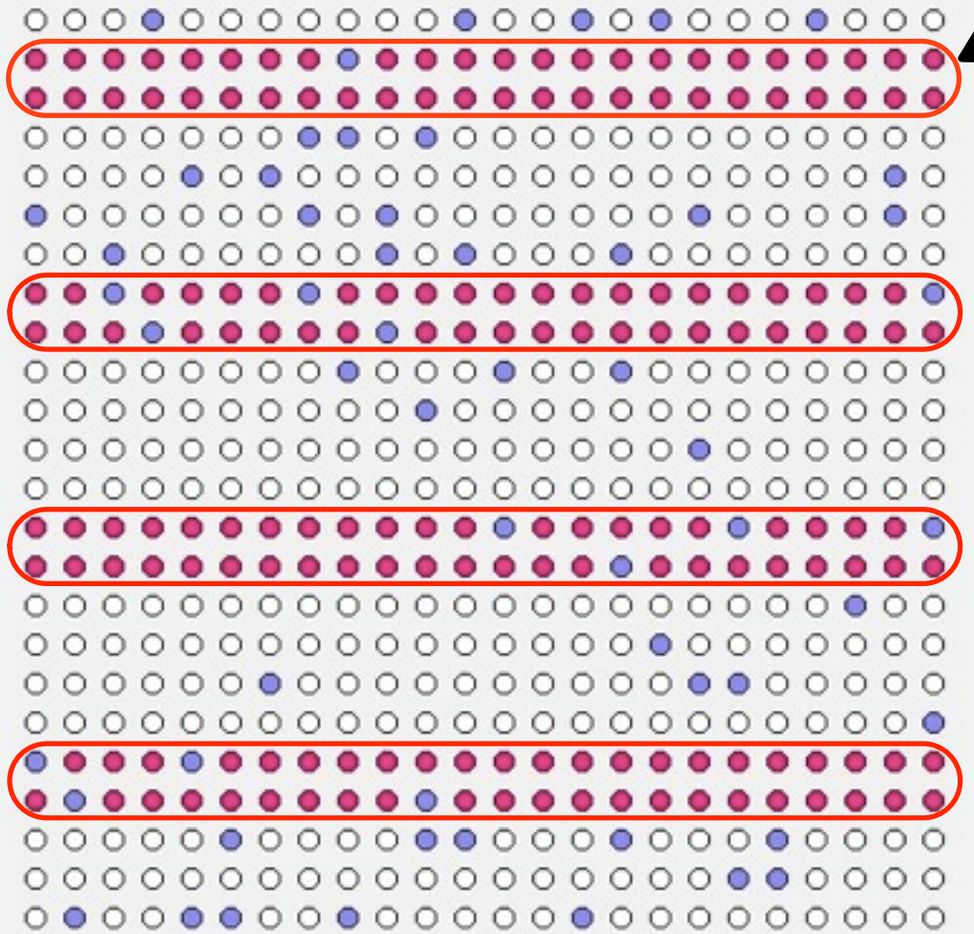
Al


-3.703
-3.71
-3.718
-3.726
-3.734
-3.742
Energy[eV/atom]
90
67.5
45
22.5
0
SFE[mJ/m²]
2H
4H
6H
8H
3C
stacking sequence ratio


-1.52
-1.53
-1.54
-1.55
Energy[eV/atom]
0
0.2
0.4
0.6
0.8
1.0
2H
18R
3C
stacking sequence ratio

