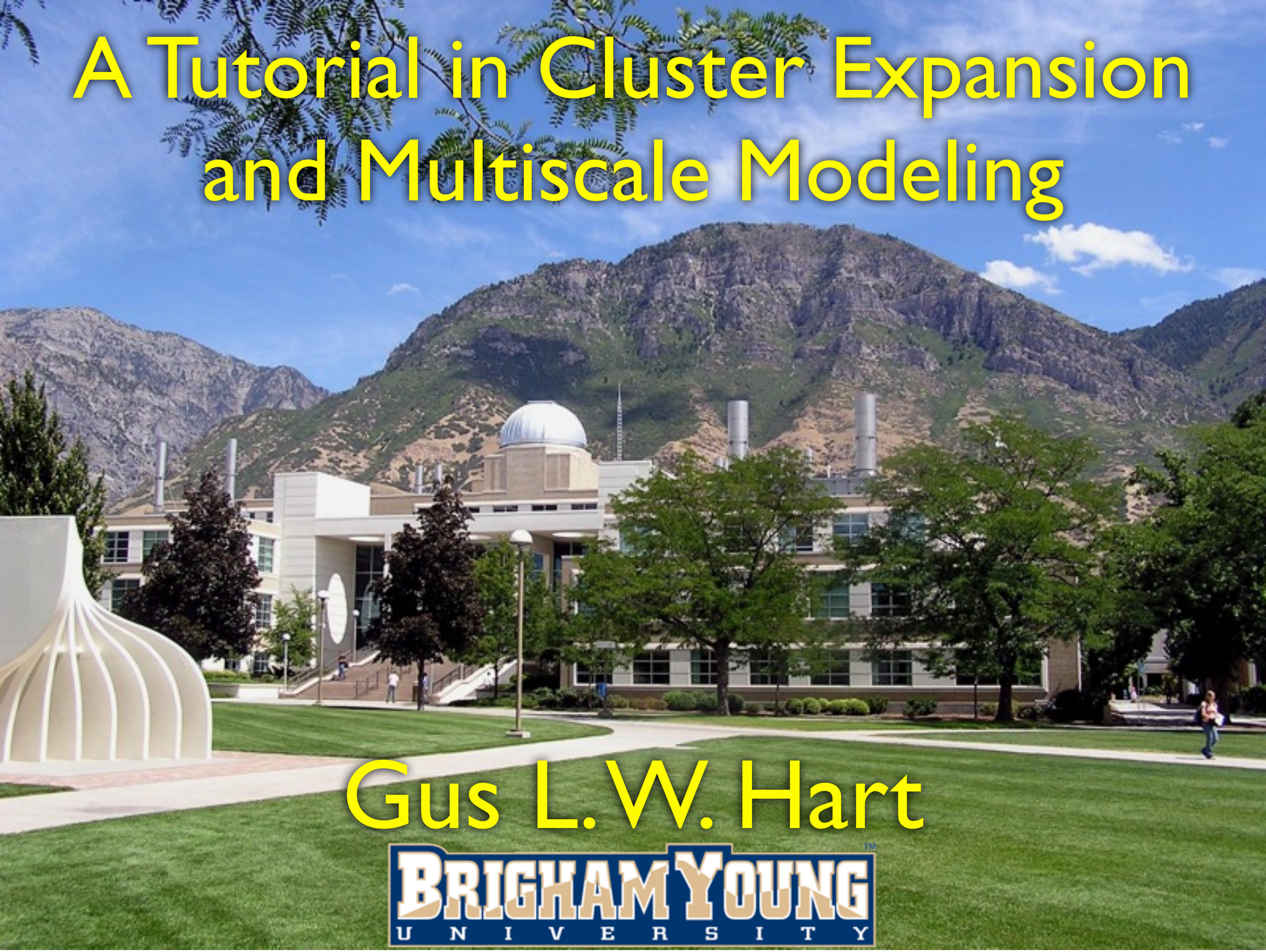
Monday, July 18, 2011

A Tutorial in Cluster Expansion and Multiscale Modeling

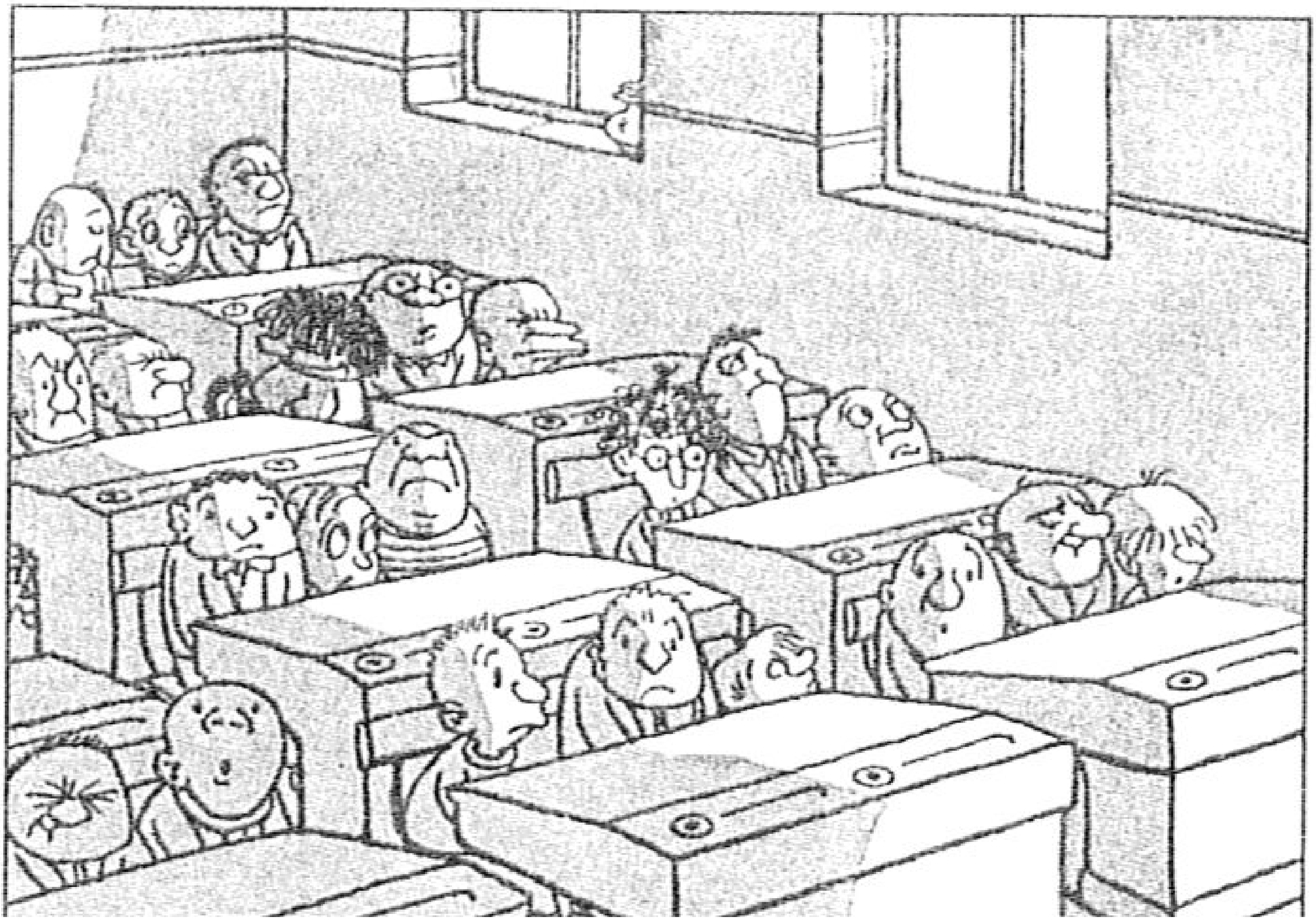


Gus L. W. Hart

BRIGHAM YOUNG UNIVERSITY


A Tutorial

A Tutorial



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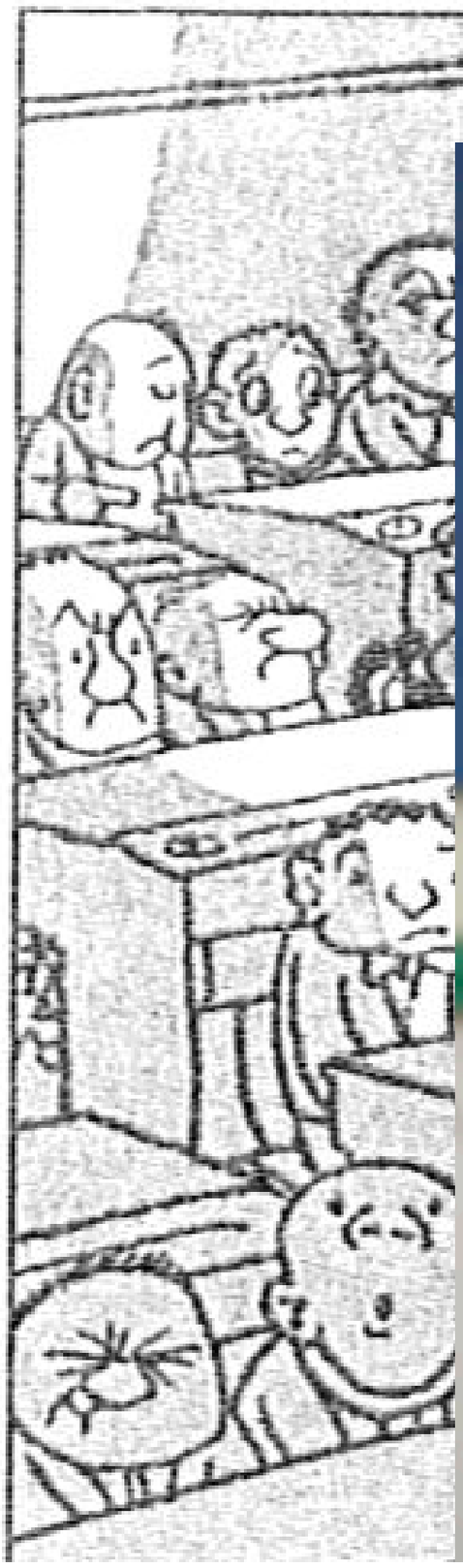
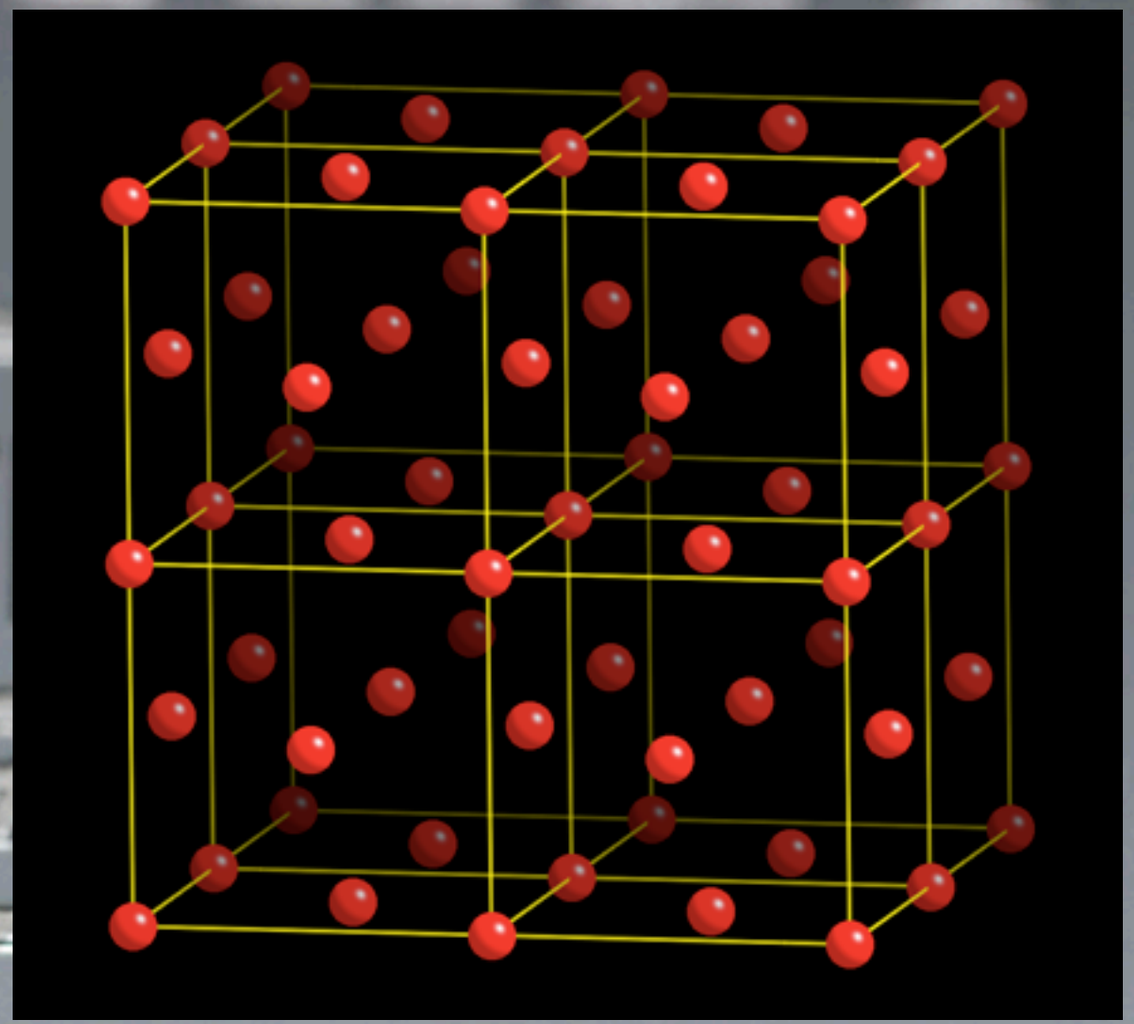


Interrupt me, please!

PLATINUM

9995

1 OUNCE TROY

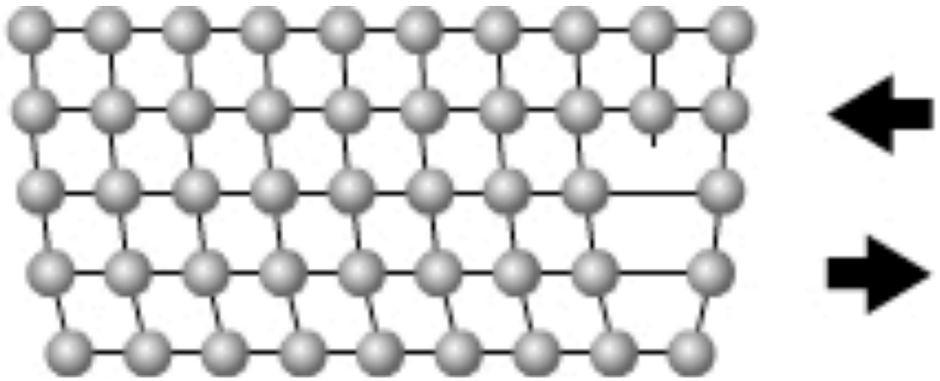


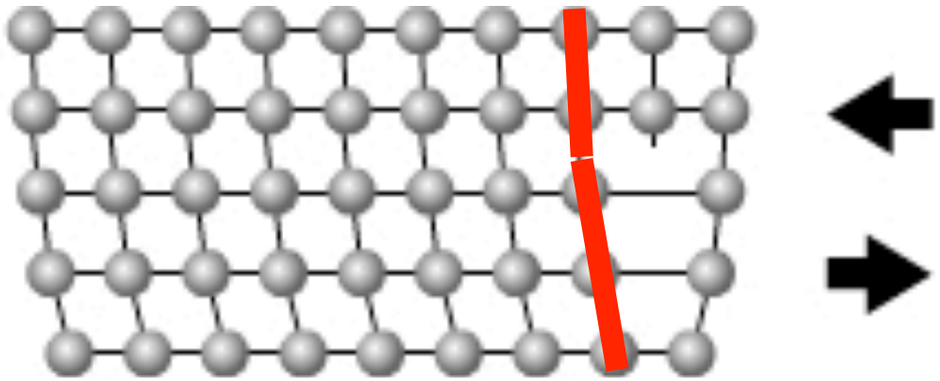
PLAT

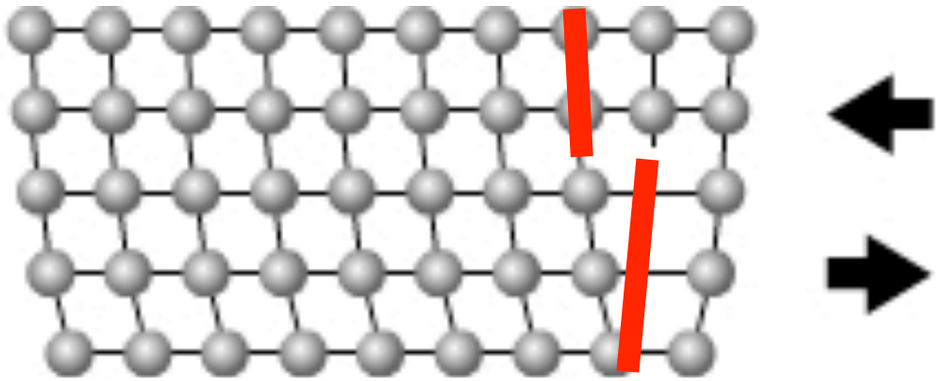
1 OUNCE TROY

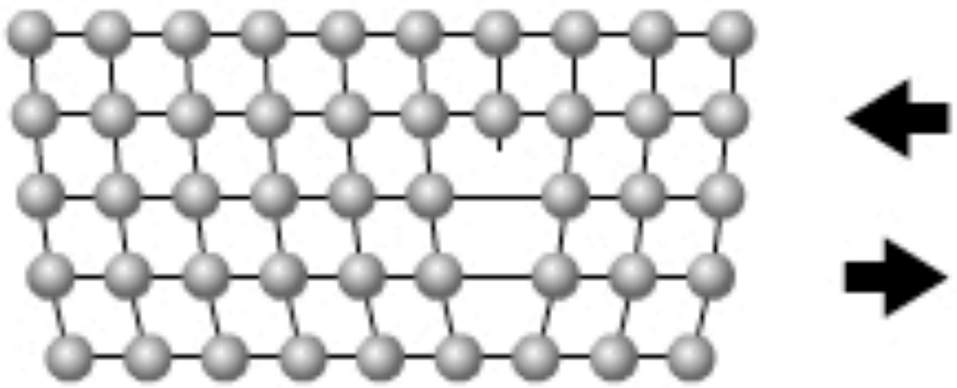
Monday, July 18, 2011

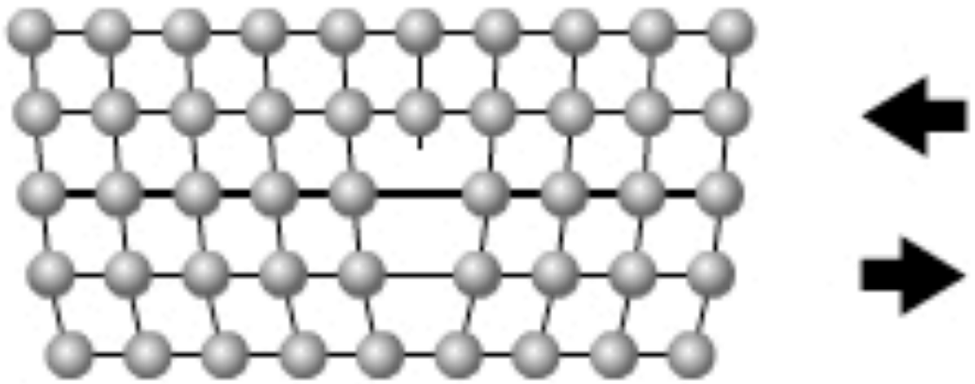
What makes a metal “soft”?