- Two Scenarios

- Controlling process
  - Stacking fault
  - Zn-Y pair diffusion or ordering



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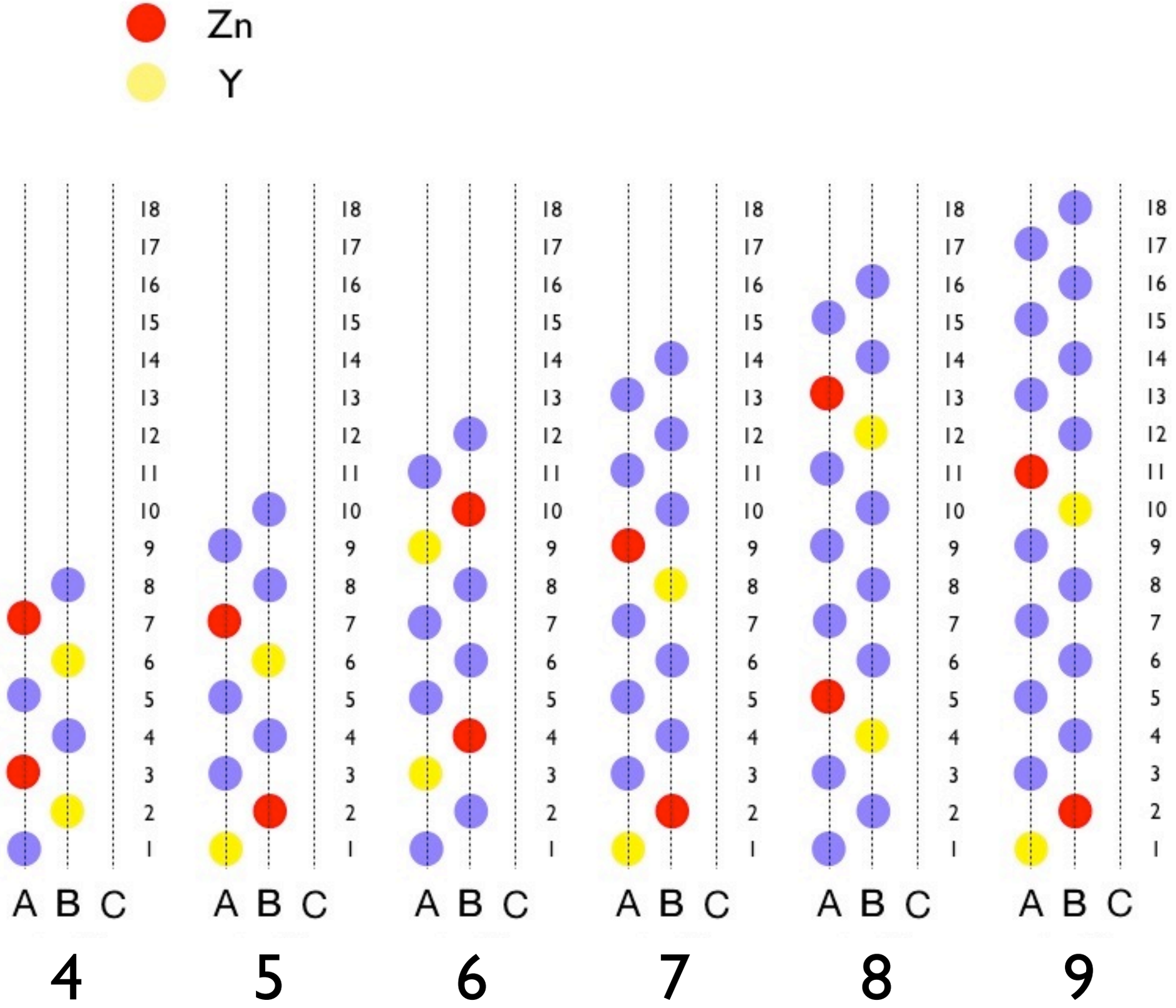