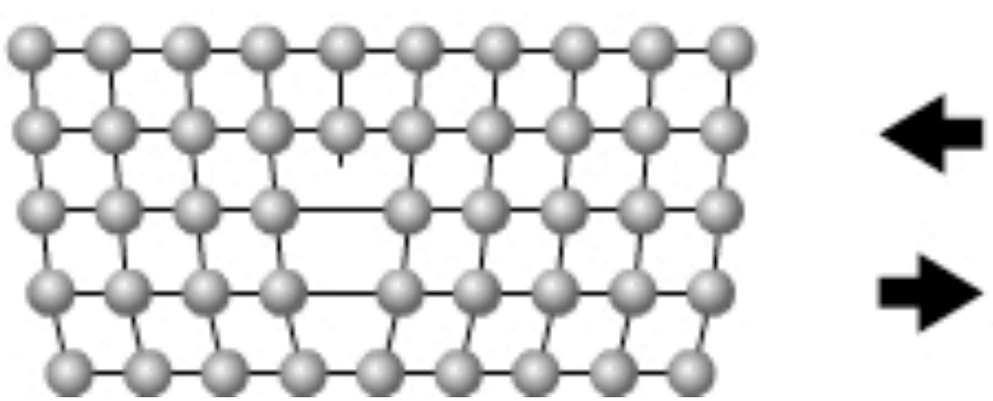


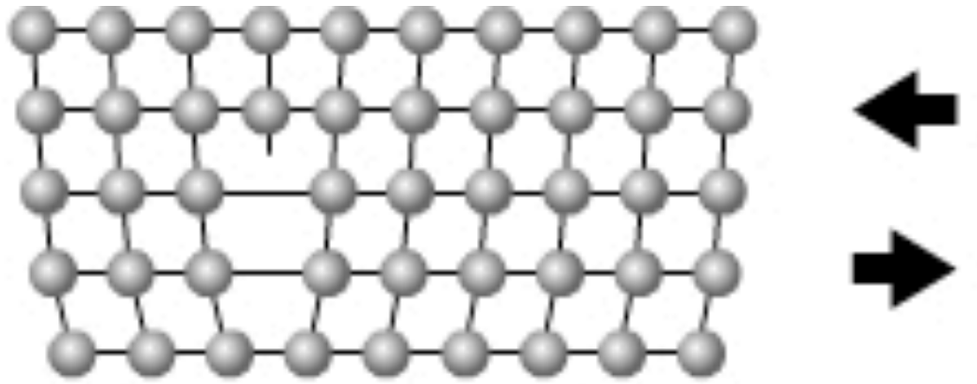


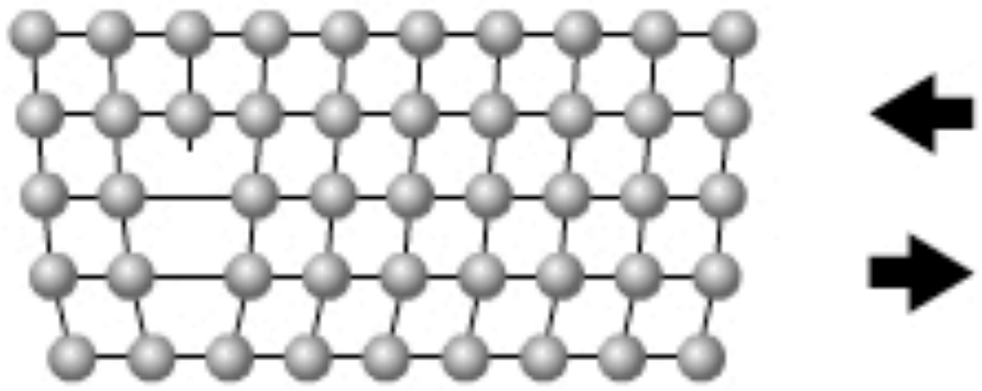


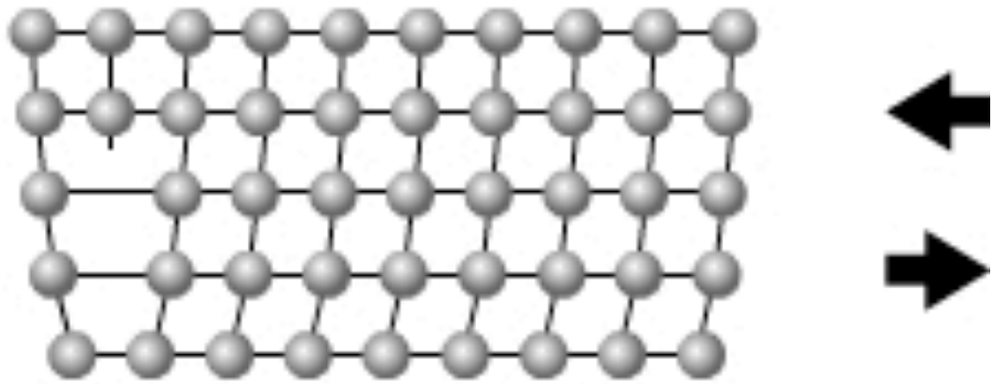


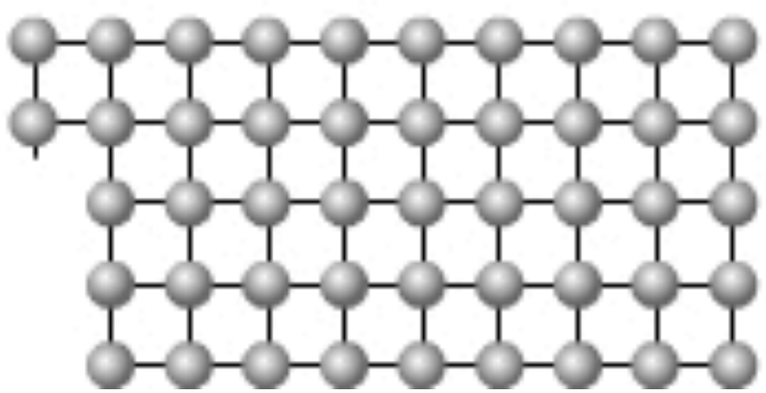




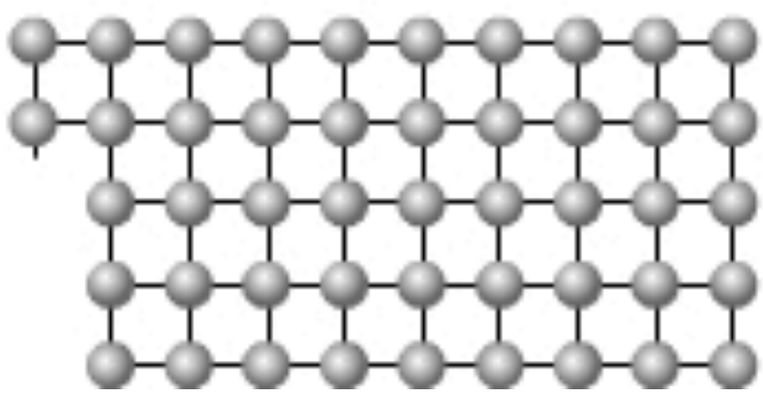








Dislocation motion leads to plastic deformation



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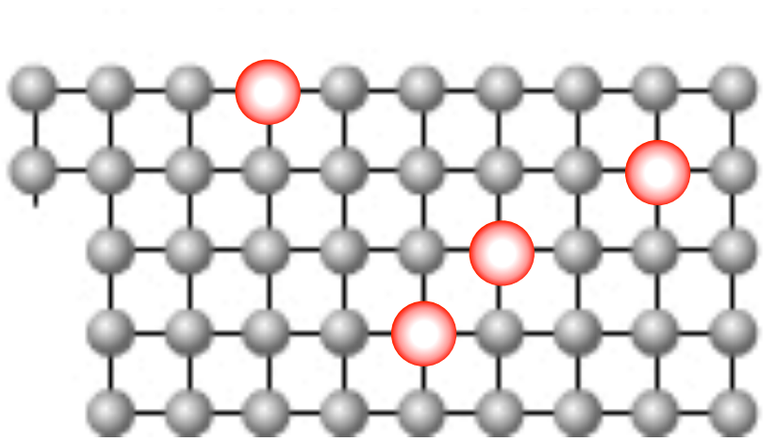
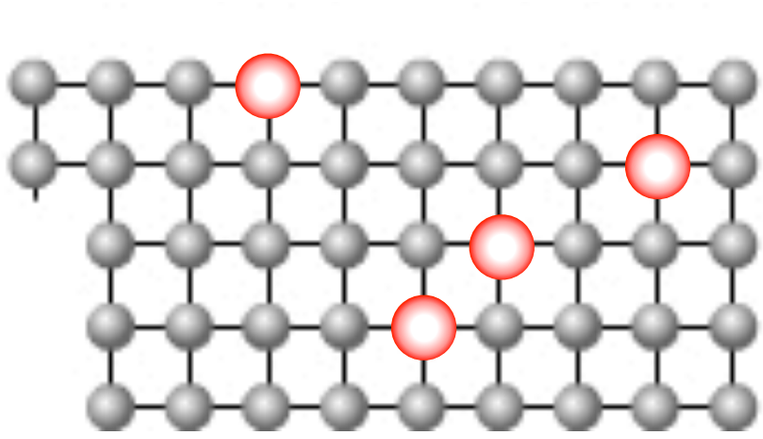
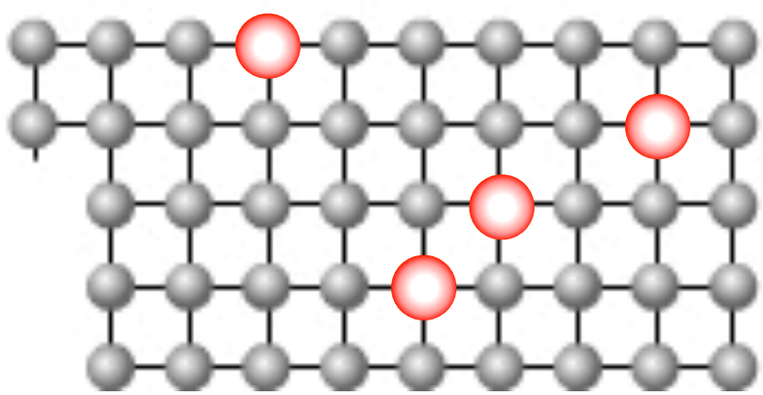


Dislocation motion leads to plastic deformation

Forming a solid solution inhibits dislocations



$$\leq 5\%$$



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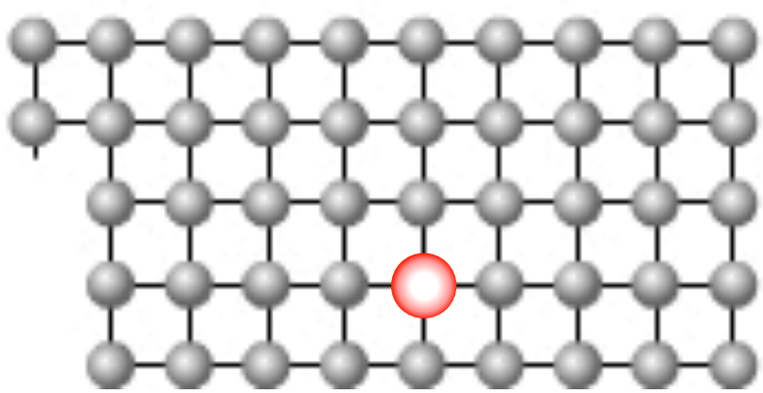
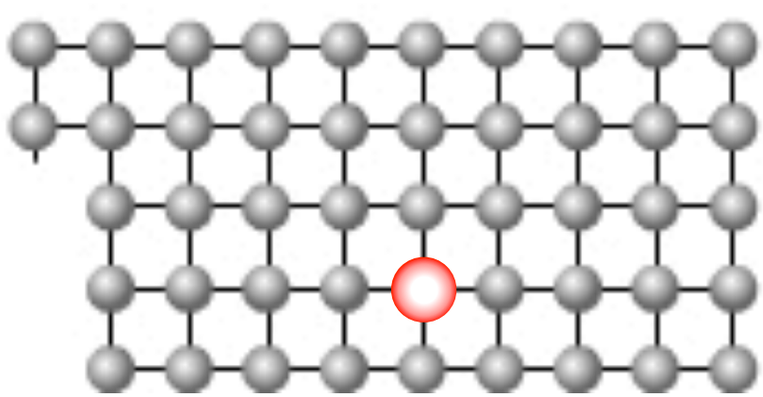
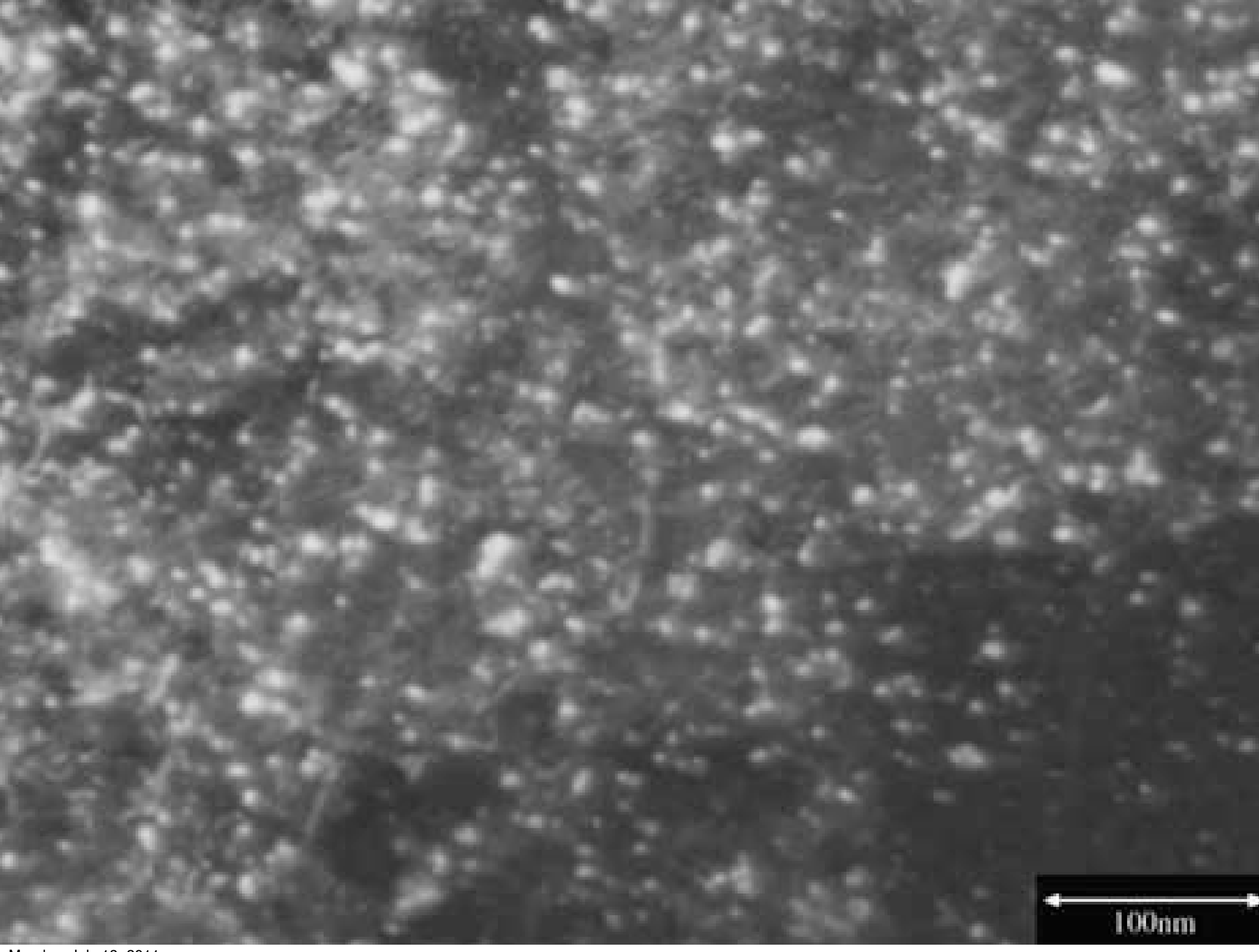
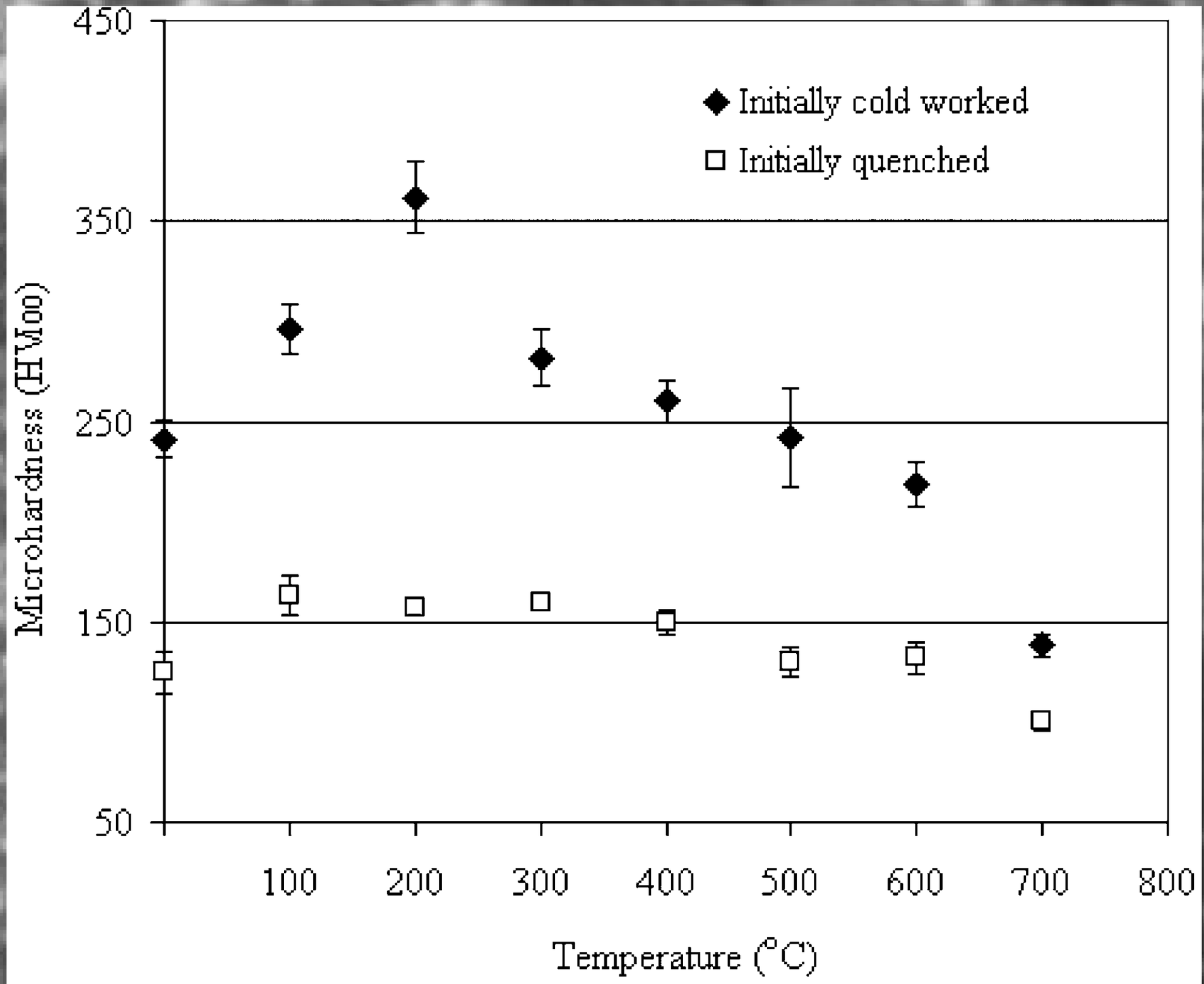


$$\underline{\leq} 5\%$$

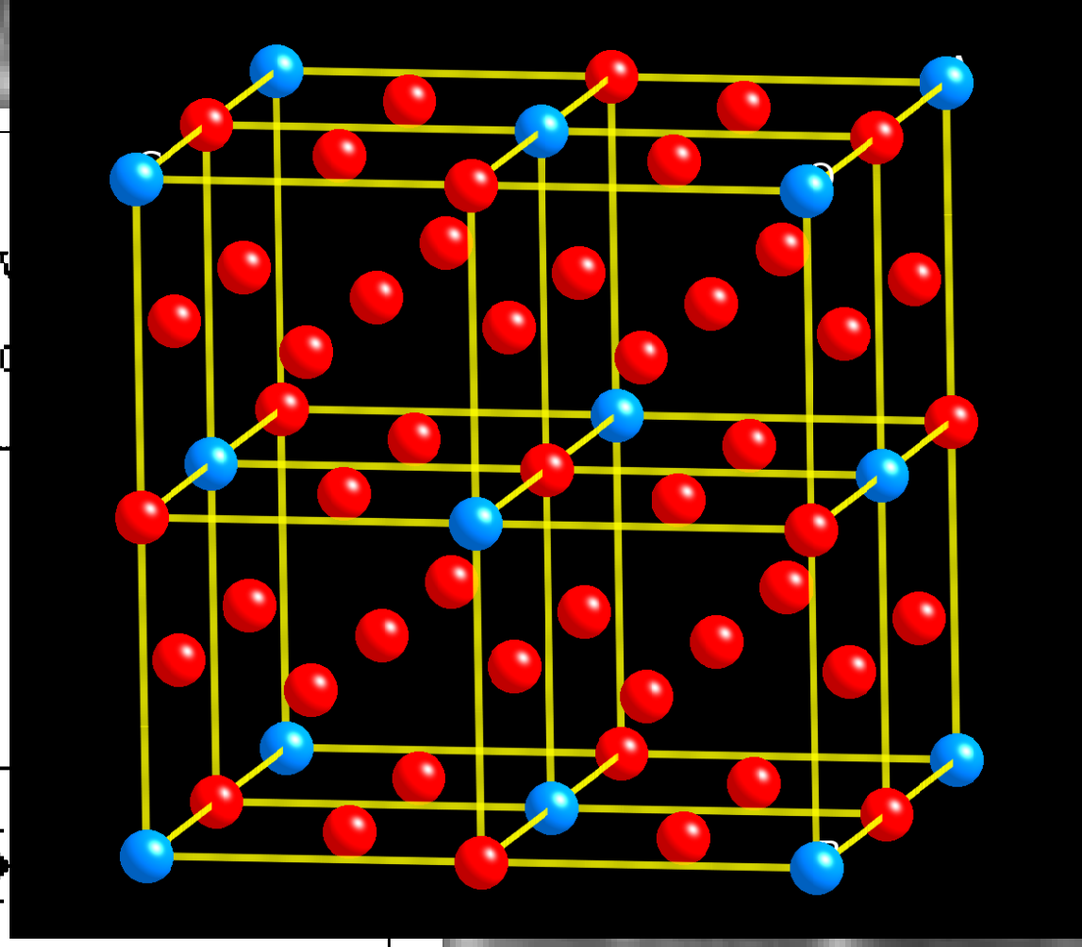
Solid solution hardening is ineffective jewelry alloys

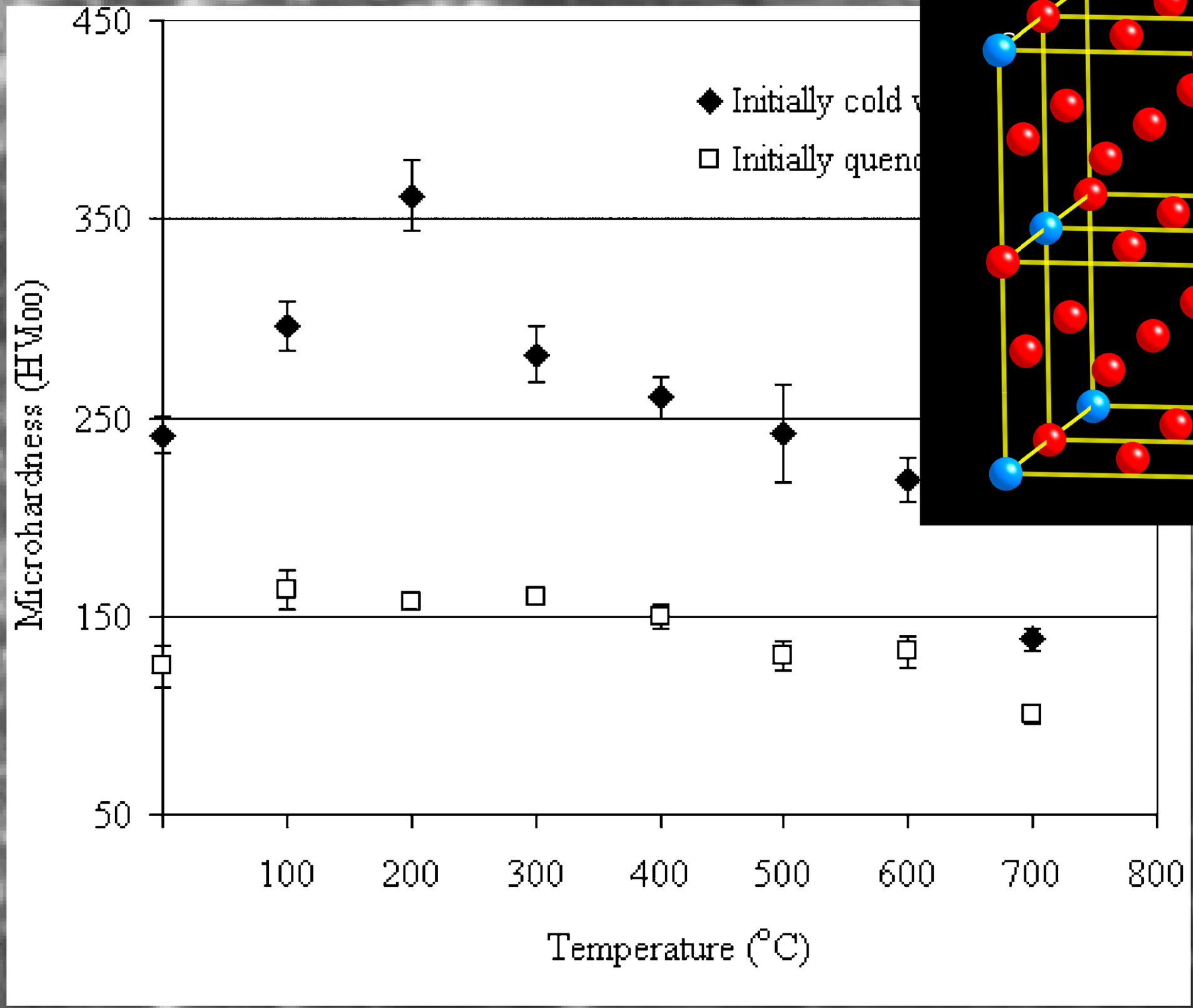



100nm


450
350
250
150
50
Microhardness (HV100)
Initially cold worked
Initially quenched
100
200
300
400
500
600
700
800
Temperature (°C)

100nm




450
350
250
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Microhardness (HV100)
Initially cold
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200
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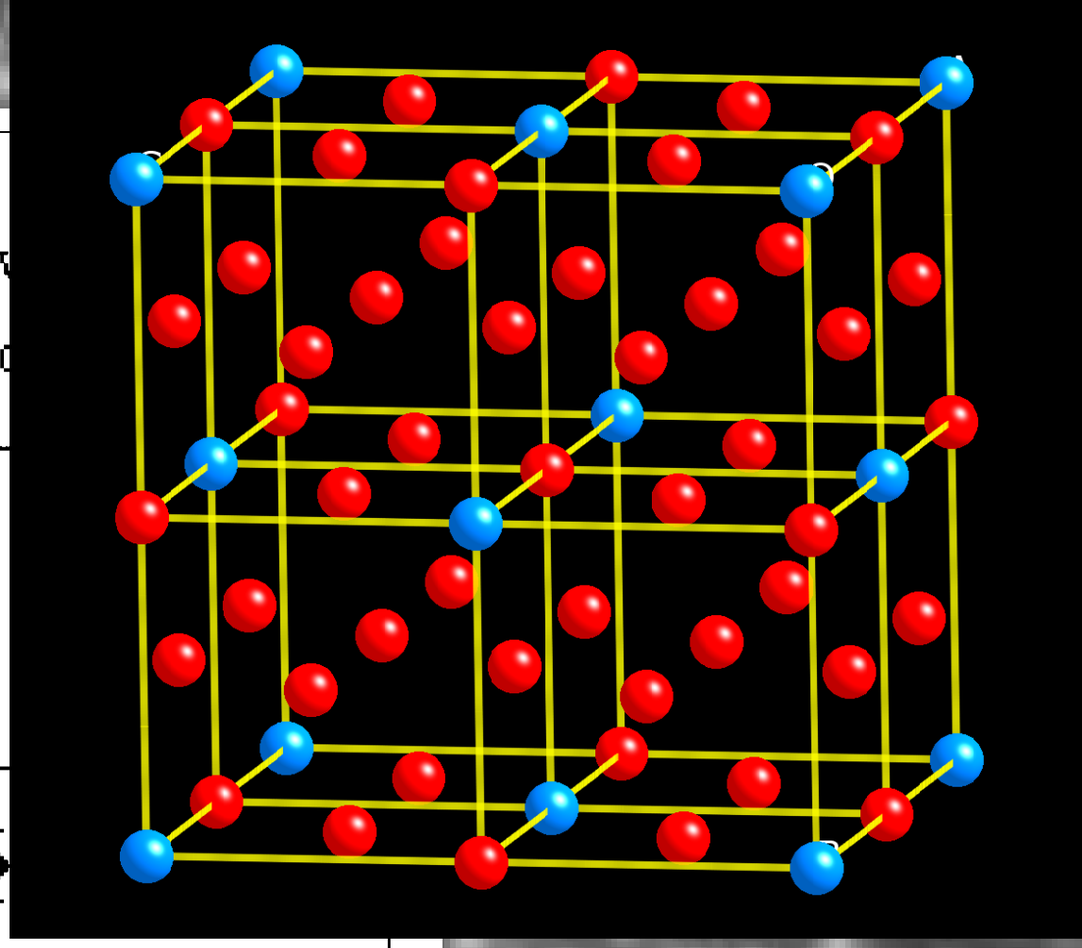
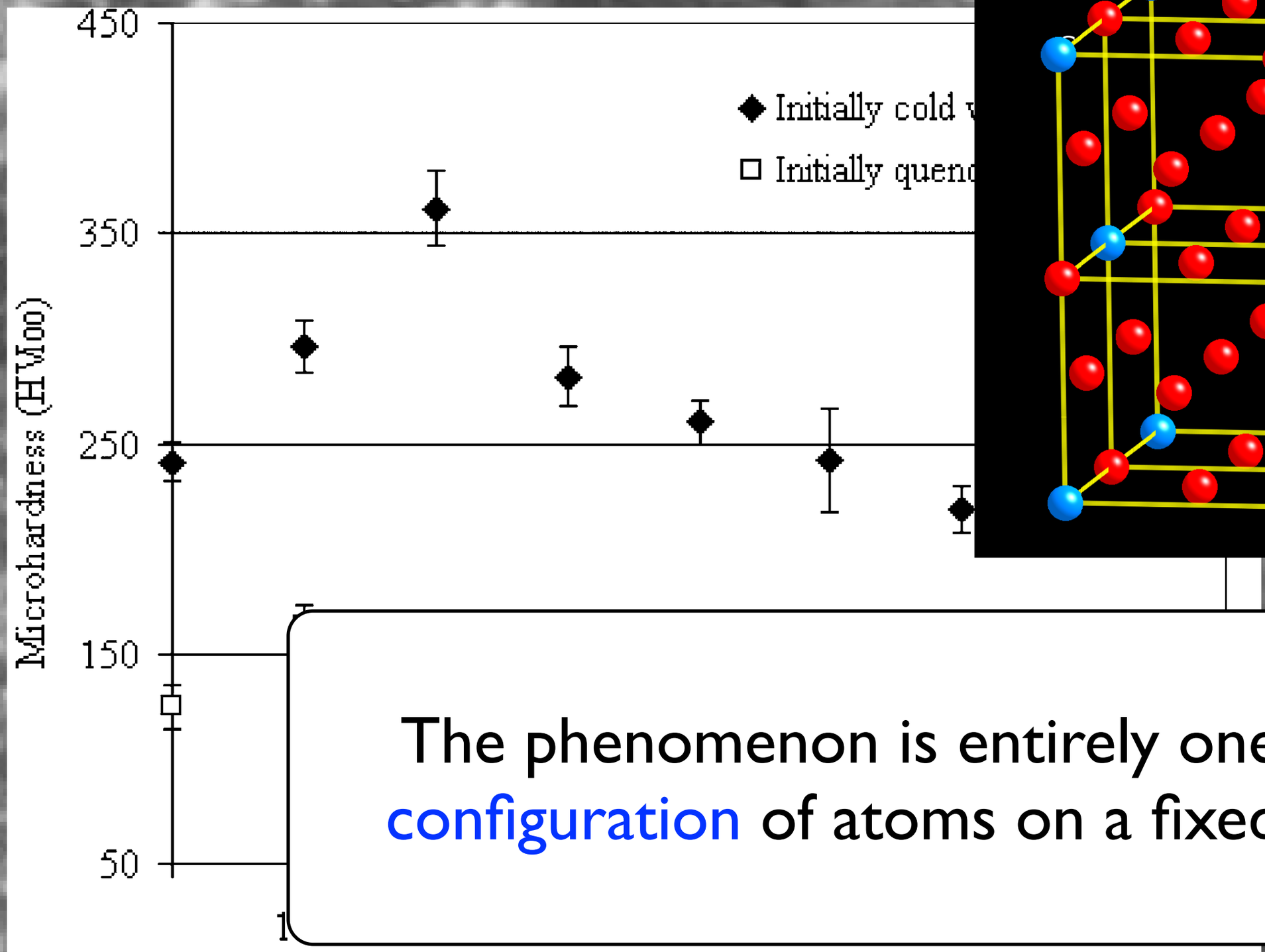
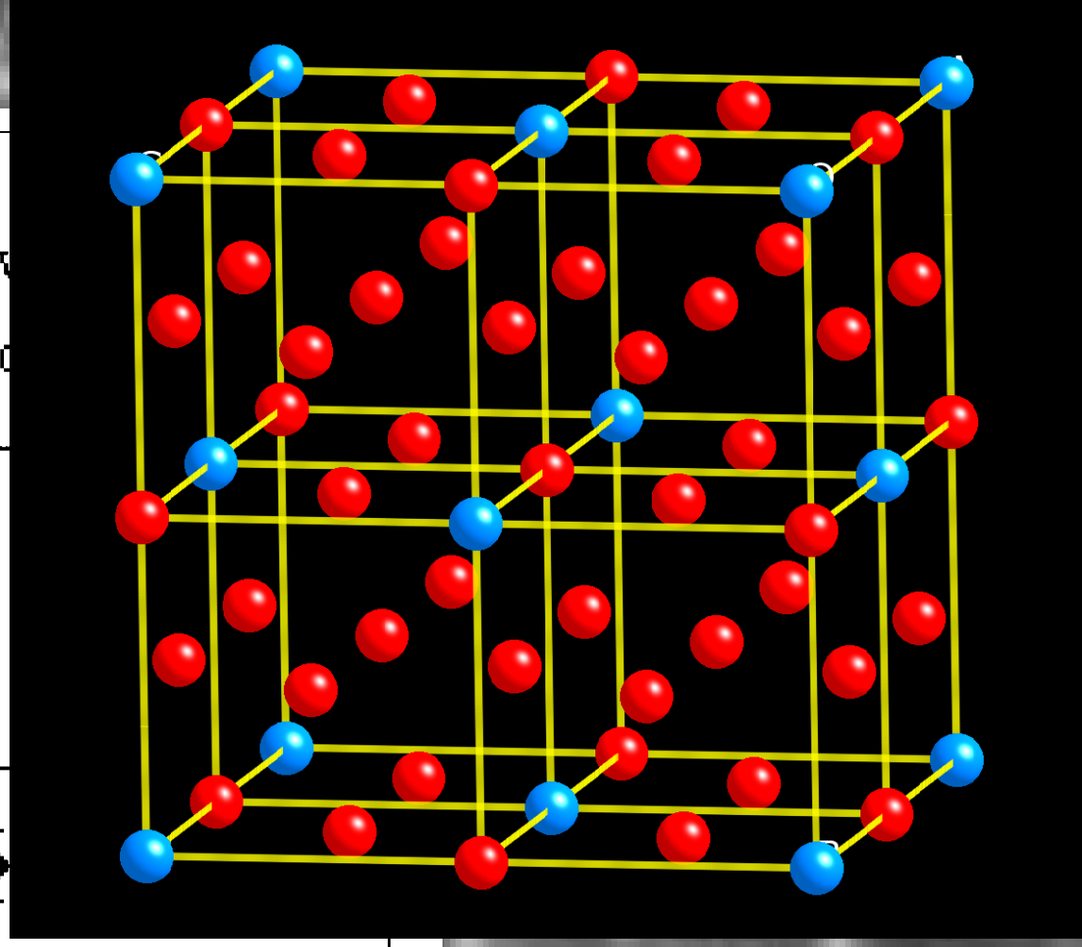
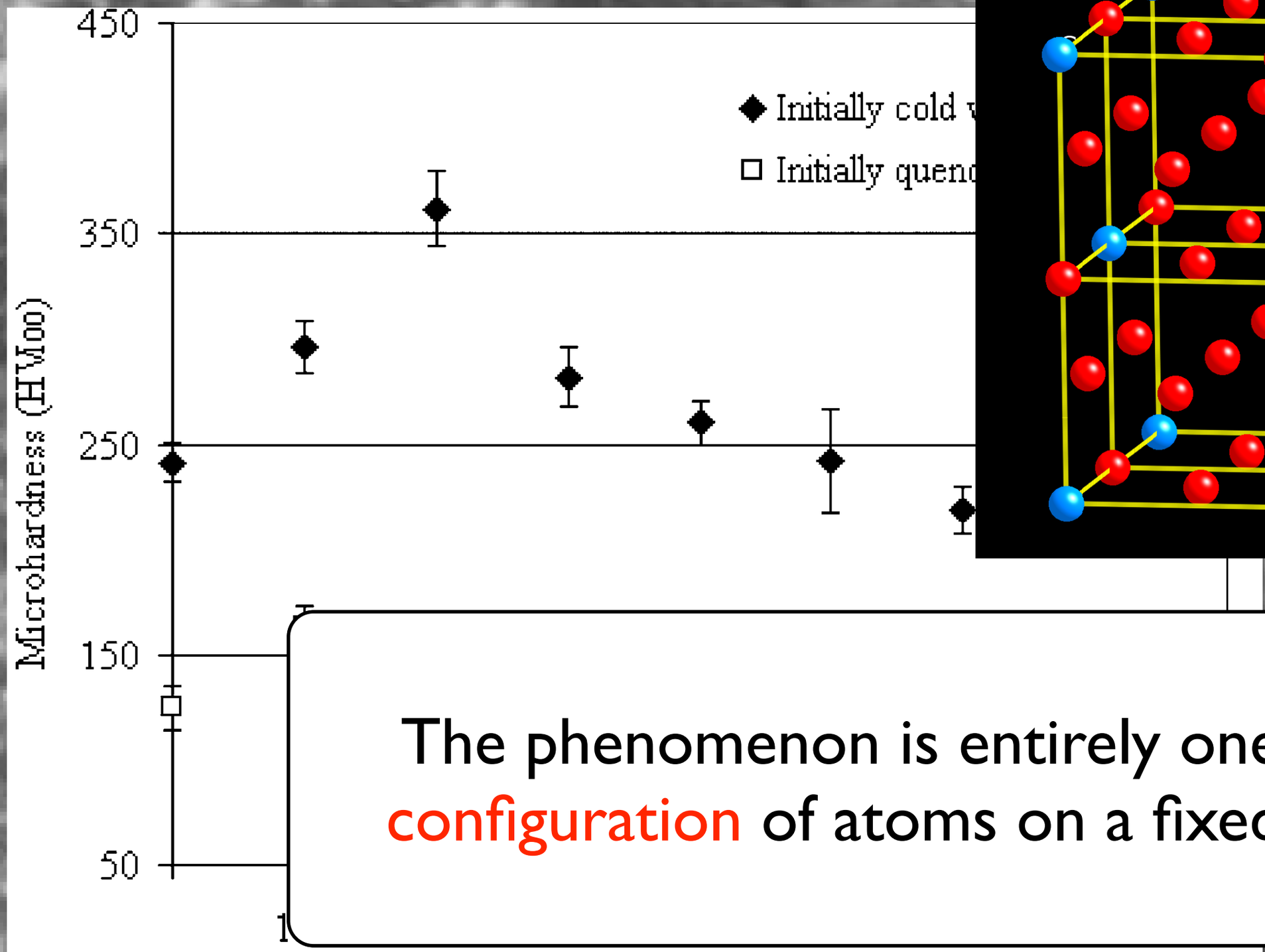
100nm





The phenomenon is entirely one of the configuration of atoms on a fixed lattice.





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Configurational problems

- Precipitate hardening (Pt-Cu, Al-Cu)
- New phases in metallic alloys (8:1)
- Vacancies in TiC, ScS, etc.
- Oxygen diffusion in fuel cell materials
- Hydrogen in storage materials
- Li in battery materials

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Can you think of other problems that are configurational in nature?
Other lattice problems?

Configurational problems

- Precipitate hardening (Pt-Cu, Al-Cu)

Interrupt me, please!

configurational in nature?
Other lattice problems?

If we had a fast lattice Hamiltonian...

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3. Build a kinetic simulation (to model time evolution)

One-Dim. configurational problem

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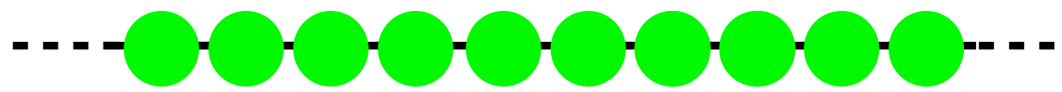

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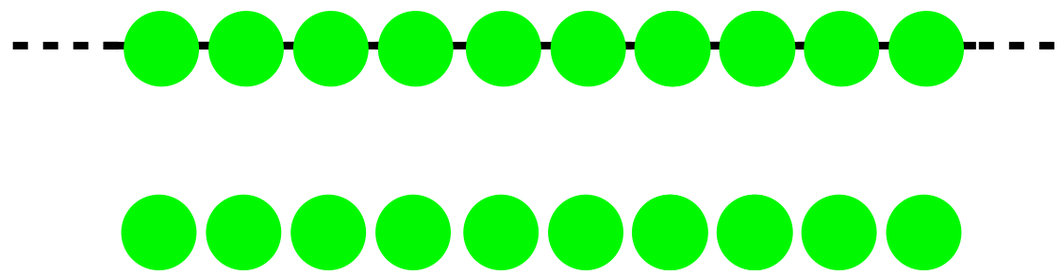

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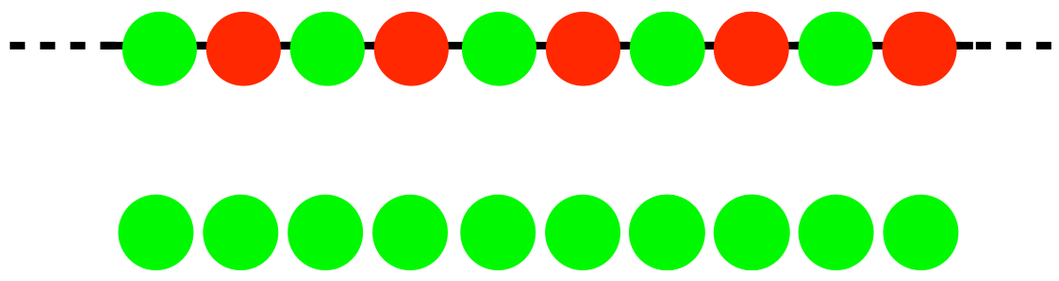

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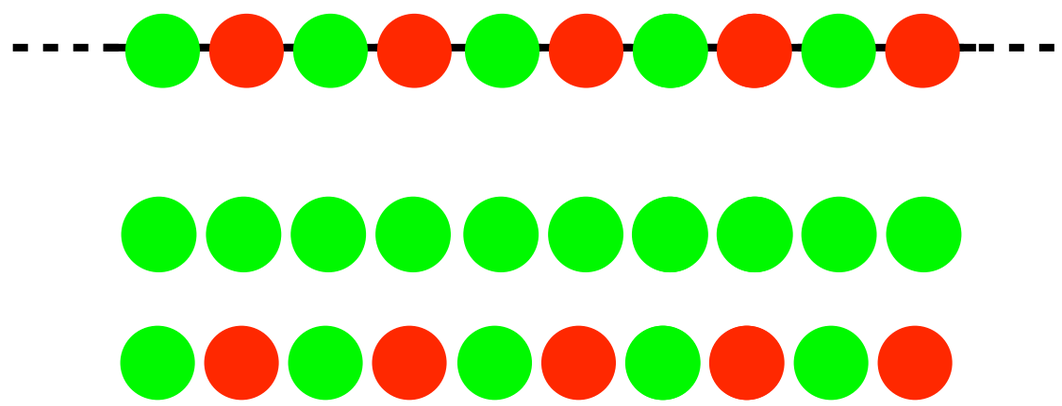

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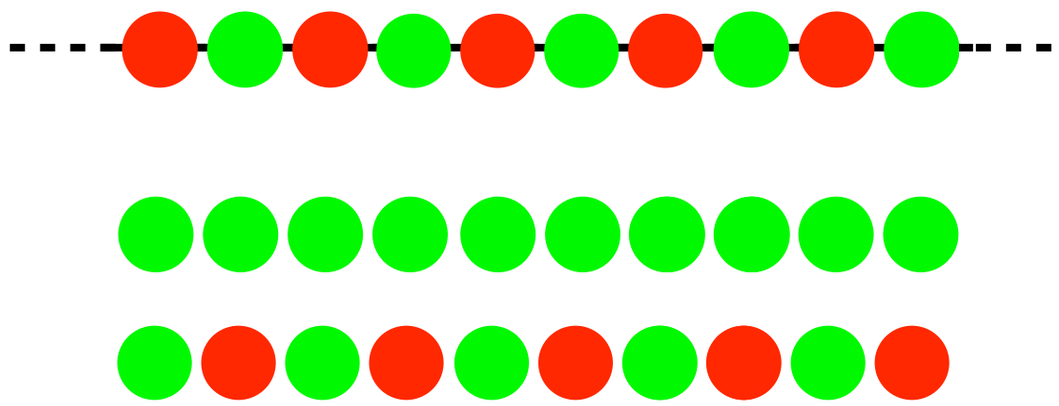
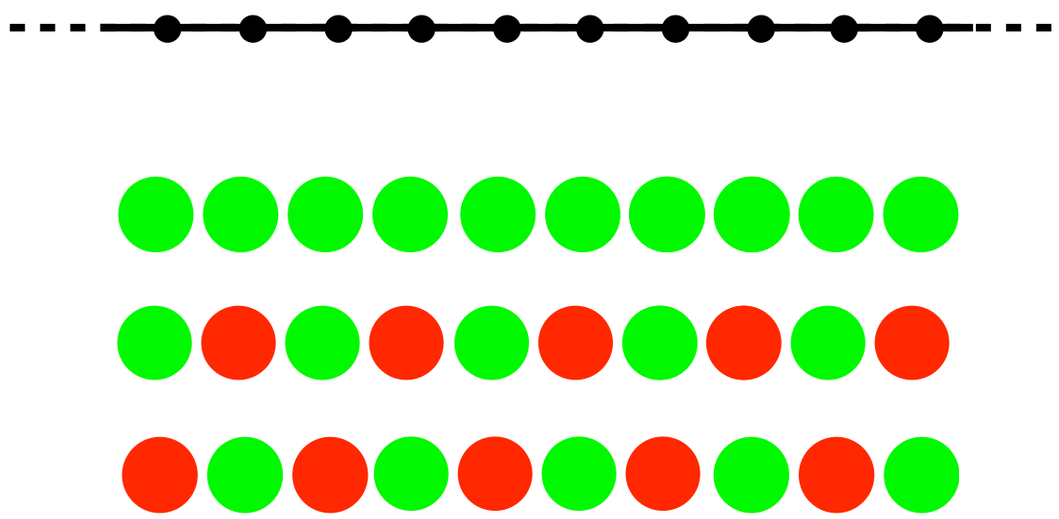


One-Dim. configurational problem



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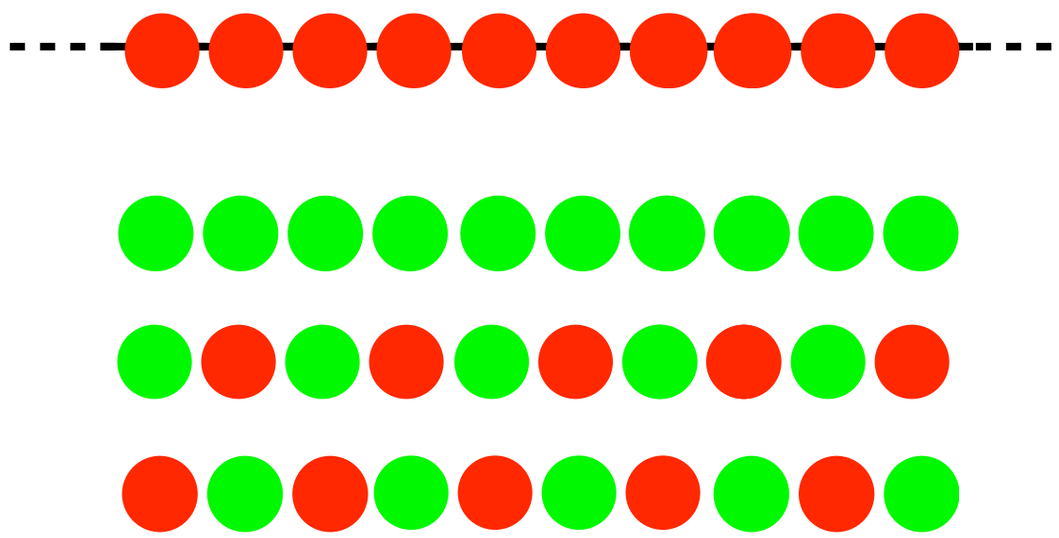