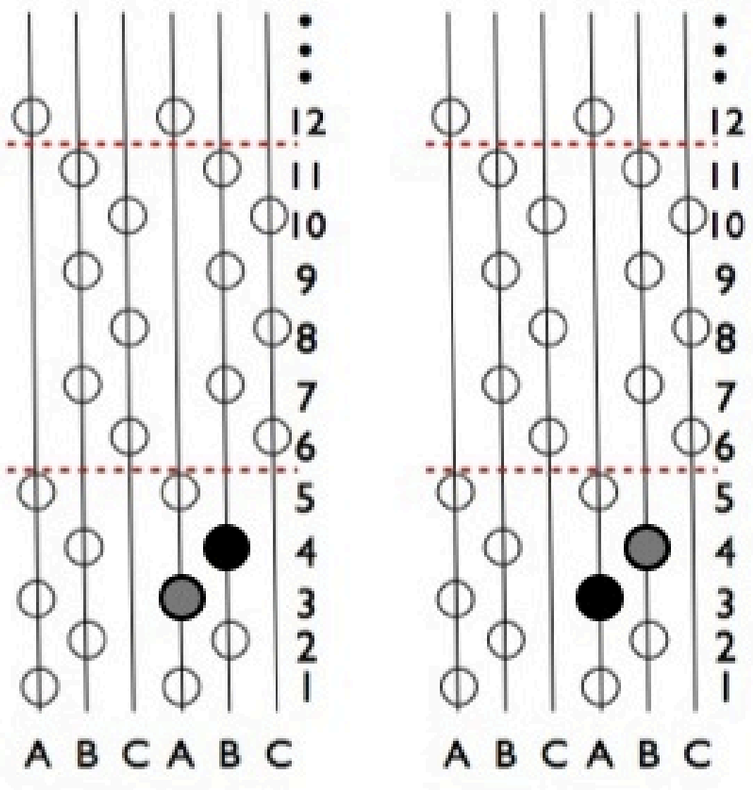
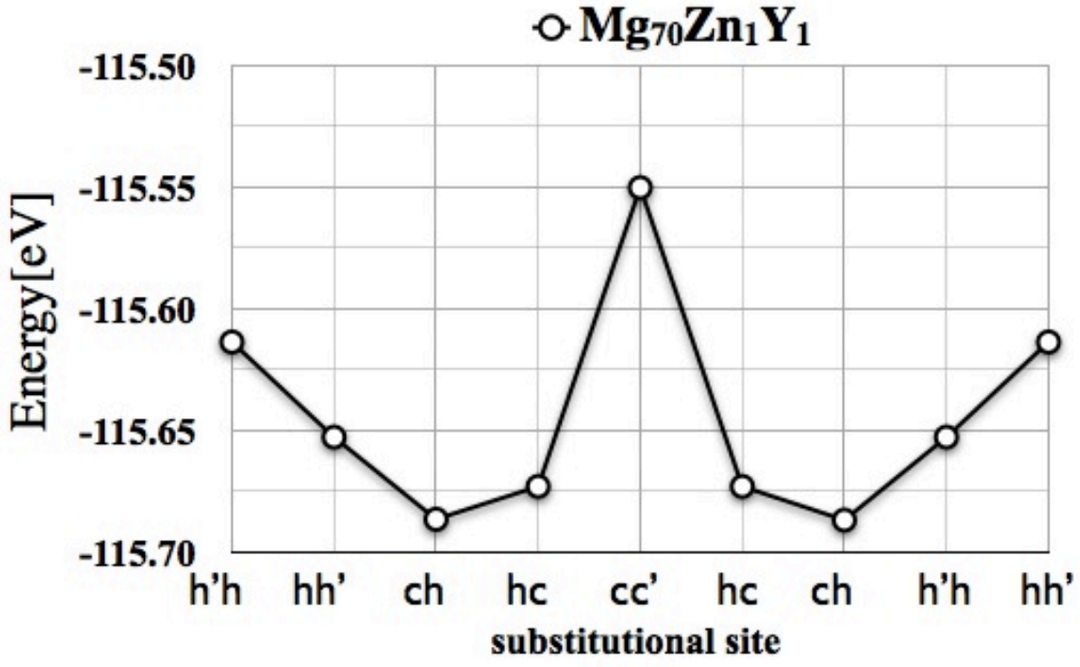
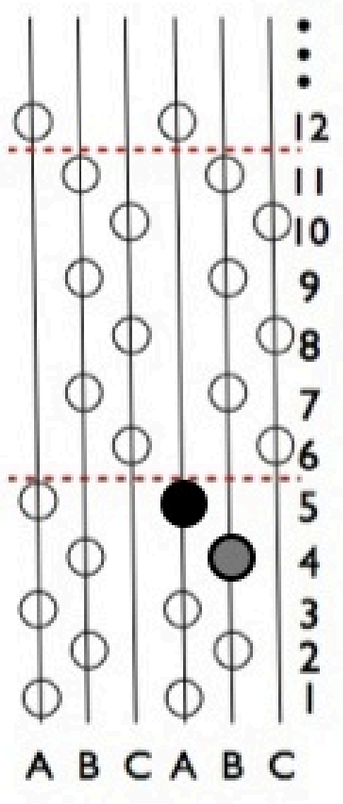
- Zn, Y solute pair ordering? in hcp-Mg