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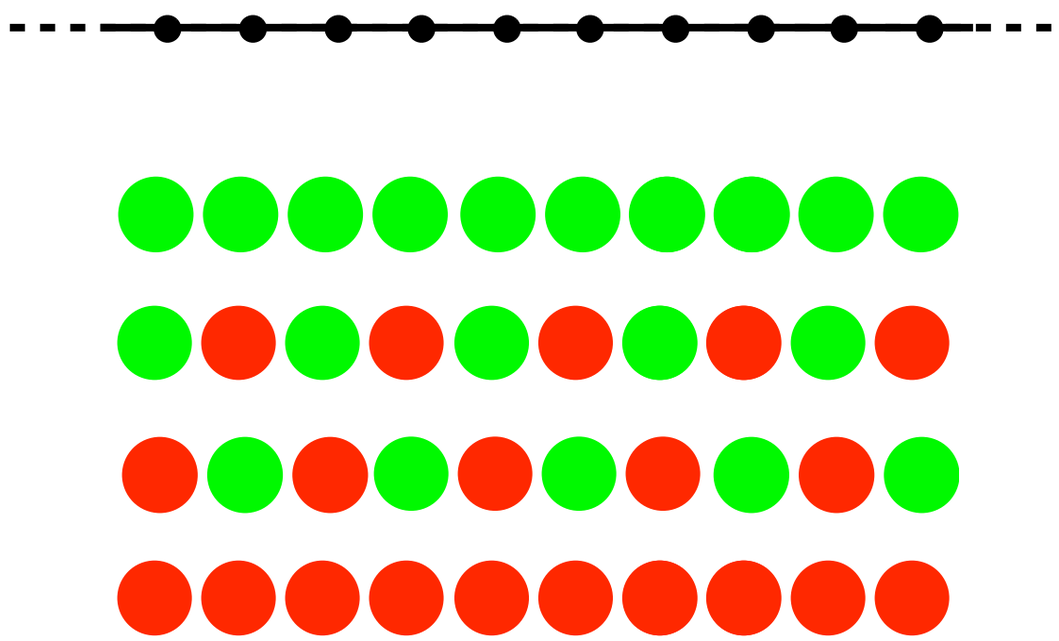

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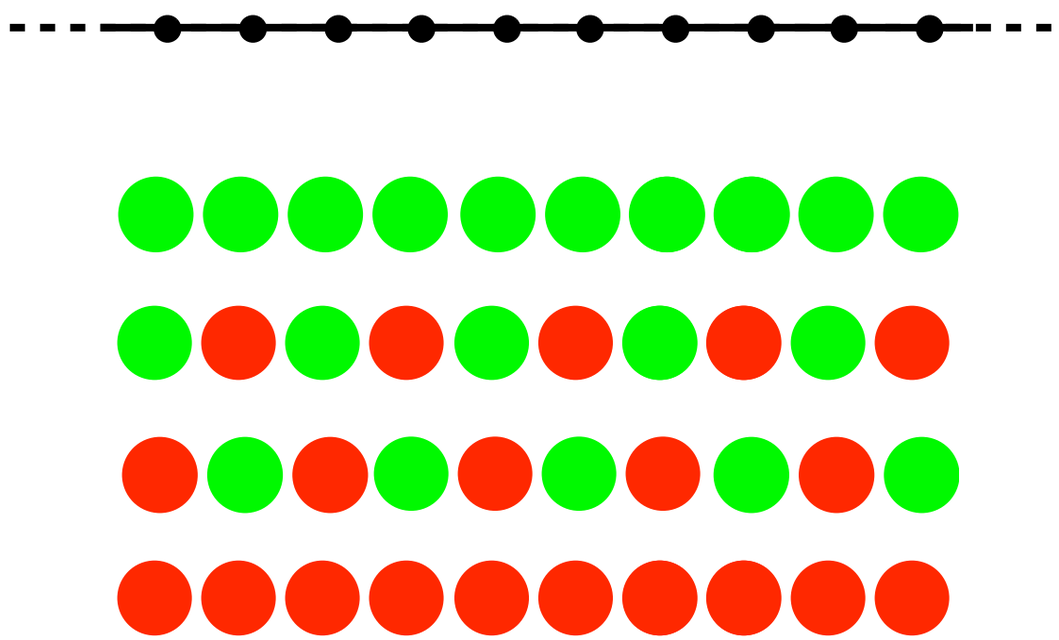


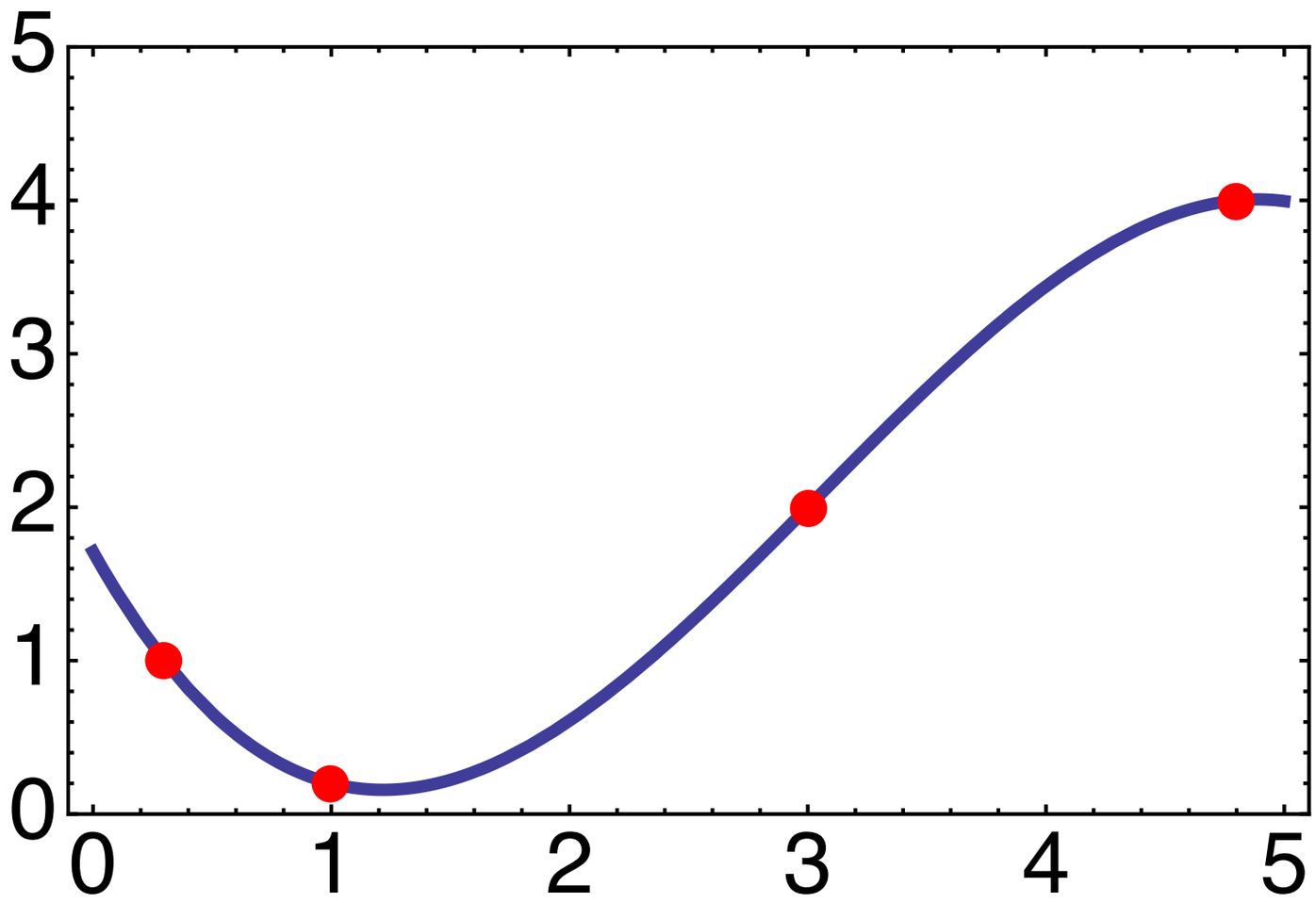
$$f(\bullet\bullet) = E_1$$

$$f(\bullet\bullet) = E_2$$

$$f(\bullet\bullet) = E_3$$

$$f(\bullet\bullet) = E_4$$

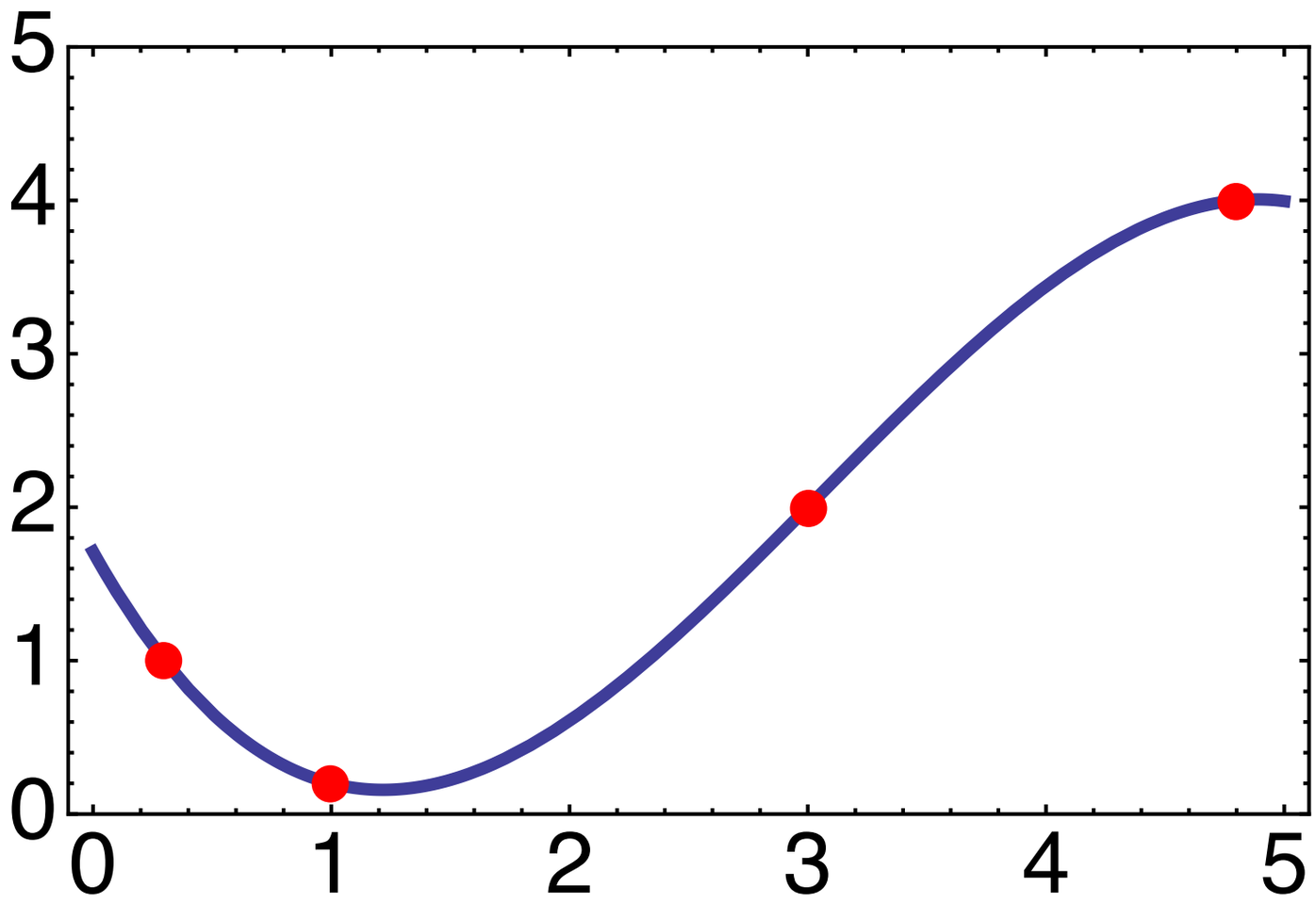
Expanding in a power series



$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

optimize $\{a_0, a_1, a_2, \ldots\}$ to minimize error

Expanding in a power series

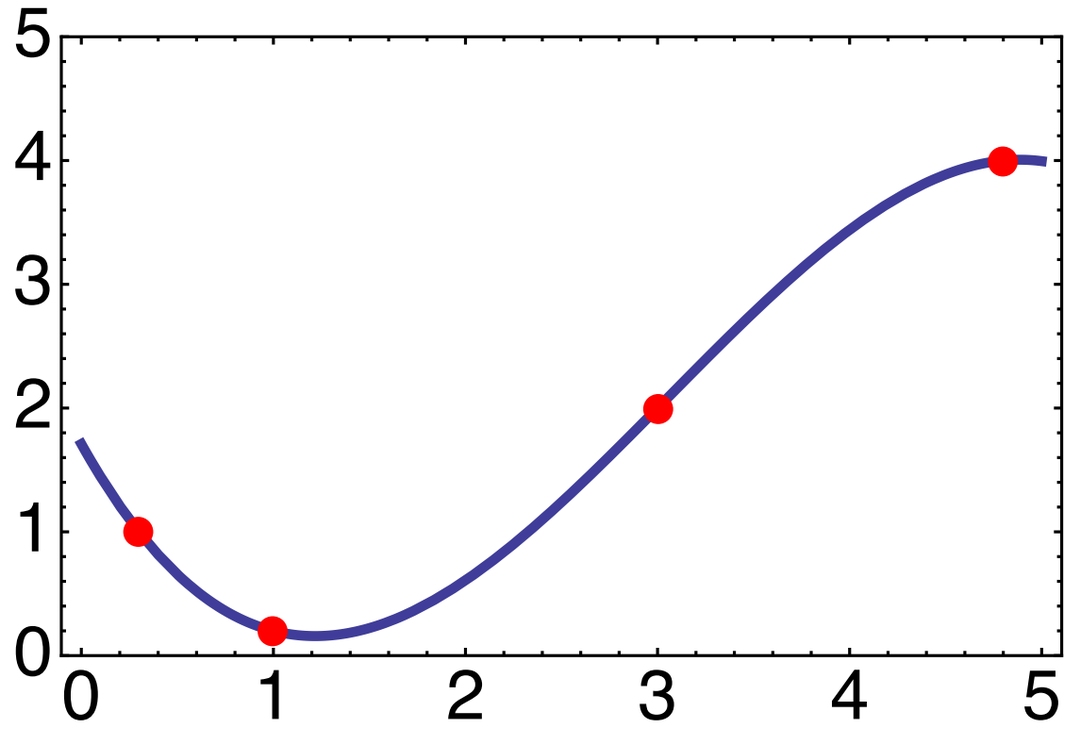


$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

optimize $\{a_0, a_1, a_2, \ldots\}$ to minimize error

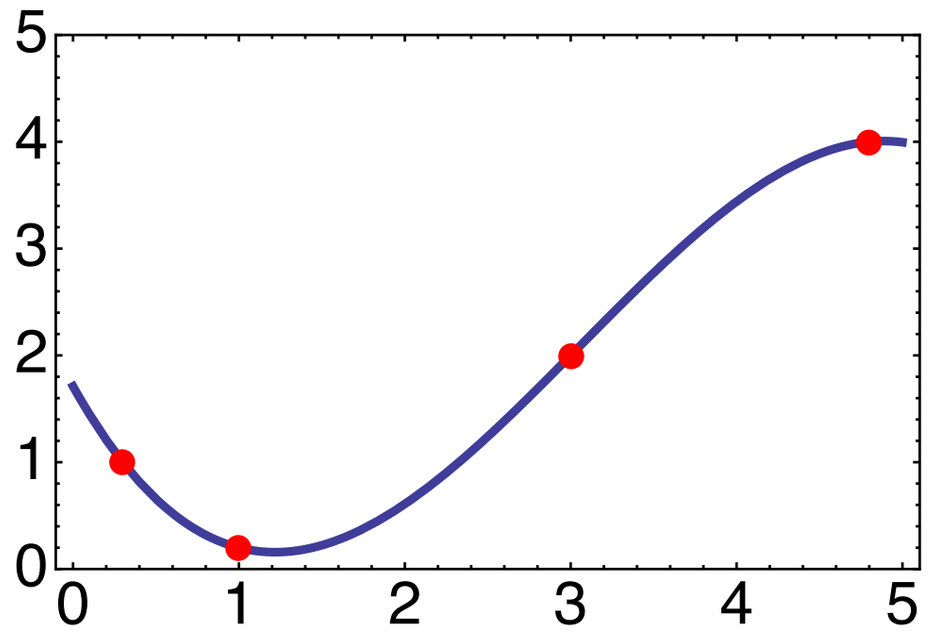
How do we find the coefficients?

Expanding in a power series



$$
\begin{aligned}
f(x_1) &= a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3 \\
f(x_2) &= a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3 \\
f(x_3) &= a_0 + a_1 x_3 + a_2 x_3^2 + a_3 x_3^3 \\
f(x_4) &= a_0 + a_1 x_4 + a_2 x_4^2 + a_3 x_4^3
\end{aligned}
$$

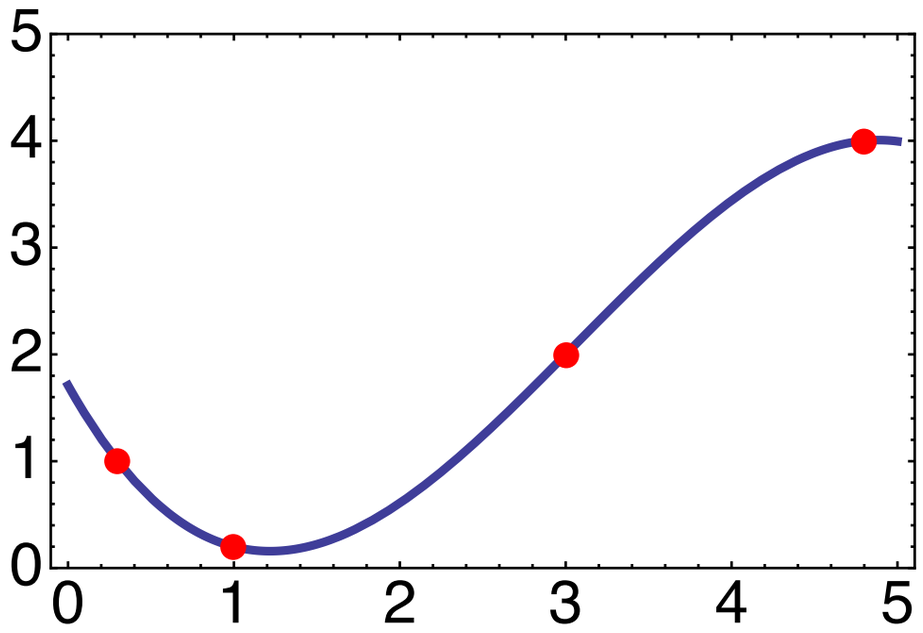
Expanding in a power series



$$\begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

Expanding in a power series

Data



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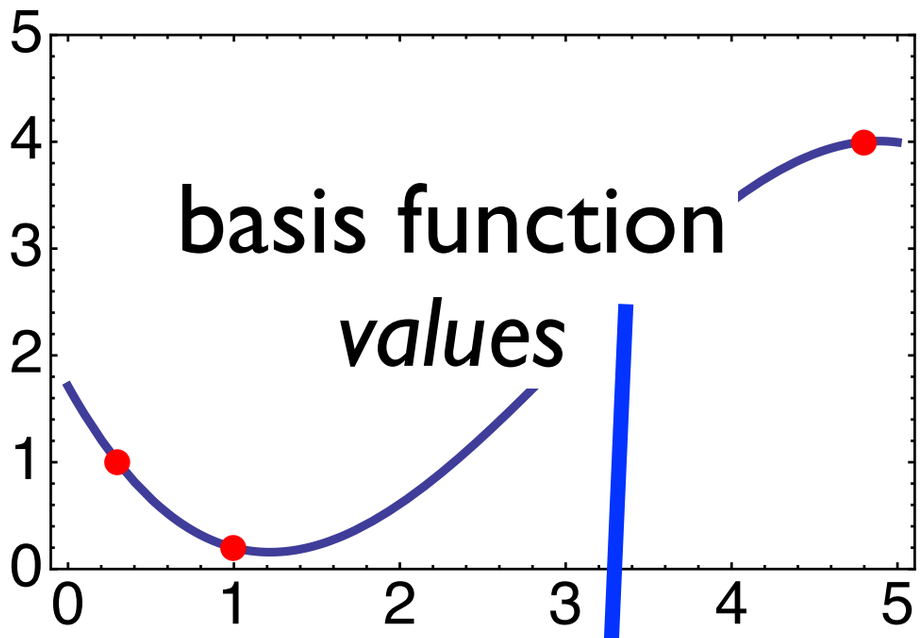

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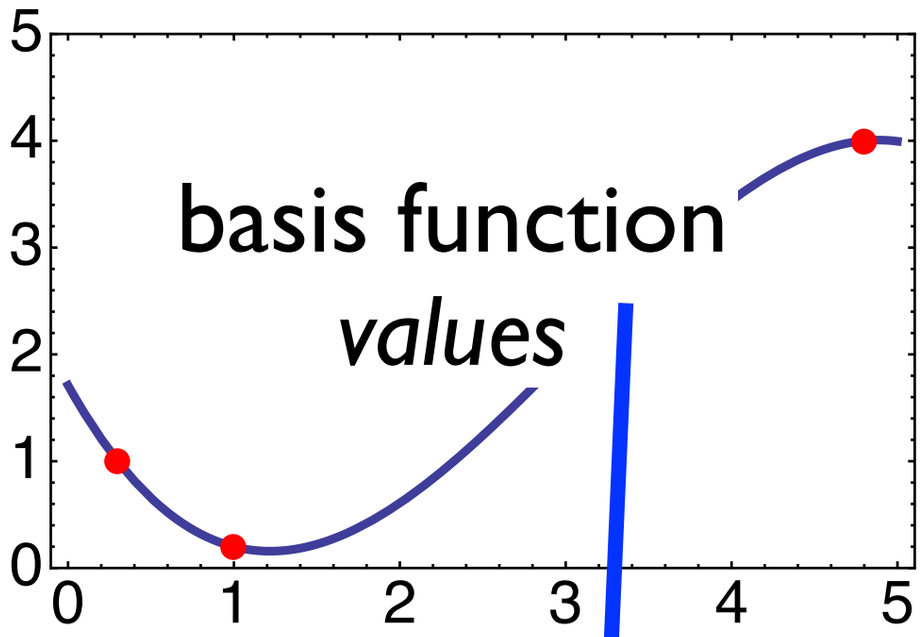
Expanding in a power series

Data



coefficients of the model

$$\begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

Expanding configurational functions

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N} \overset{\circ\circ\circ\circ}{\sum_i} 1 + J_1 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i + J_2 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i \bigcirc_{i+1} + J_3 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1 \bar{\Pi}^{\circ} + J_2 \bar{\Pi}^{\circ\circ} + J_3 \bar{\Pi}^{\circ\circ\circ} + \cdots$$

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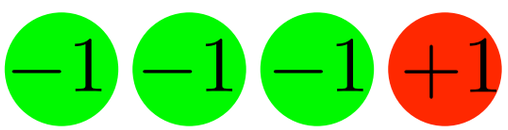
Expanding configurational functions

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N} \overset{\circ\circ\circ\circ}{\sum_i} 1 + J_1 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i + J_2 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i \bigcirc_{i+1} + J_3 \overset{\circ\circ\circ\circ}{\sum_i} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1 \bar{\Pi}^{\circ} + J_2 \bar{\Pi}^{\circ\circ} + J_3 \bar{\Pi}^{\circ\circ\circ} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 \bigcirc + J_1 \bigcirc + J_2 \bigcirc\bigcirc + J_3 \bigcirc\bigcirc\bigcirc + \cdots$$



Expanding configurational functions

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_{i}^{\circ\circ\circ\circ} 1 + J_1\sum_{i}^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_{i}^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1} + J_3\sum_{i}^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1}\,\bigcirc_{i+2} + \cdots$$

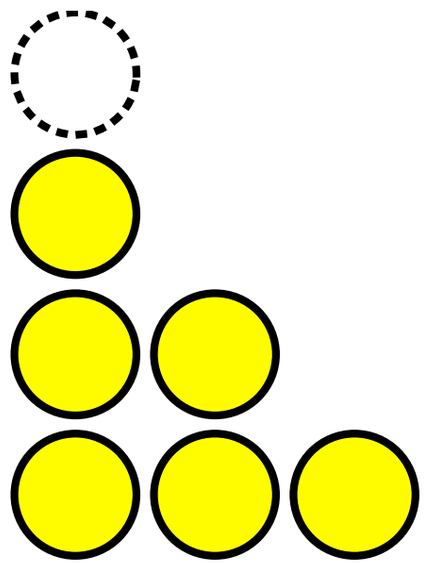
$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1\bar{\Pi}^{\circ} + J_2\bar{\Pi}^{\circ\circ} + J_3\bar{\Pi}^{\circ\circ\circ} + \cdots$$

$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$ $+ J_1$  $+ J_2$ $+ J_3$ $+ \cdots$

These are the
"effective cluster interactions"
(unknown expansion coefficients)

$$\{J_0, J_1, J_2, J_3, \cdots\}$$

These are the "clusters" or
"figures" (basis functions)

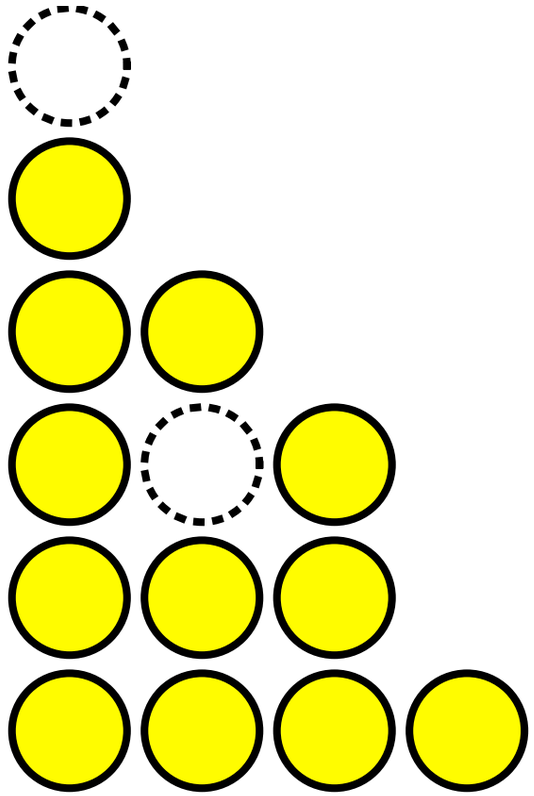


Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1}\bigcirc_{i+2} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1\bar{\Pi}^{\circ} + J_2\bar{\Pi}^{\circ\circ} + J_3\bar{\Pi}^{\circ\circ\circ} + \cdots$$

$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$ ◌ $+ J_1$ ● $+ J_2$ ●● $+ J_3$ ●●● $+ \cdots$



Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1}\,\bigcirc_{i+2} + \cdots$$

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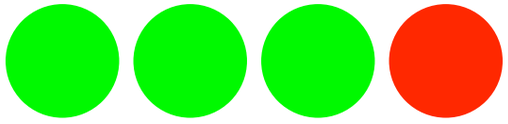
$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$ $+ J_1$ $+ J_2$ $+ J_3$ $+ \cdots$

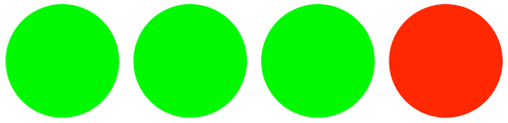


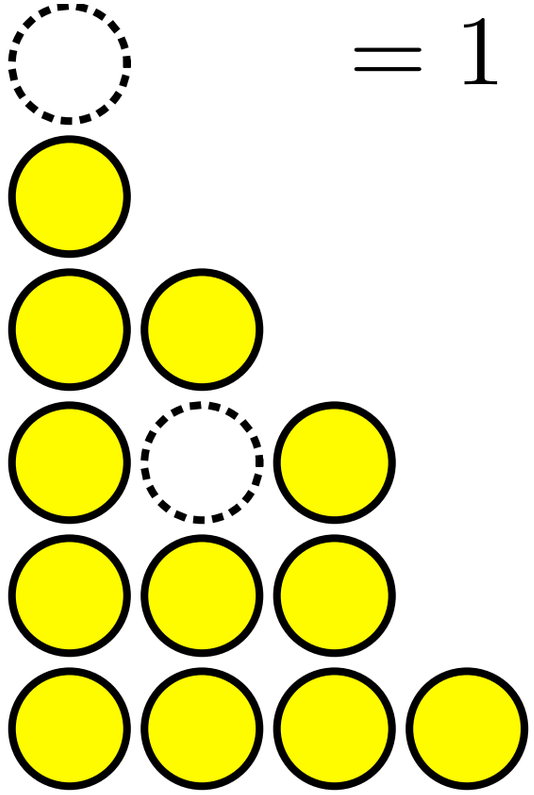
Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\,\bigcirc_{i+1}\,\bigcirc_{i+2} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1\bar{\Pi}^{\circ} + J_2\bar{\Pi}^{\circ\circ} + J_3\bar{\Pi}^{\circ\circ\circ} + \cdots$$

$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$ ○ $+ J_1$ ● $+ J_2$ ●● $+ J_3$ ●●● $+ \cdots$





Cluster Expansion: Example

$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$

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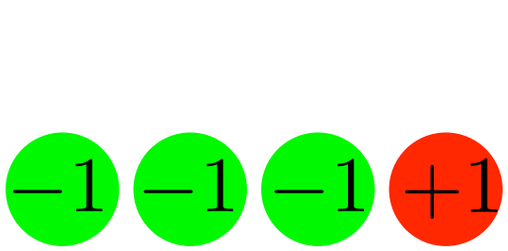

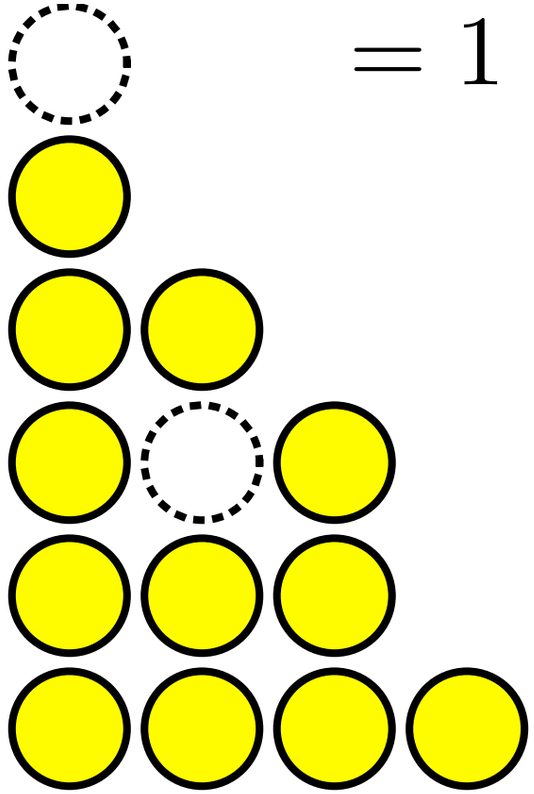

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

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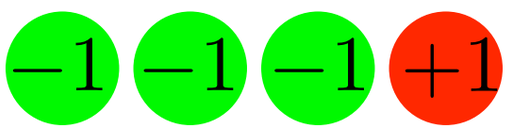

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1}\bigcirc_{i+2} + \cdots$$

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$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$  $+ J_1$ $+ J_2$ $+ J_3$ $+ \cdots$

$= 1$

$= -\frac{1}{2}$

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_{i}^{\circ\circ\circ\circ} 1 + J_1 \sum_{i}^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_{i}^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_{i}^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

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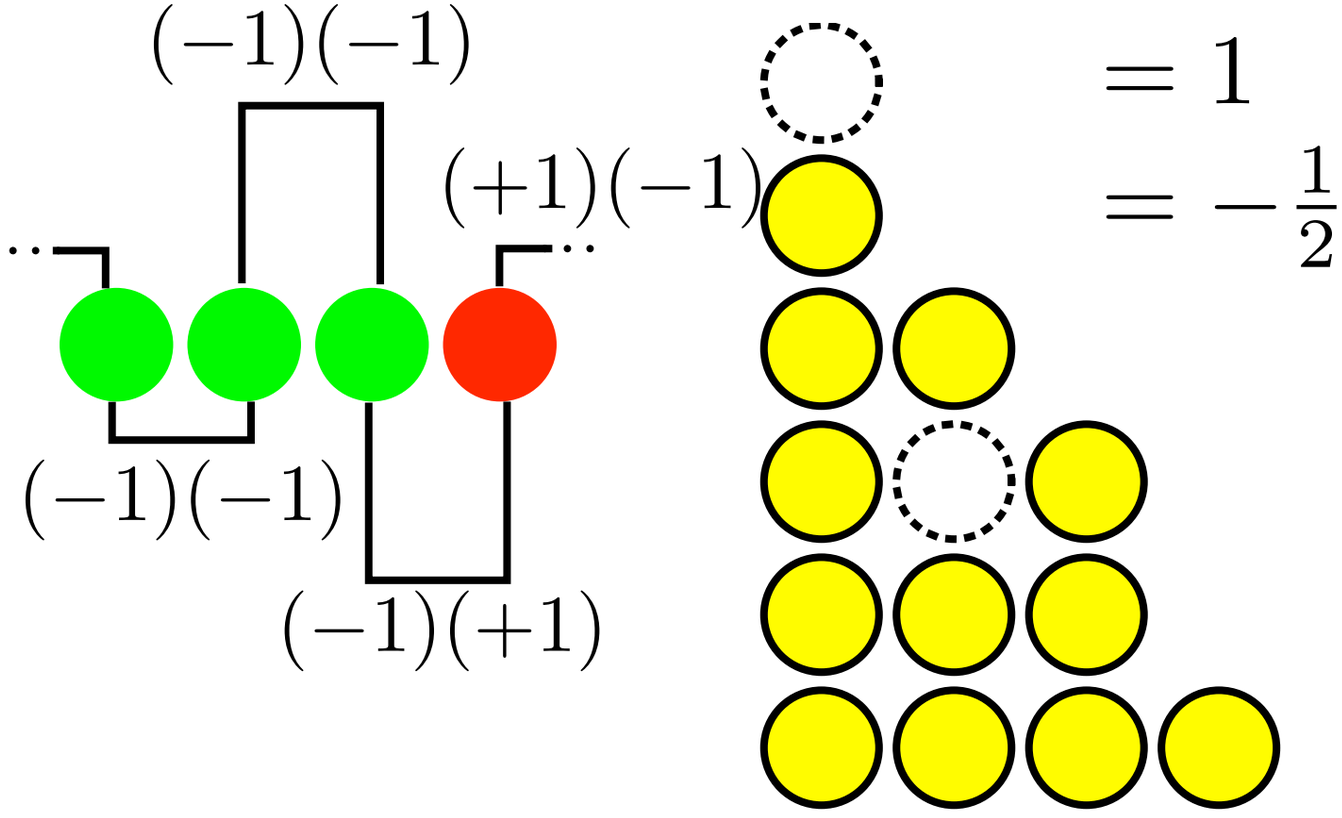

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

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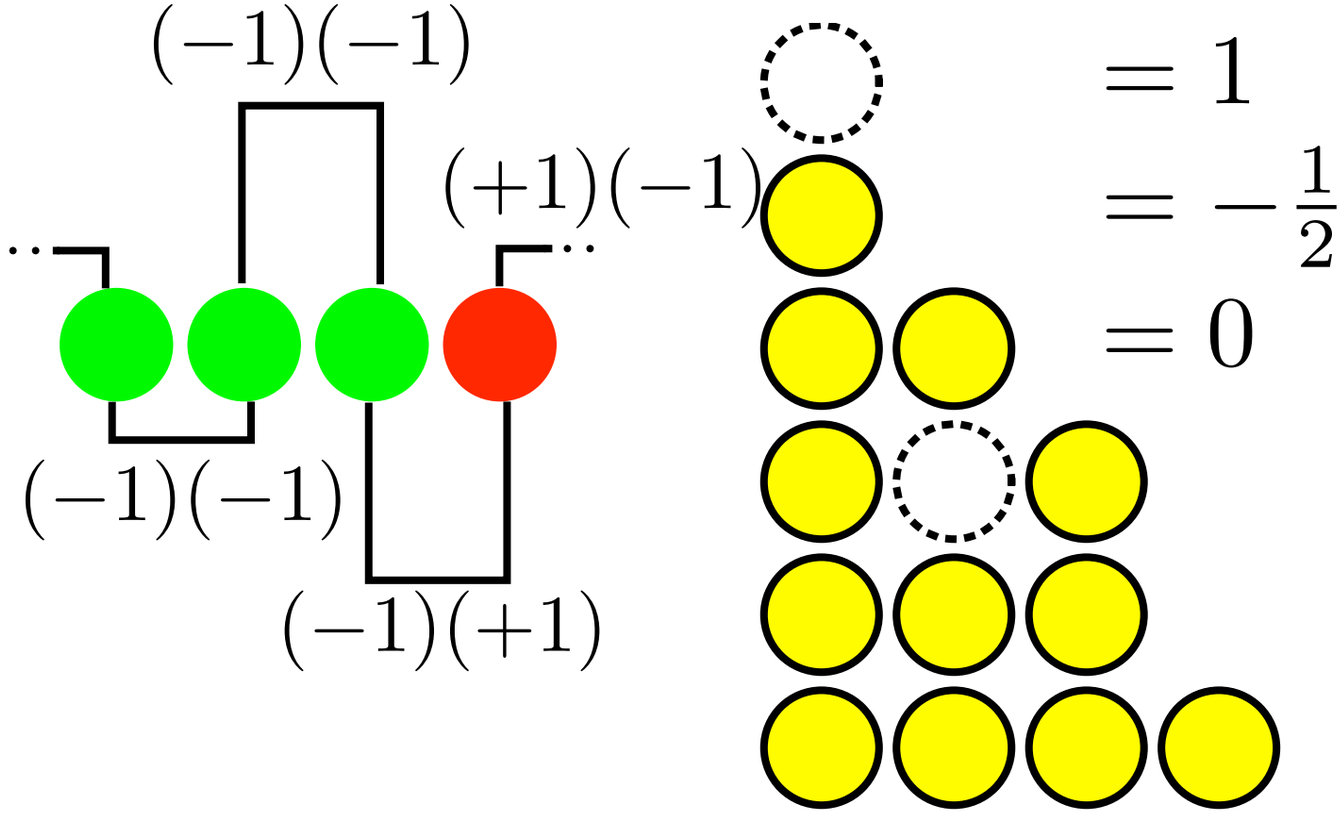

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1}\bigcirc_{i+2} + \cdots$$

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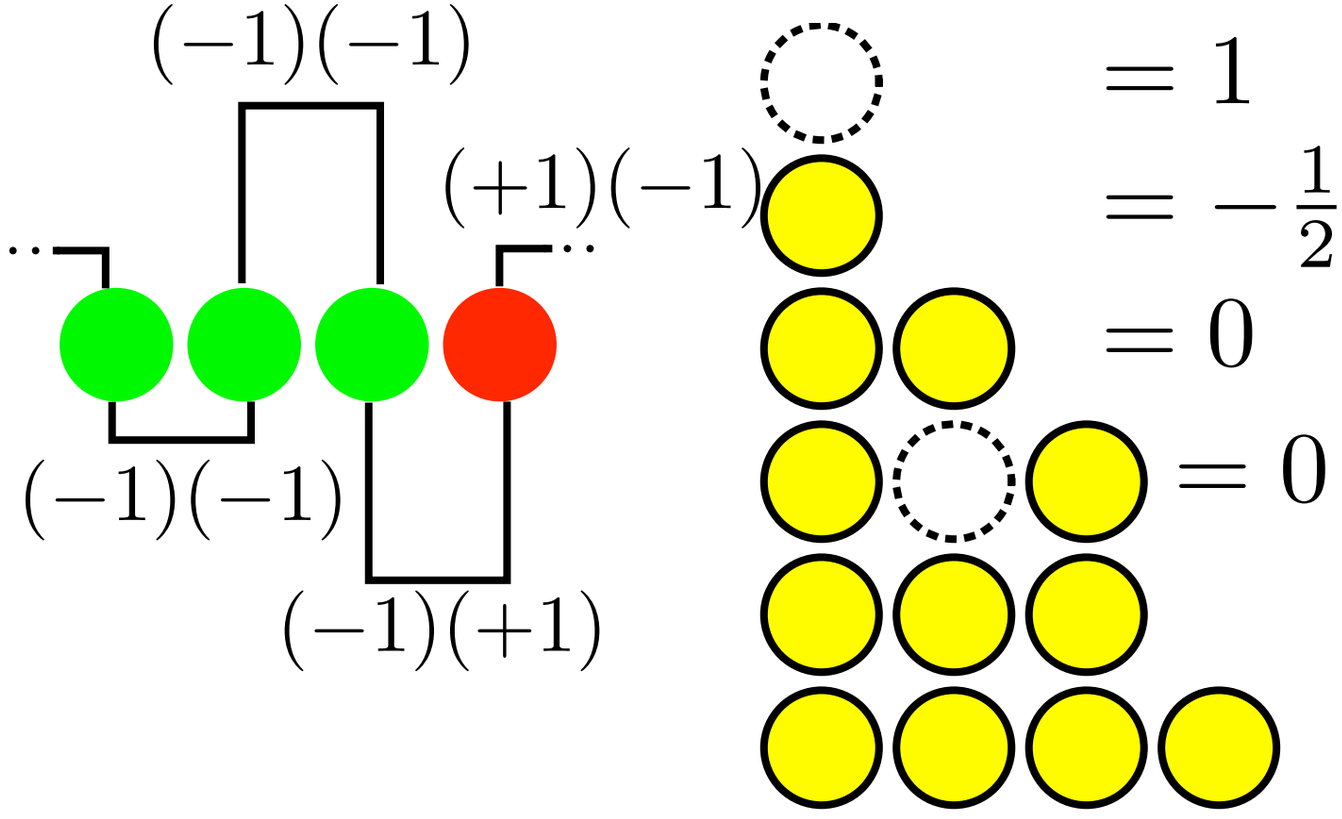

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

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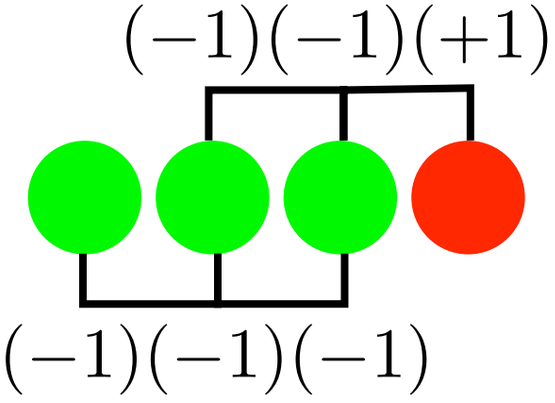

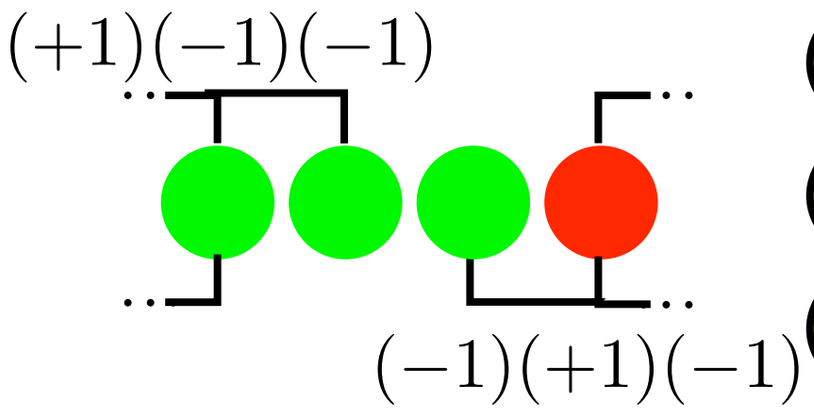

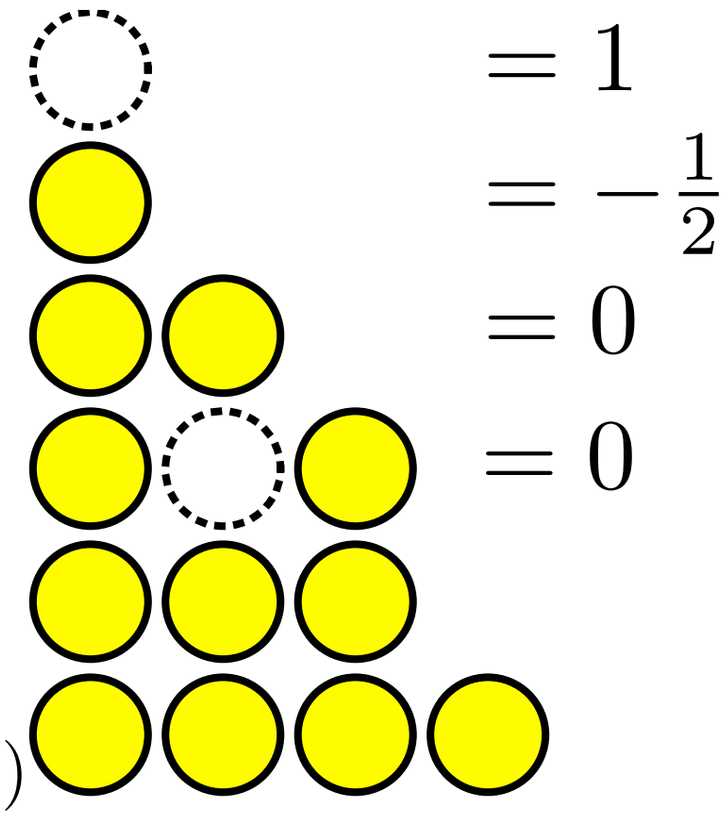

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1}\bigcirc_{i+2} + \cdots$$

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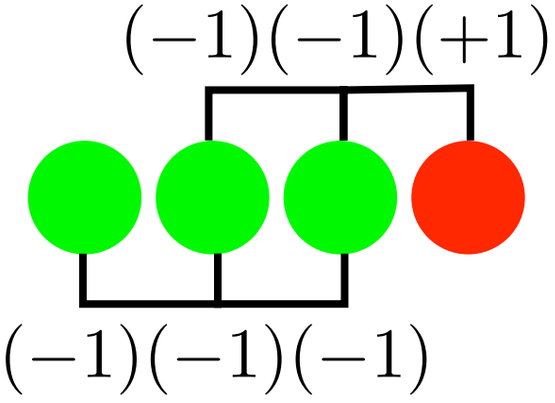