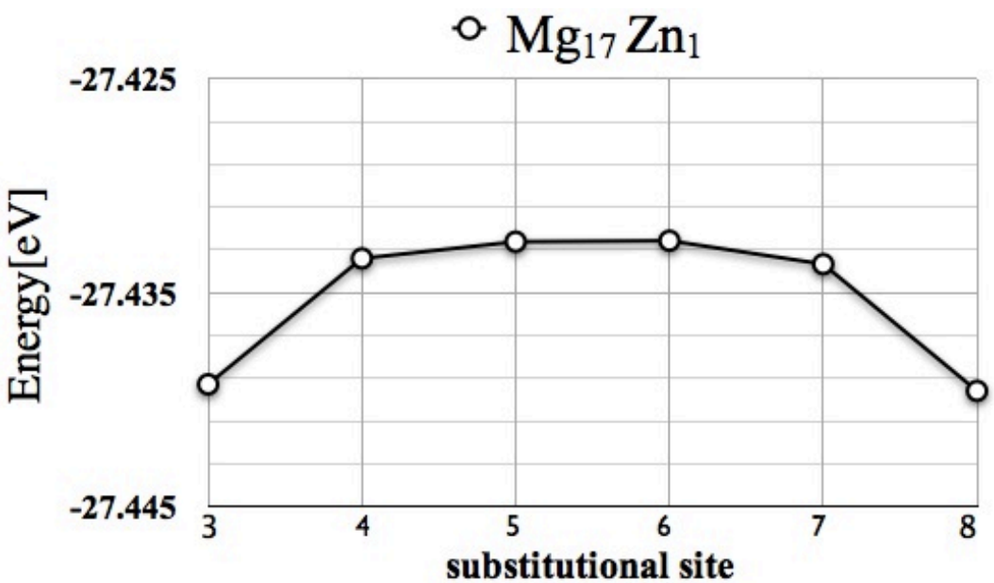


◆ Zn, Y in 18R-Mg

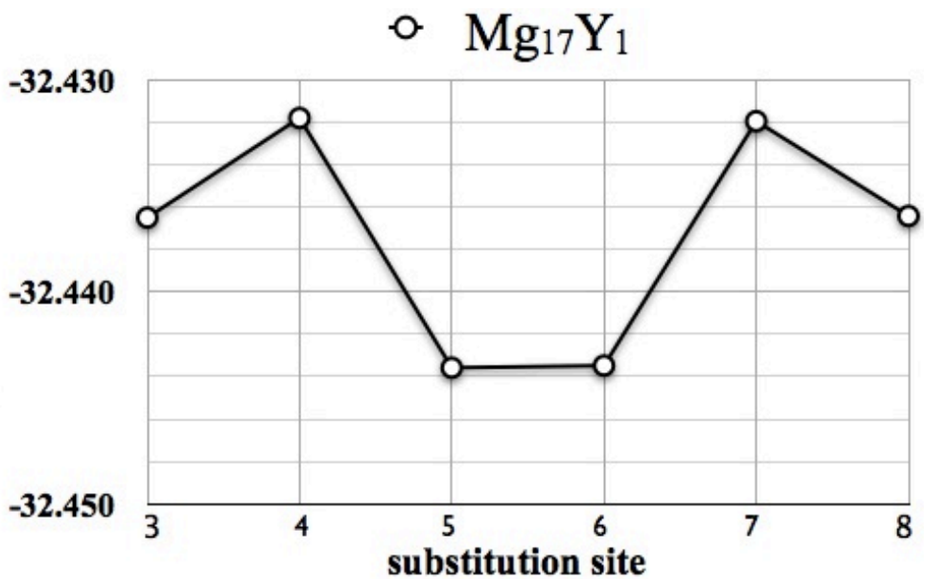








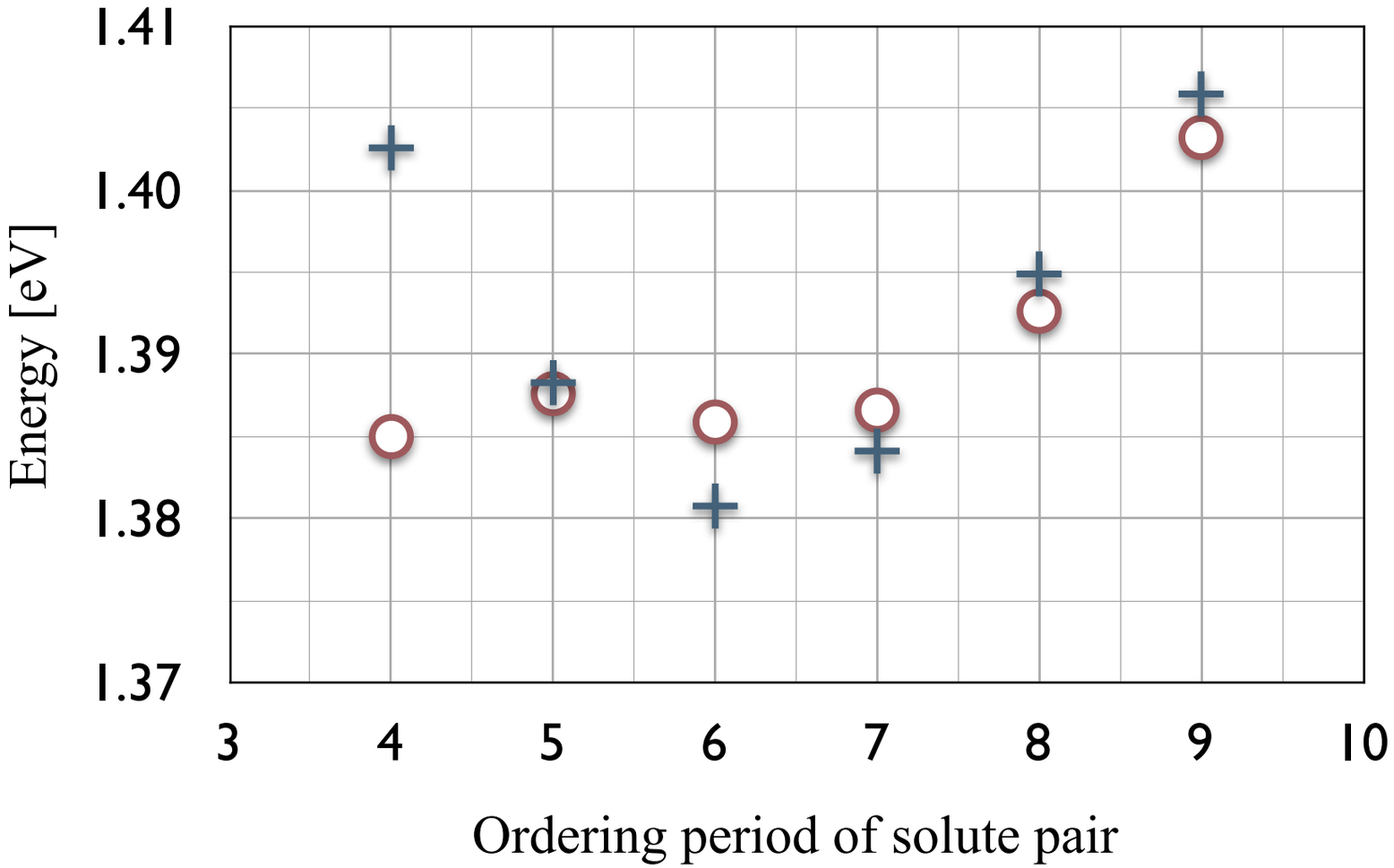
(a)