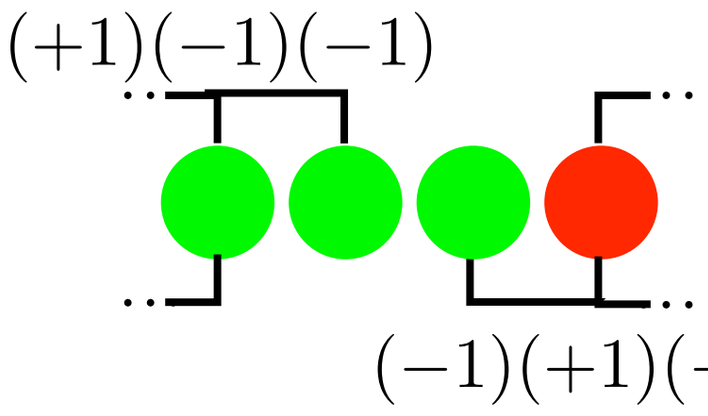

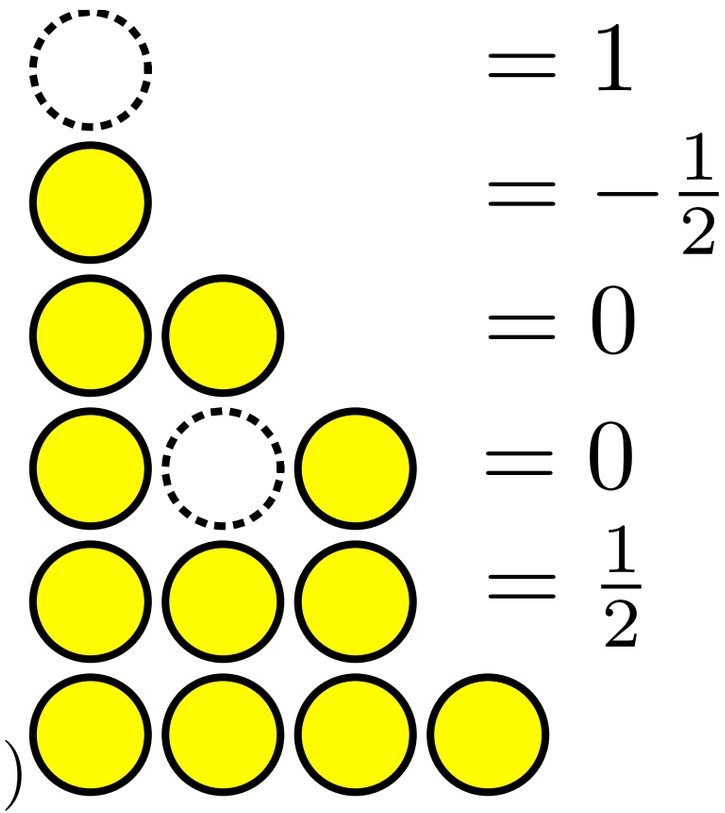

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1\sum_i^{\circ\circ\circ\circ}\bigcirc_i + J_2\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1} + J_3\sum_i^{\circ\circ\circ\circ}\bigcirc_i\bigcirc_{i+1}\bigcirc_{i+2} + \cdots$$

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1\bar{\Pi}^{\circ} + J_2\bar{\Pi}^{\circ\circ} + J_3\bar{\Pi}^{\circ\circ\circ} + \cdots$$

$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0$ ◌ $+ J_1$ ● $+ J_2$ ●● $+ J_3$ ●●● $+ \cdots$

◌ $= 1$

● $= -\frac{1}{2}$

●● $= 0$

●◌● $= 0$

●●● $= \frac{1}{2}$

●●●● $= -1$

Cluster Expansion: Example

$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots$$

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◌ $= 1$

● $= -\frac{1}{2}$

●● $= 0$

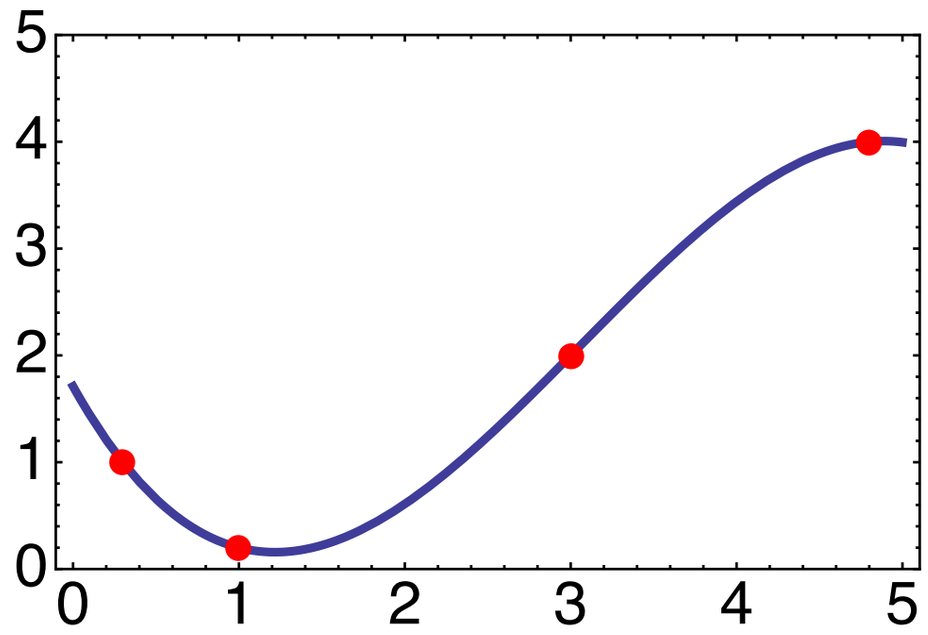
●◌● $= 0$

●●● $= \frac{1}{2}$

●●●● $= -1$

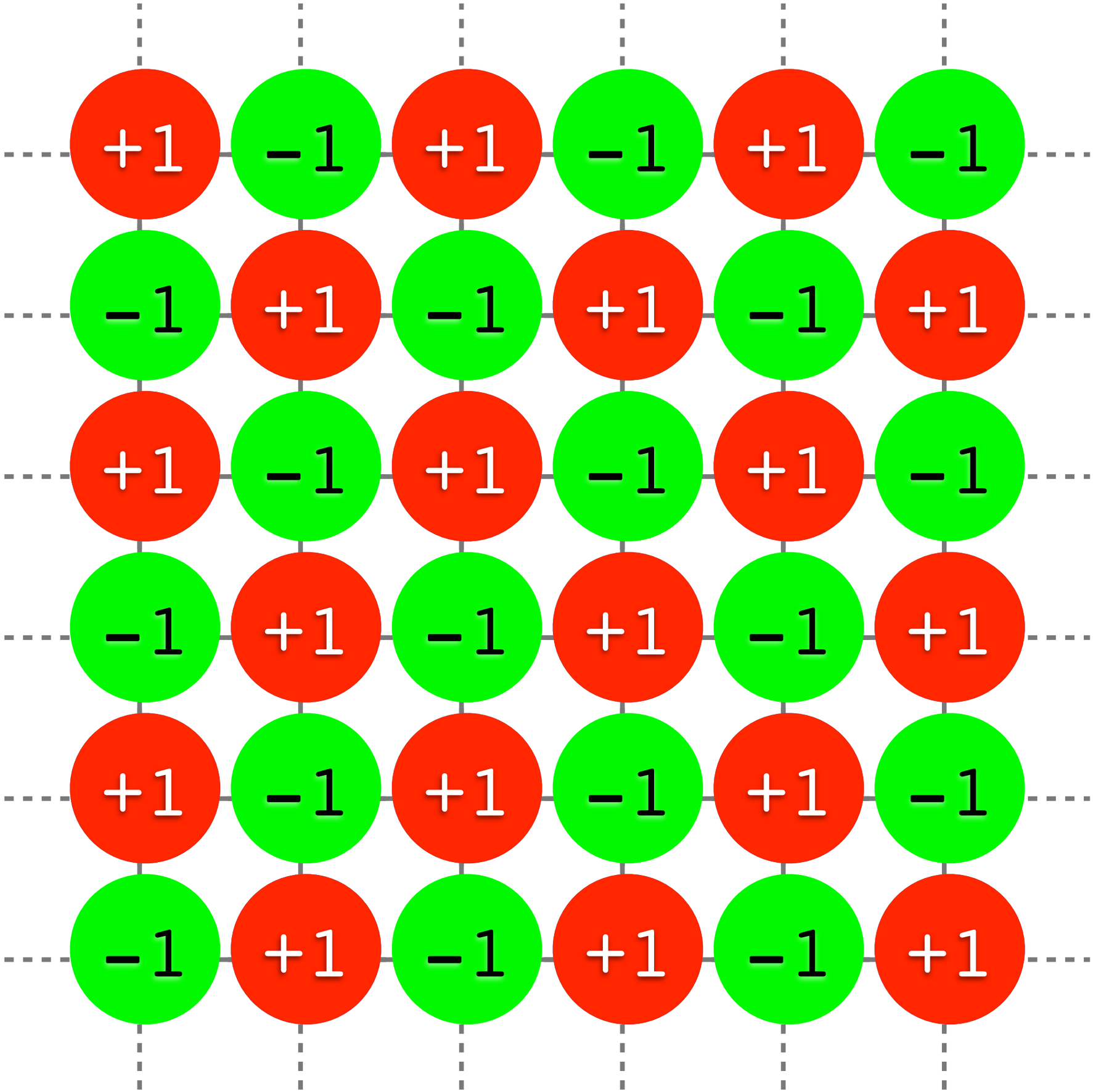
$$\begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & -1 \end{pmatrix}$$

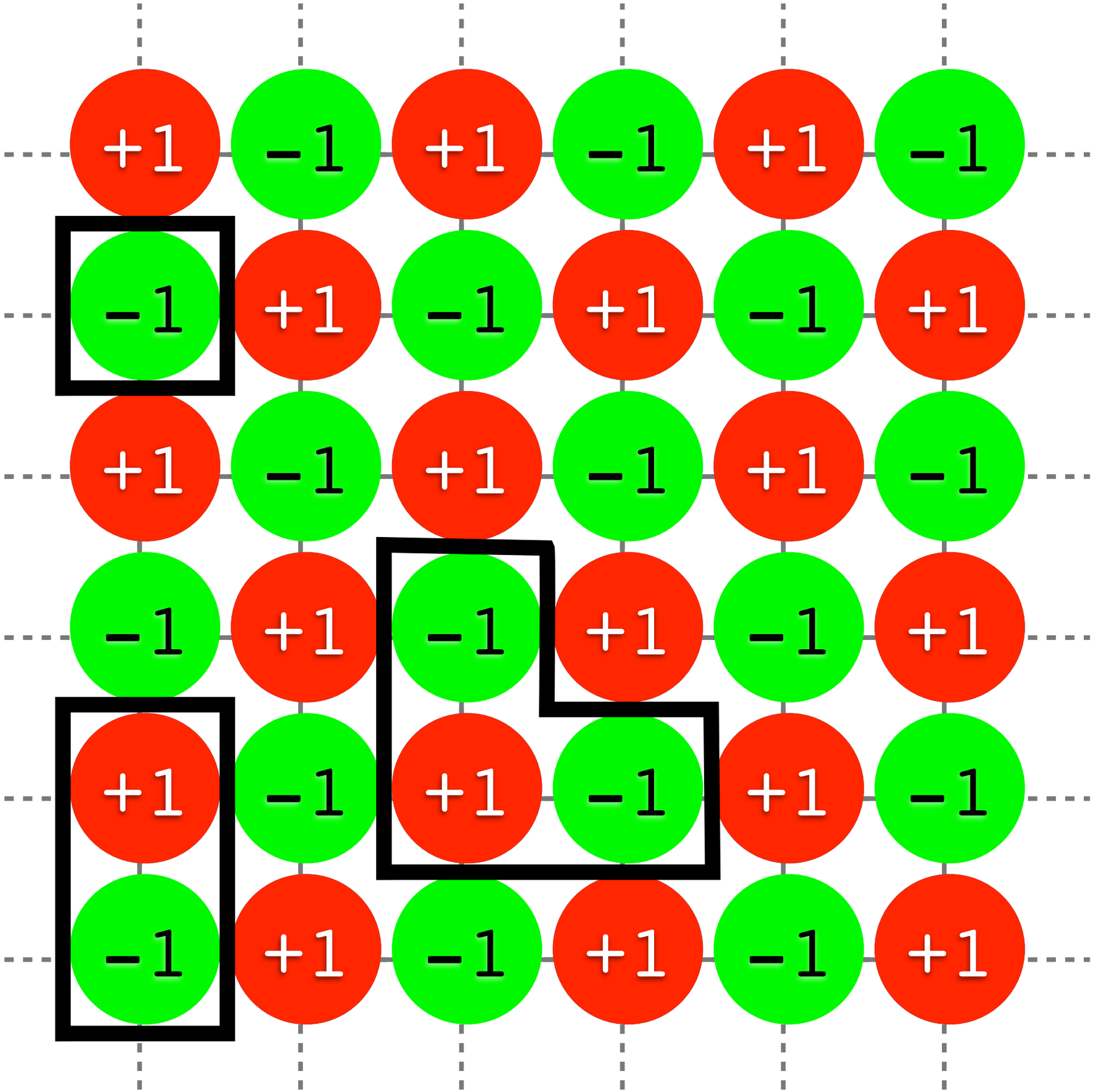
Expanding in a power series



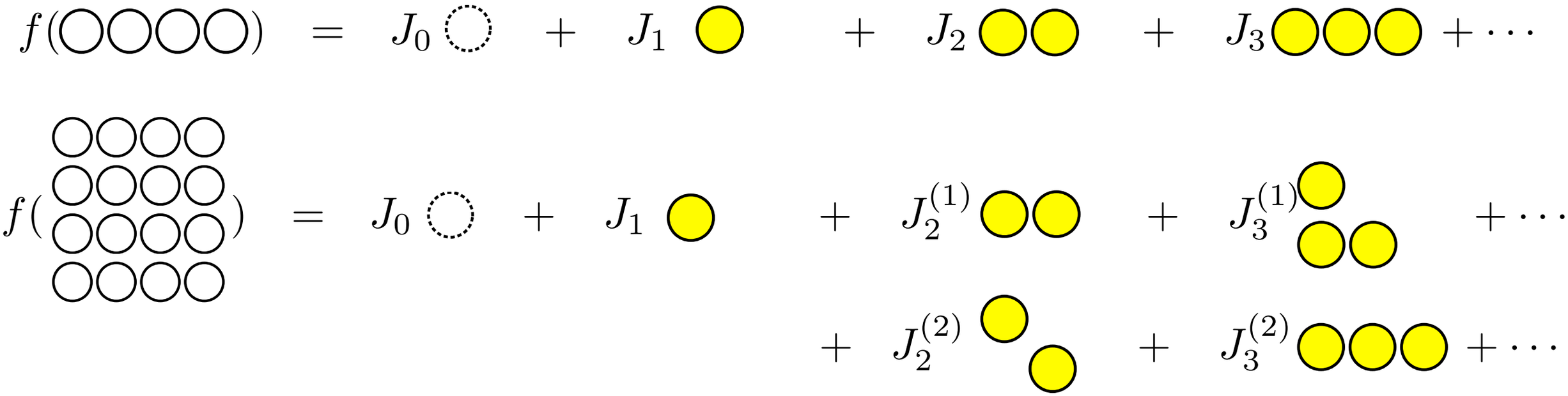
$$\begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\vec{\Pi} = \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & -1 \end{pmatrix}$$

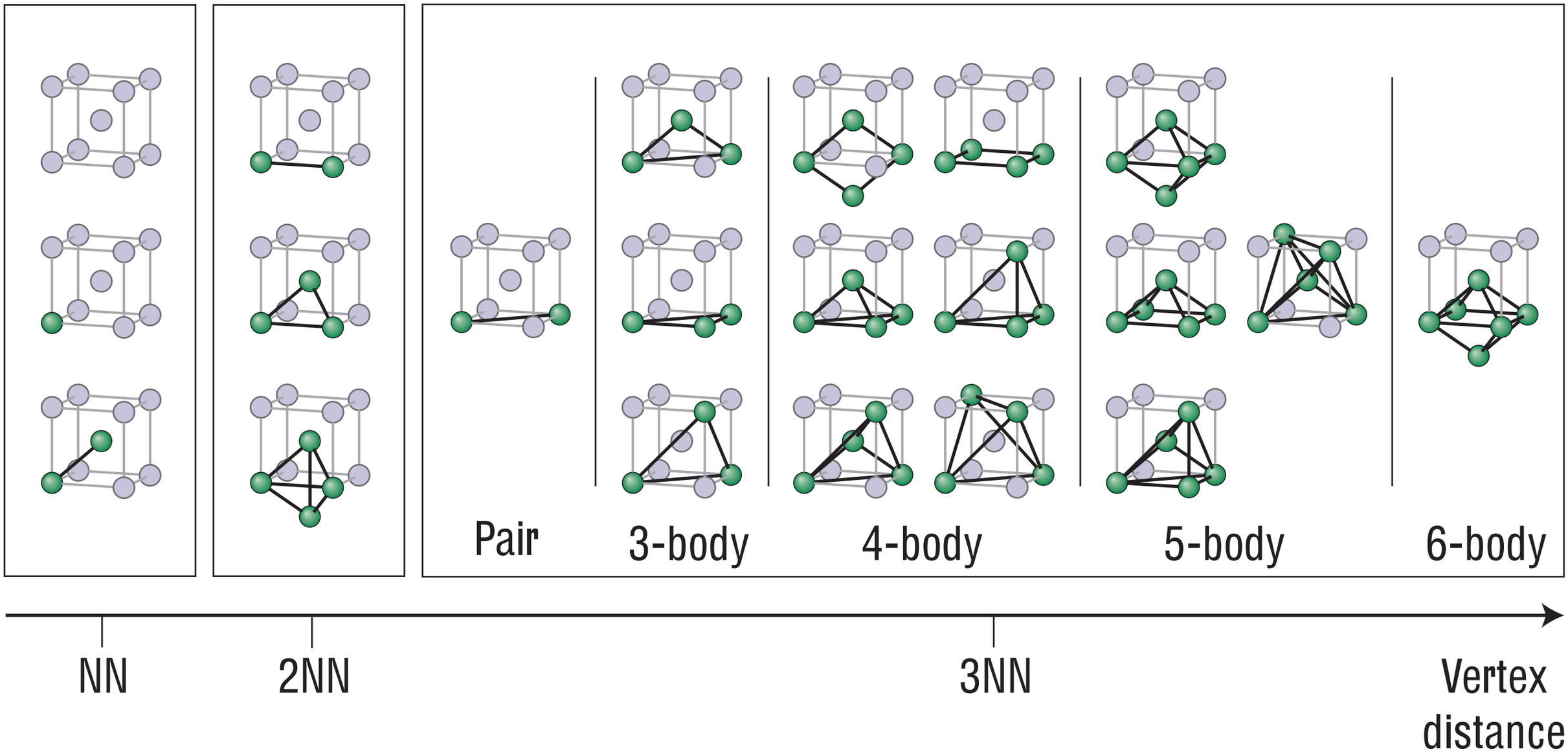

+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1
+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1
+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1


+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1
+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1
+1 −1 +1 −1 +1 −1
−1 +1 −1 +1 −1 +1

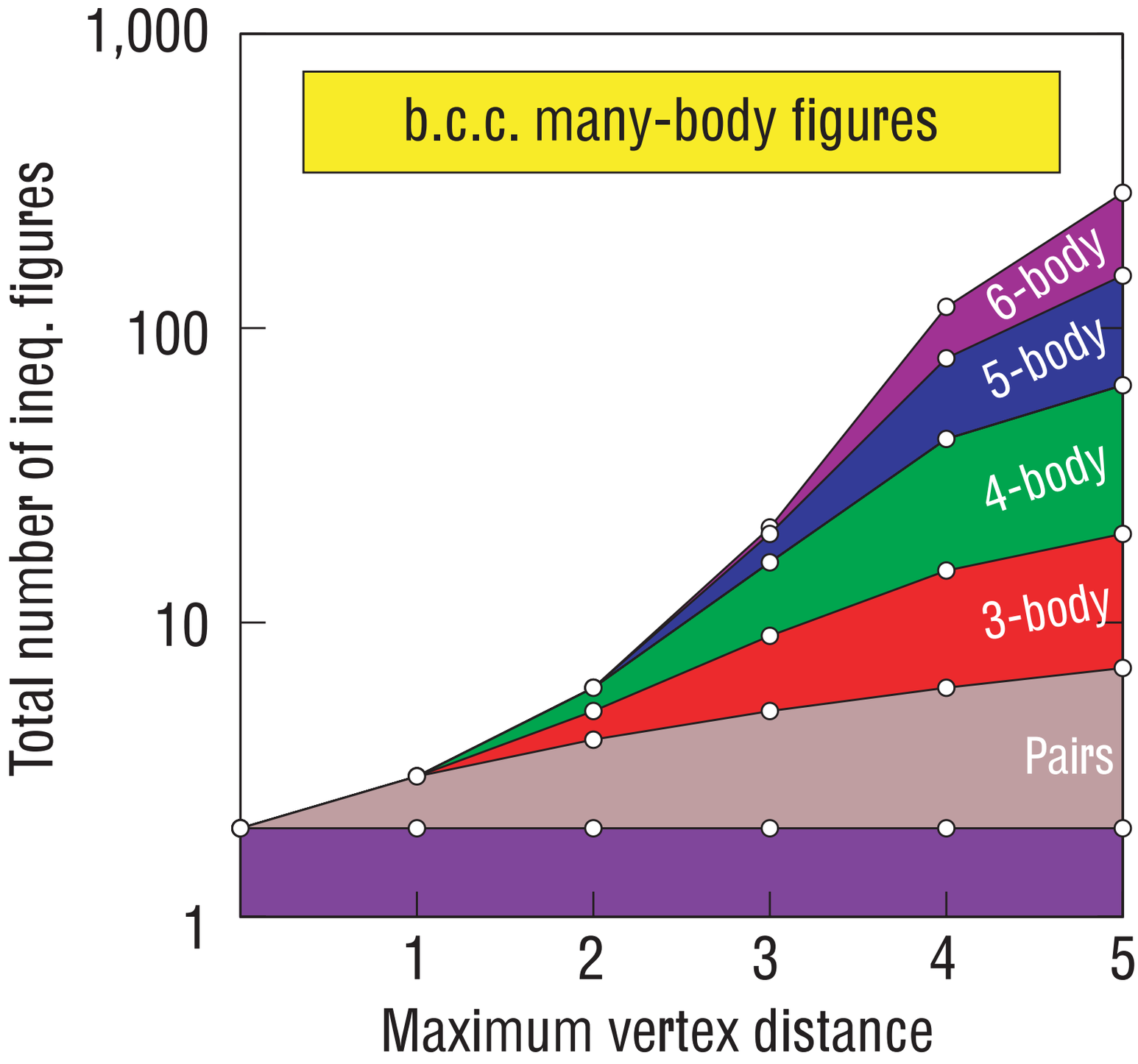
In more than one dimension...



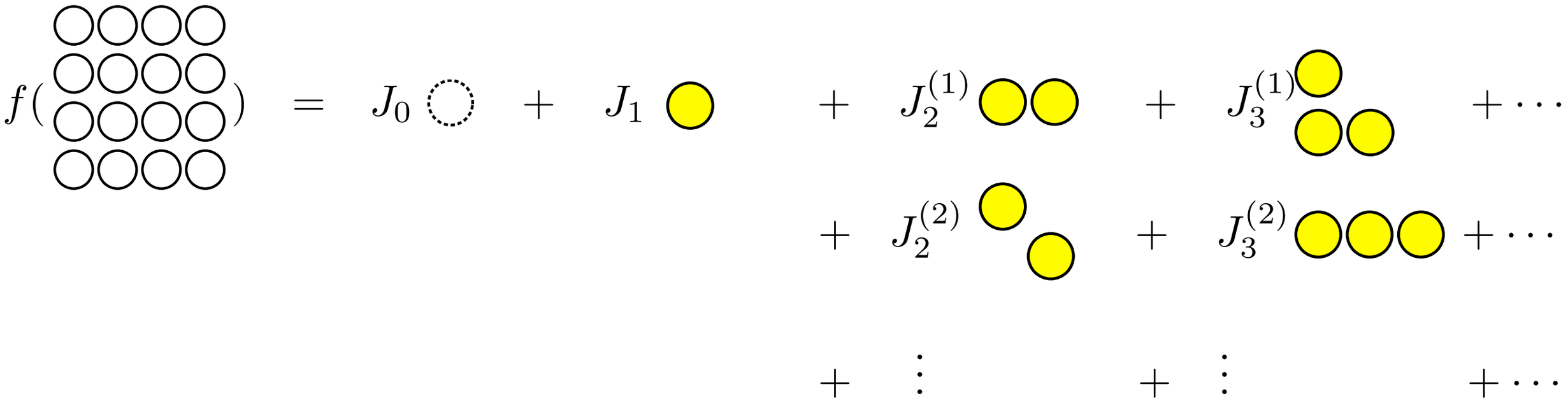
In three dimensions...



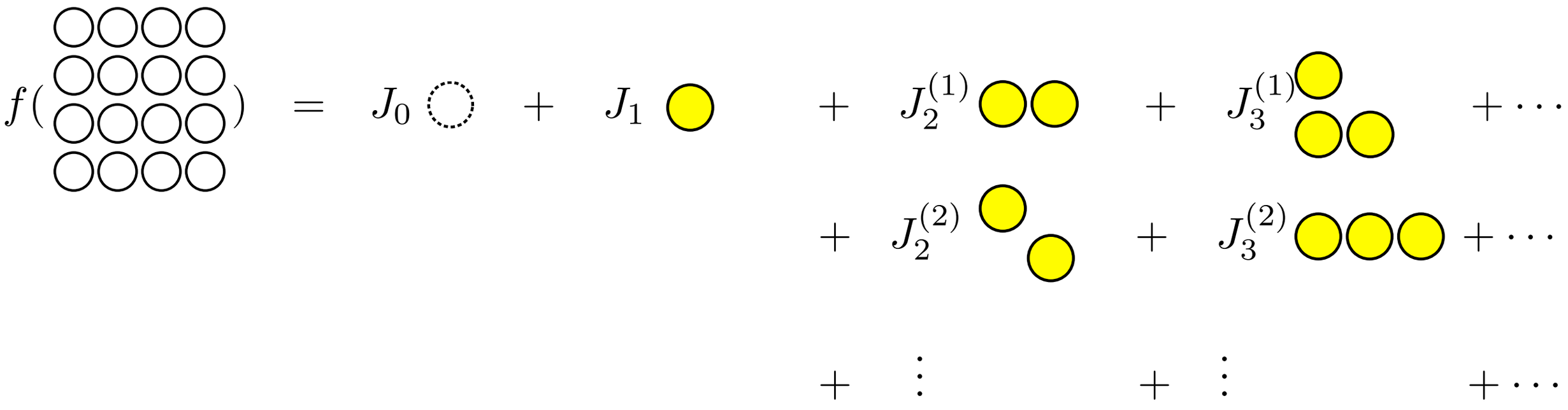
In three dimensions...



In more than one dimension...

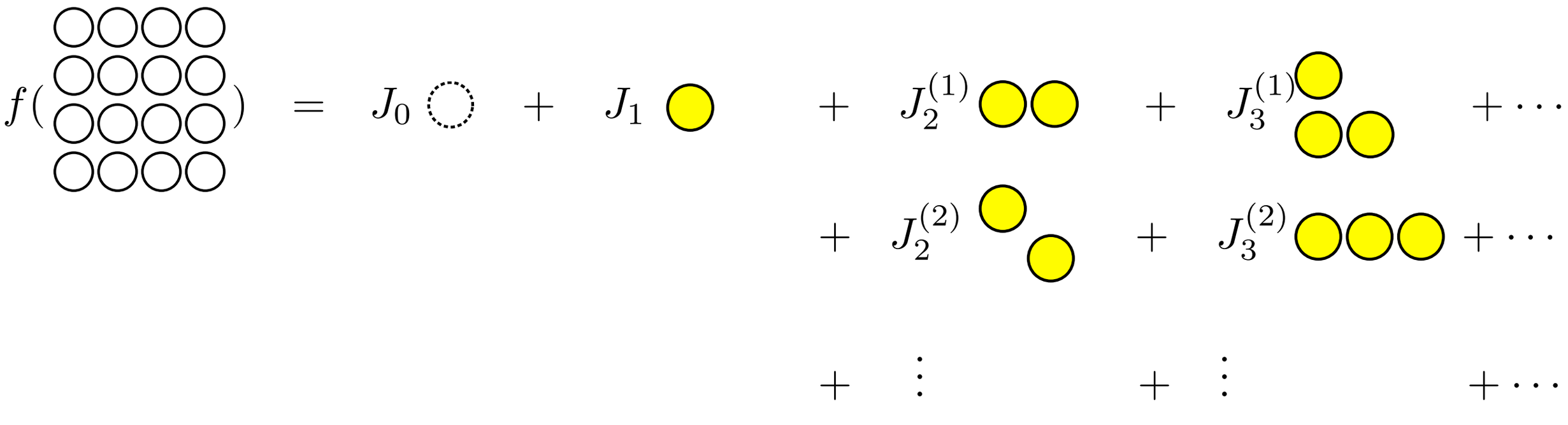


In more than one dimension...



How do we select the clusters that are relevant?

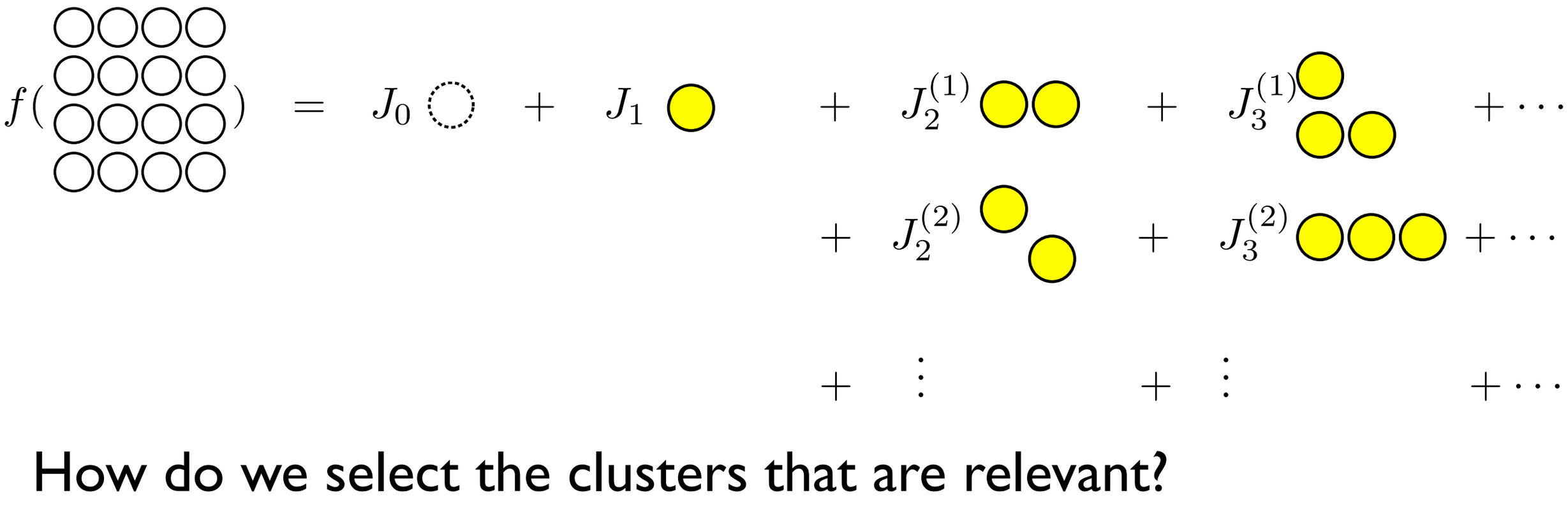
In more than one dimension...



How do we select the clusters that are relevant?

$$\binom{400}{10} \approx 10^{19}$$

In more than one dimension...



How do we select the clusters that are relevant?

$$\binom{400}{10} \approx 10^{19}$$

Impractical to try all combinations...

$$E = J_0 \; + \; J_1 \; + \; J_2^{(1)} \; + \; J_2^{(2)}$$

$$+ J_2^{(3)} \; + \cdots + \; J_3^{(2)} \; + J_3^{(3)} \; + \cdots$$

$$+ J_4^{(1)} \; + J_4^{(2)} \; + \cdots + \; J_5^{(1)} \; + \cdots$$

$$E = J_0 \; + \; J_1 \; + \; J_2^{(1)} \; + \; J_2^{(2)}$$

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$$E = J_0 + J_1 + J_2^{(1)} + J_2^{(2)}$$

$$+ J_2^{(3)} + \cdots + J_3^{(2)} + J_3^{(3)} + \cdots$$

$$+ J_4^{(1)} + J_4^{(2)} + \cdots + J_5^{(1)} + \cdots$$

1 1 1 0 1 0 0 1 0 0 1 1 0 0 0

Current population

0101000100011010 0 — Fitness score 1

1100100010001101 0 — Fitness score 2

0010001100010100 0 — Fitness score *n*

Choose 2 parents

0001001000011000 1 — Parent 1

1000100010010101 0 — Parent 2

Mating

1001100010011001 0

Mutation

0001101010011011 0

Reduction

0001100010001011 0

Child

Accept child into population if fitness score is improved

Fitness Scores:
Cross Validation (a.k.a. Rotation Estimation)

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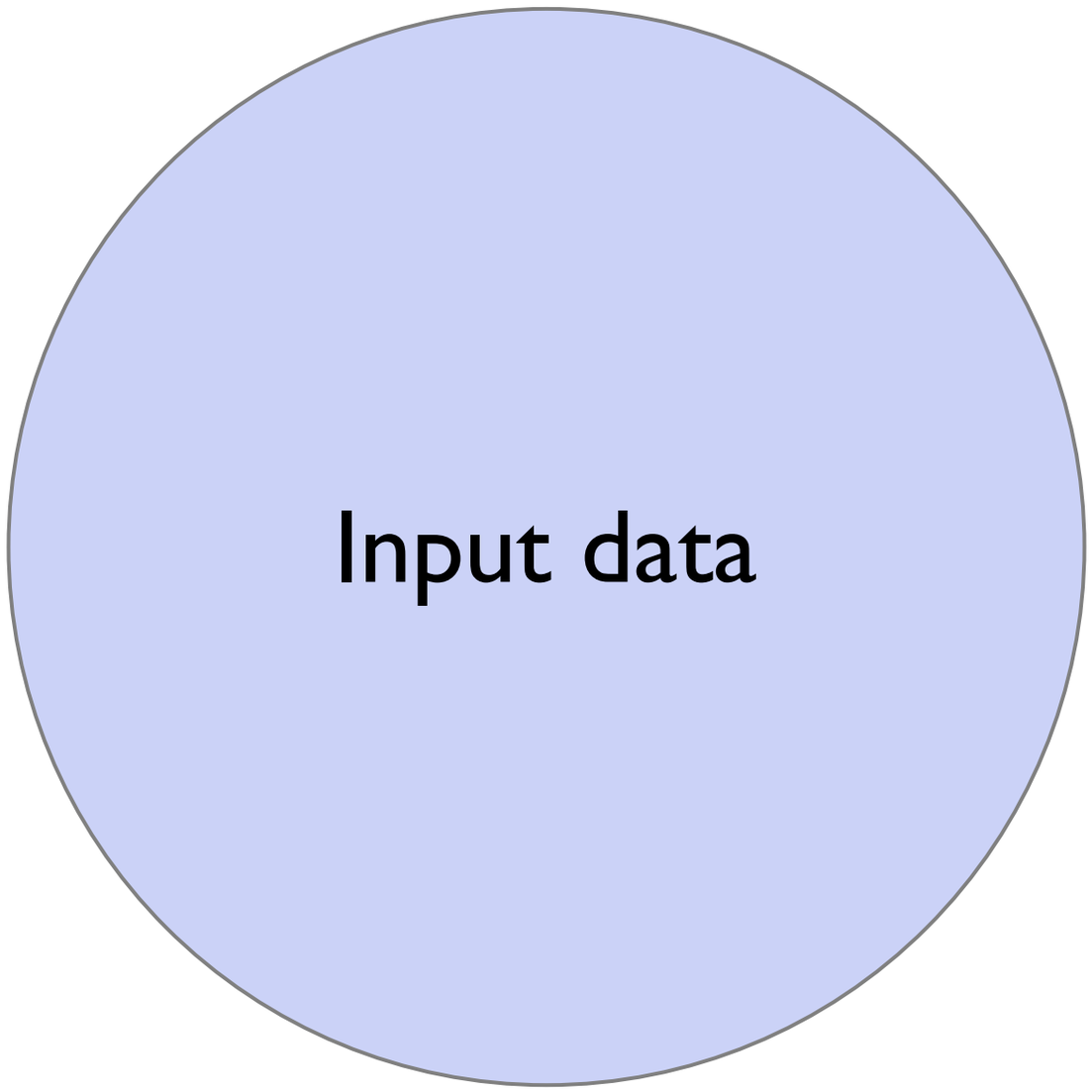
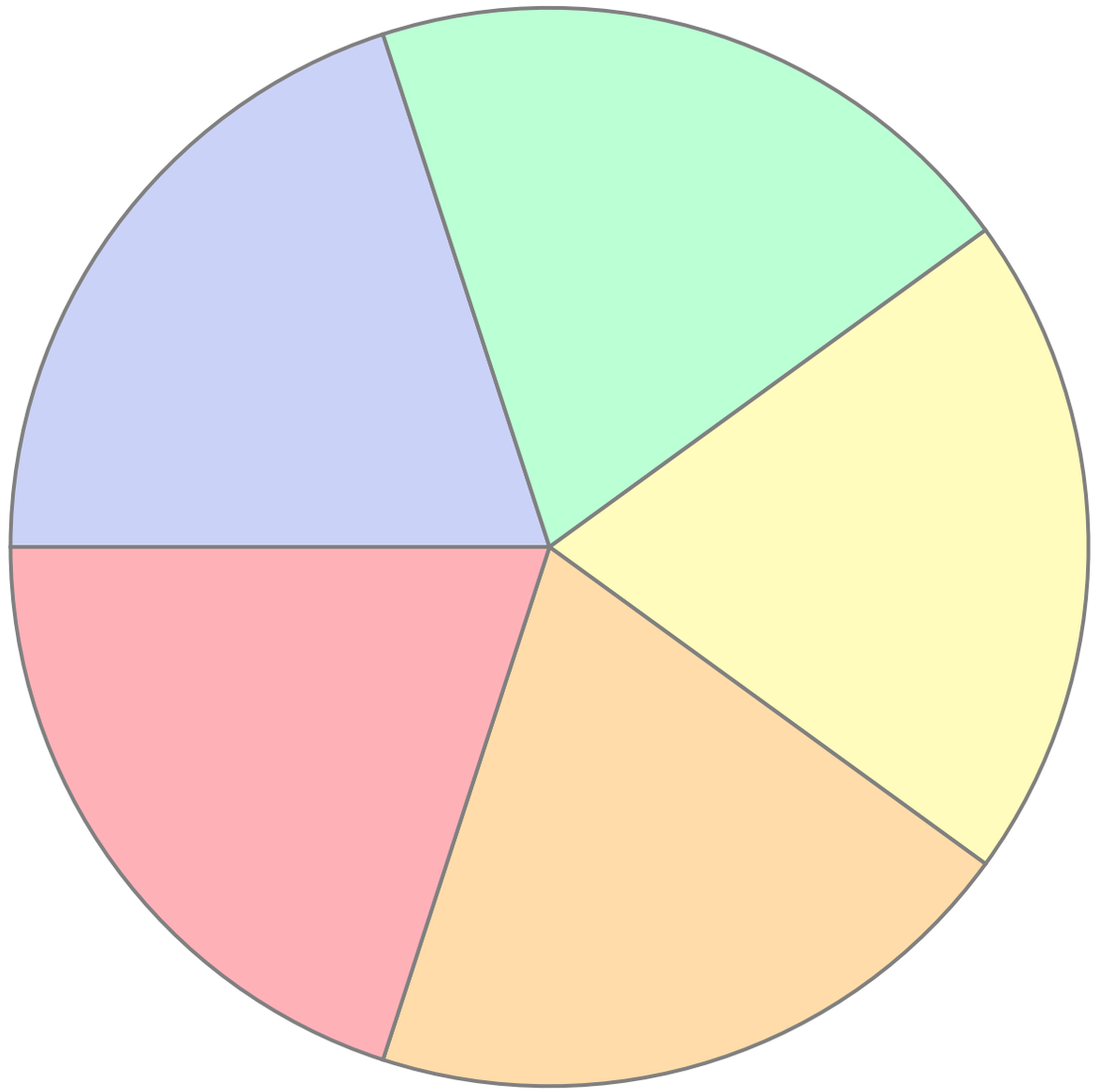
Least Square Minimization is dangerous because of overfitting

Fitness Scores:
Cross Validation (a.k.a. Rotation Estimation)



Fitness Scores:
Cross Validation (a.k.a. Rotation Estimation)



Fitness Scores:
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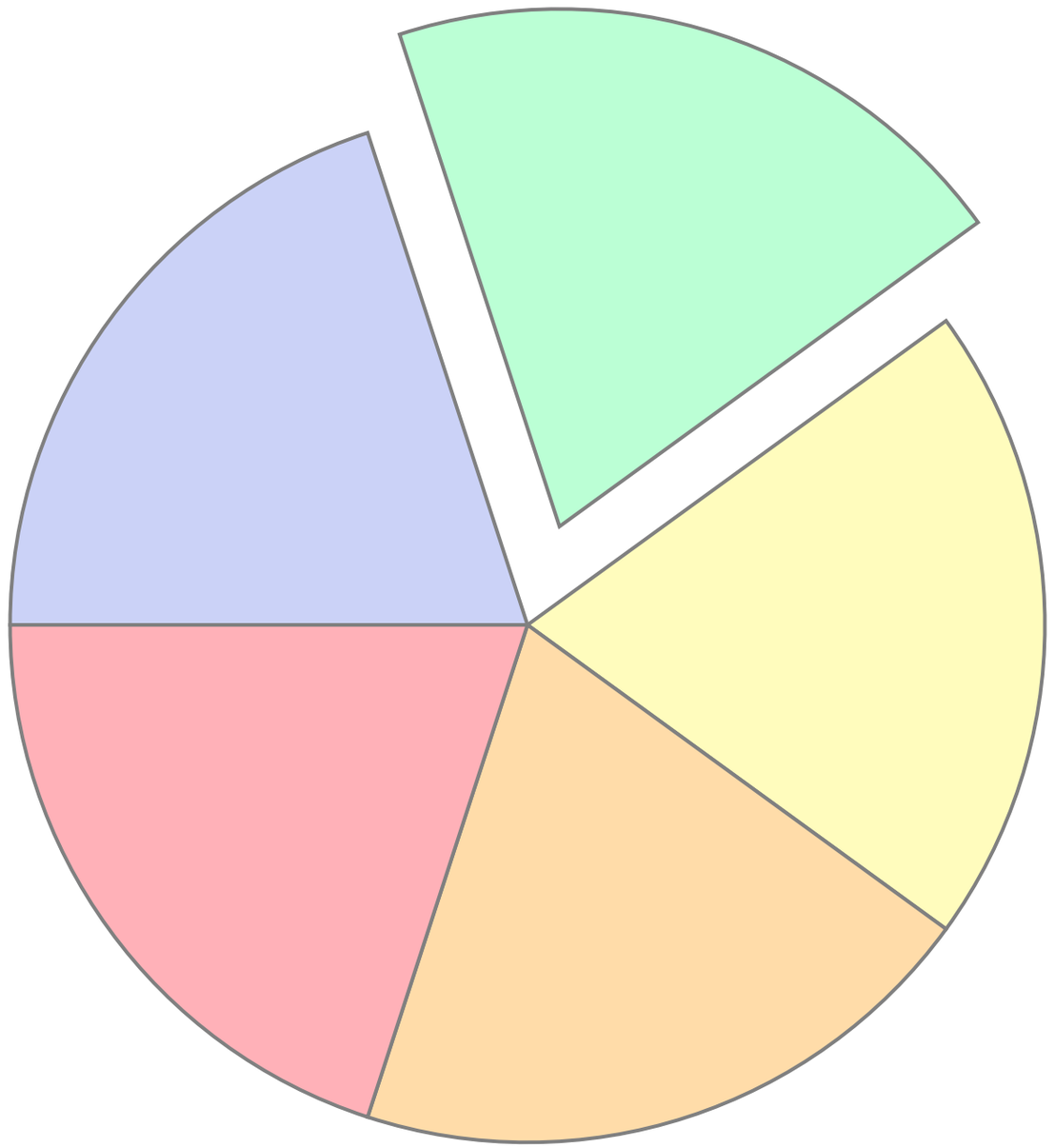