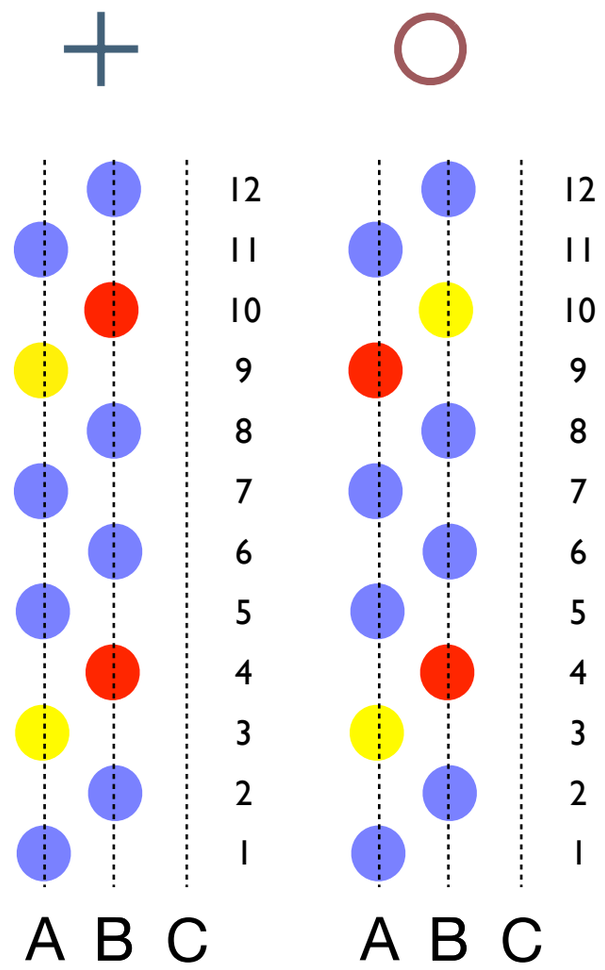


(b)

◆ Zn, Y solute ordering? in hcp-Mg

$$\Delta E = E - (nE_{\mathrm{Mg}} - mE_{\mathrm{Zn}} - mE_{\mathrm{Y}})$$





formation mechanism of LPSO, from structure energies...

- Stacking order (0.005eV)
- Zn, Y in hcp, fcc-Mg(0.05eV)
- Zn, Y in 18R-Mg (0.1eV:large but final state)
- Zn, Y solute ordering? in hcp-Mg (0.02eV:small but...)
- Synchronous effect of Stack. and Sol. Ord.

$dE_{total}(0.1eV)=$

$dE_{stacking}(0.005eV)$

$+dE_{solute}(0.02eV)$

$+dE_{synchronous\ effect}$

Synchronized LPSO Structure

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