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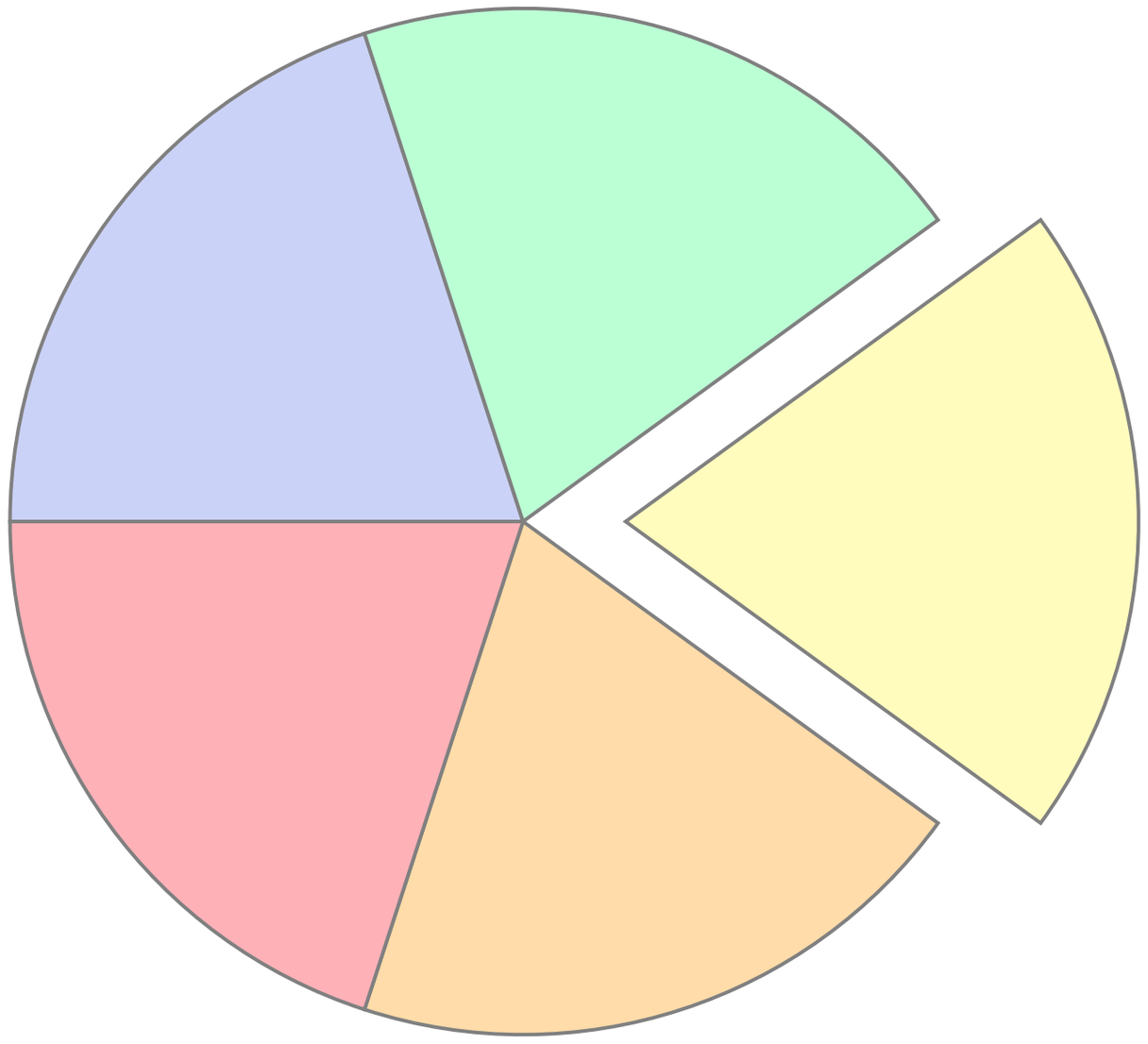


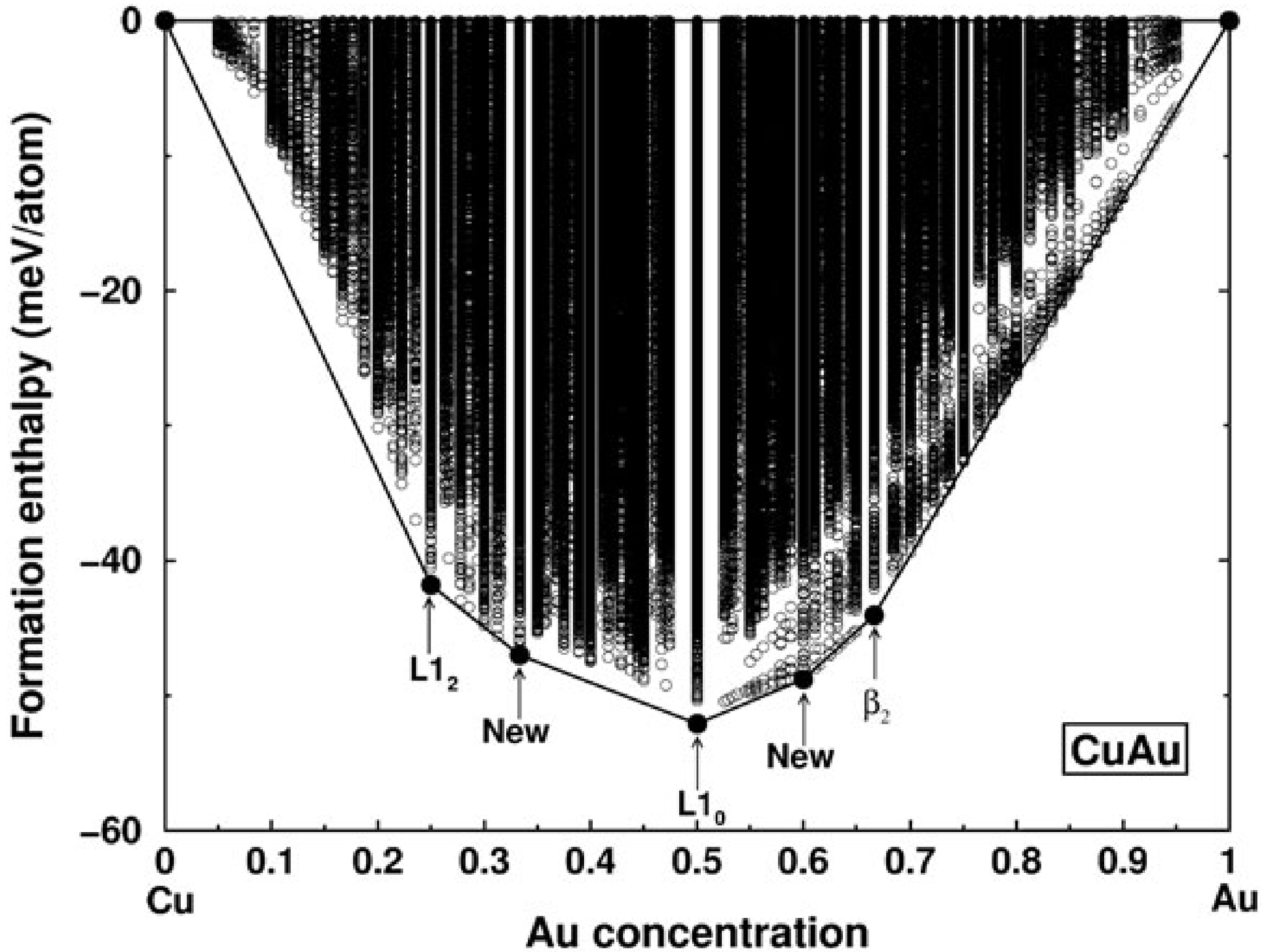
Make a model and *predict* data you already know

Once you have a good physical model, what can you do with it?

Once you have a good physical model, what can you do with it?

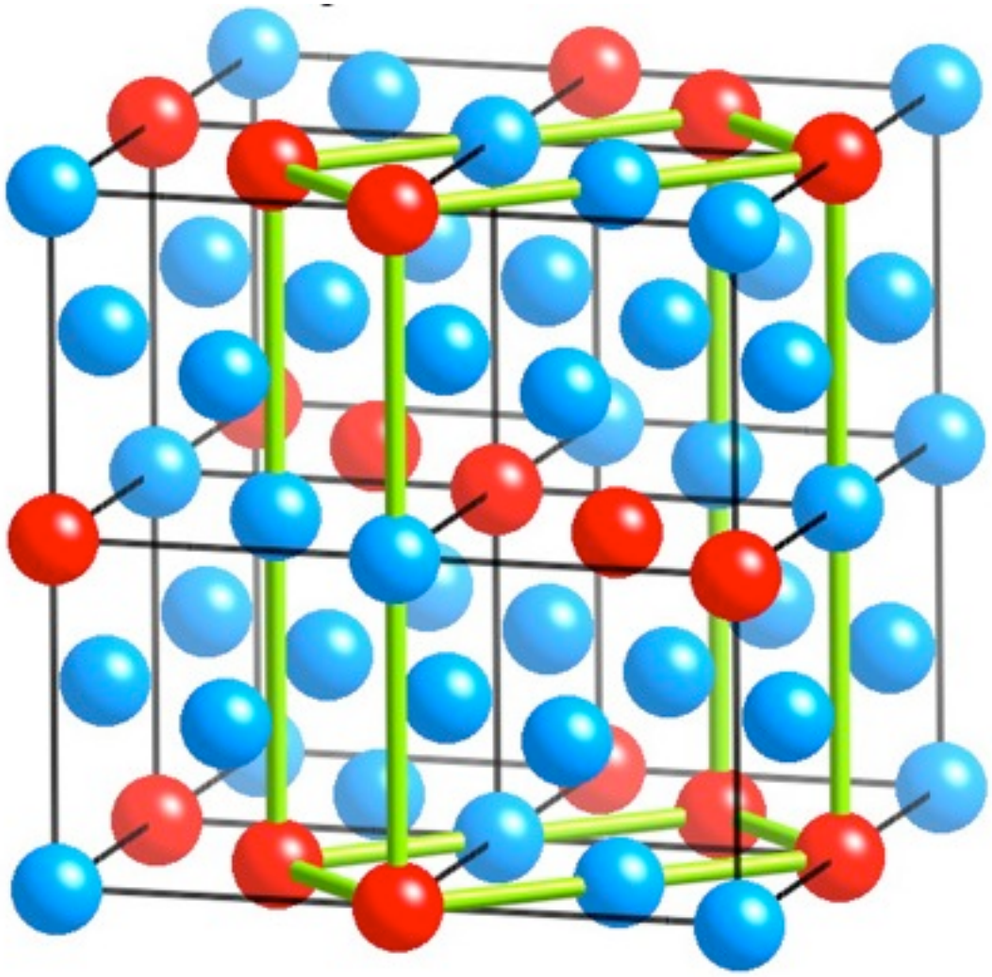
Calculate the energy of
millions of configurations

Once you have a good physical model, what can you do with it?

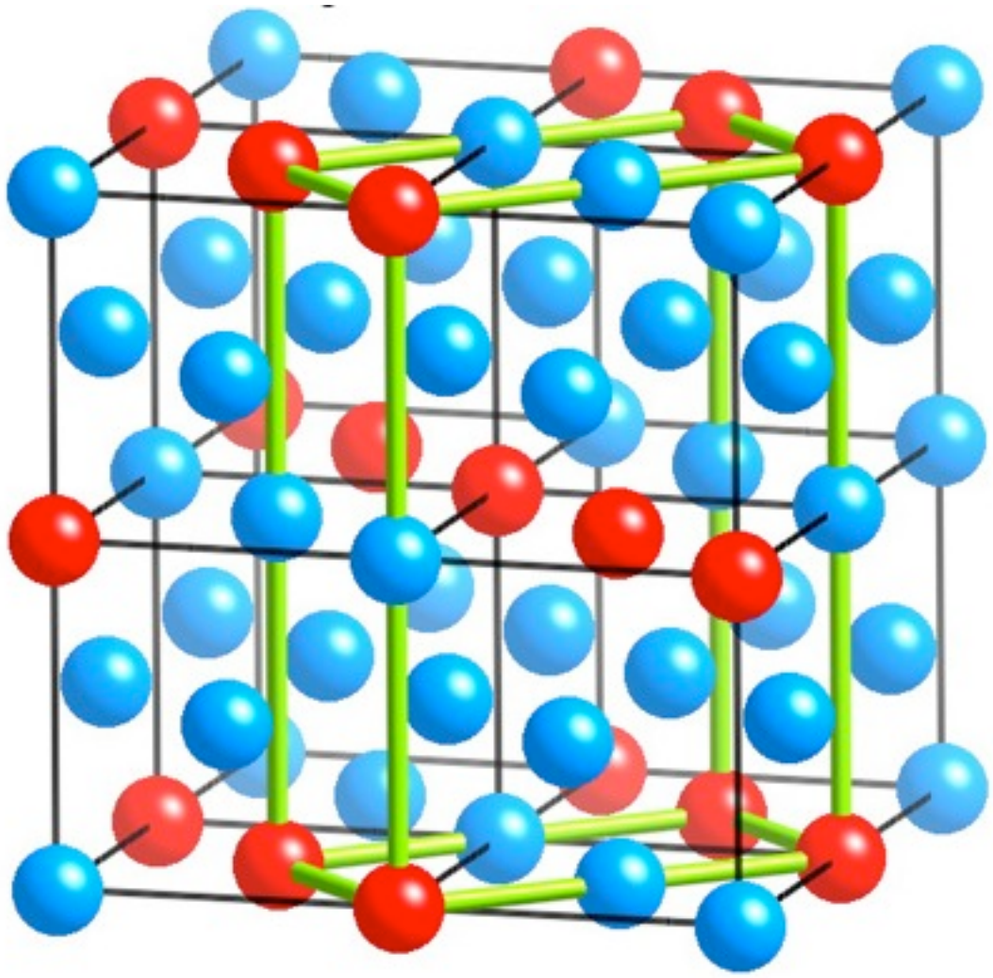


Where do you get a list of all possible configurations?

Enumerating derivative structures



Enumerating derivative structures



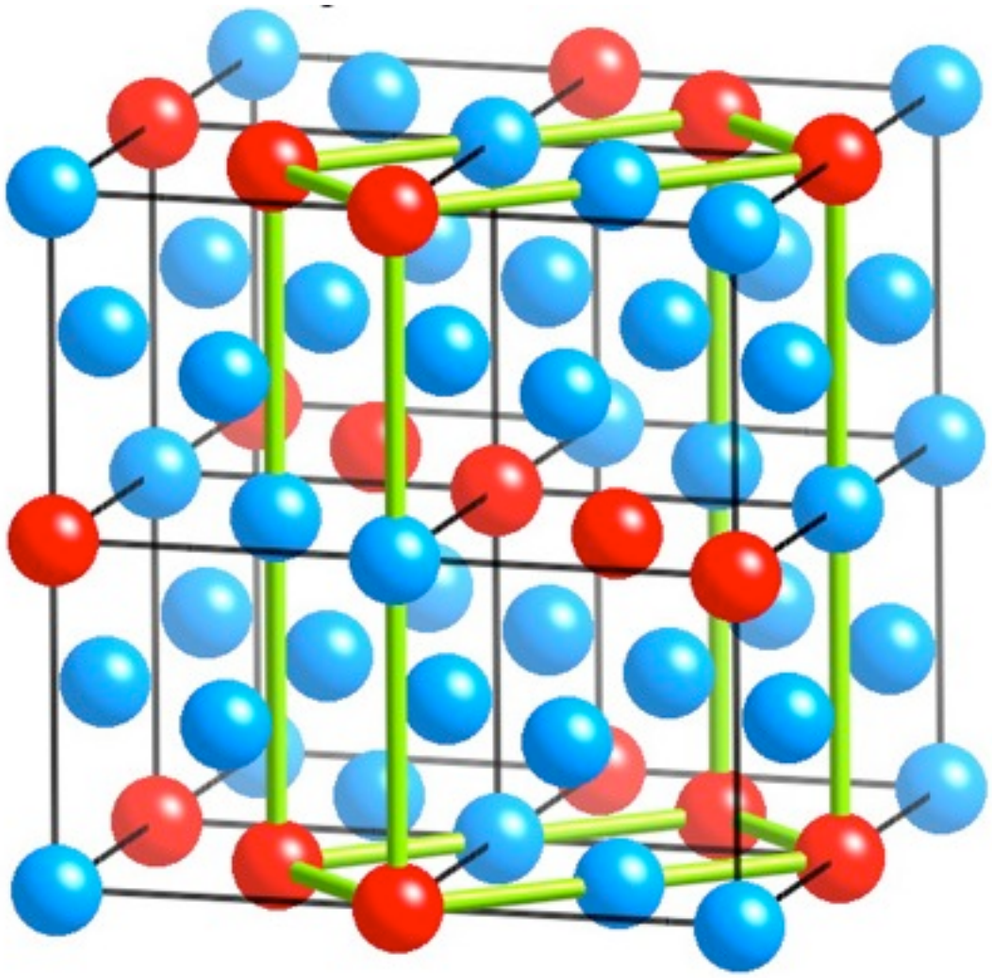
$\Rightarrow$

Hermite Normal Form

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}$$

0001

Enumerating derivative structures



$\Rightarrow$

Hermite Normal Form

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{pmatrix}$$

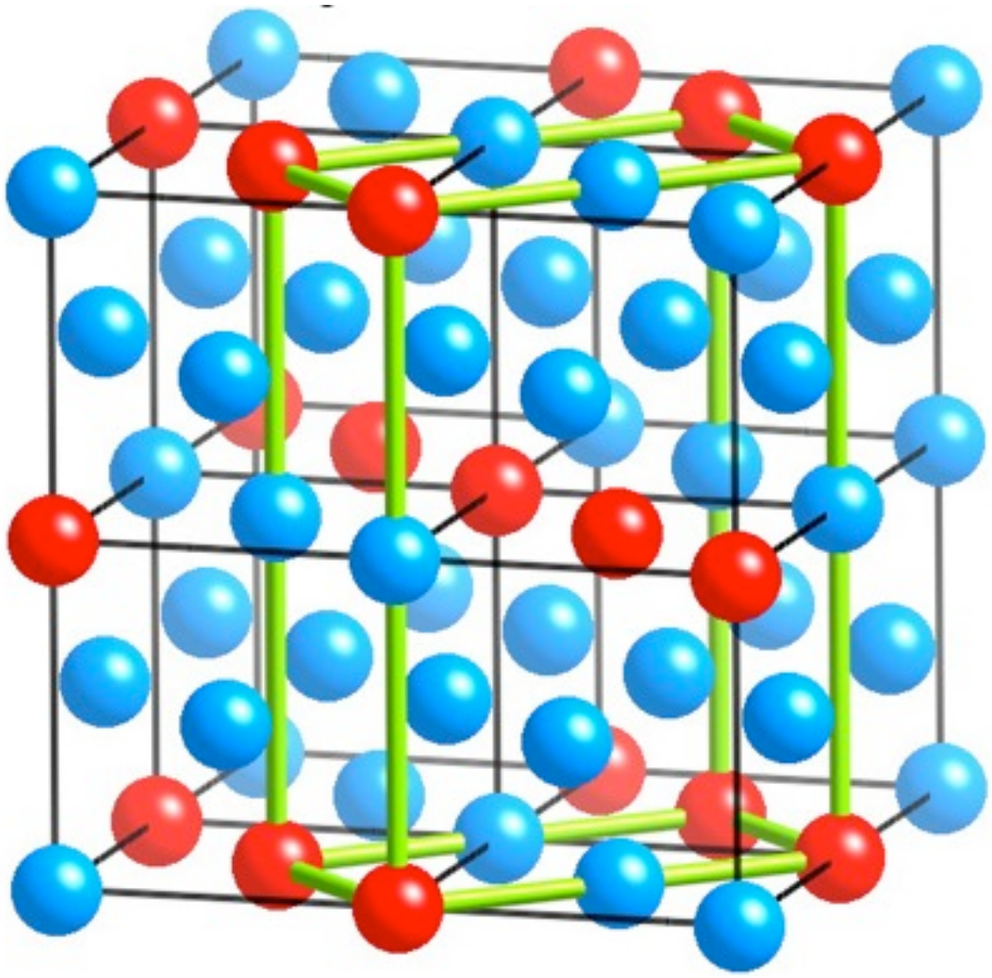
0001

$\Downarrow$

Smith Normal Form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Enumerating derivative structures



$$\mathbb{G}' = \mathbb{L}\mathbb{A}^{-1}\mathbb{R}(\mathbb{L}\mathbb{A}^{-1})^{-1}\mathbb{G}$$

$\Rightarrow$

Hermite Normal Form

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0001

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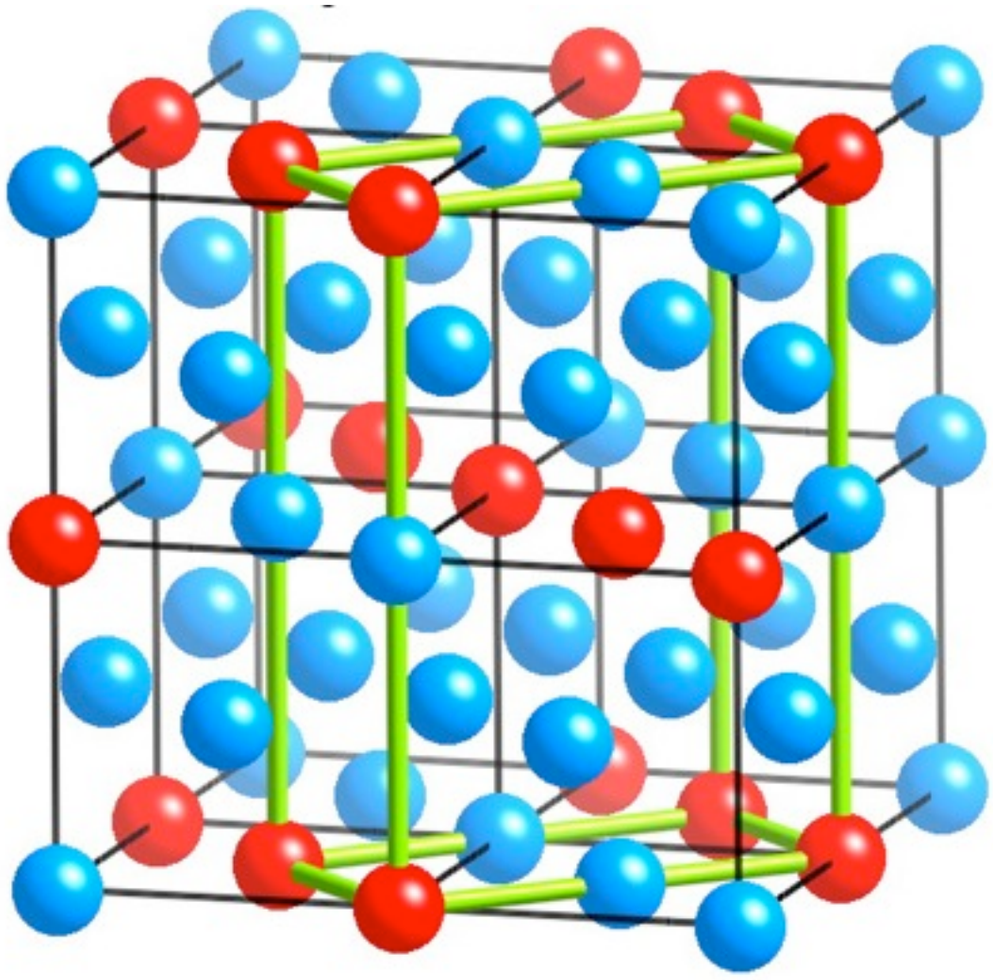
Enumerating derivative structures



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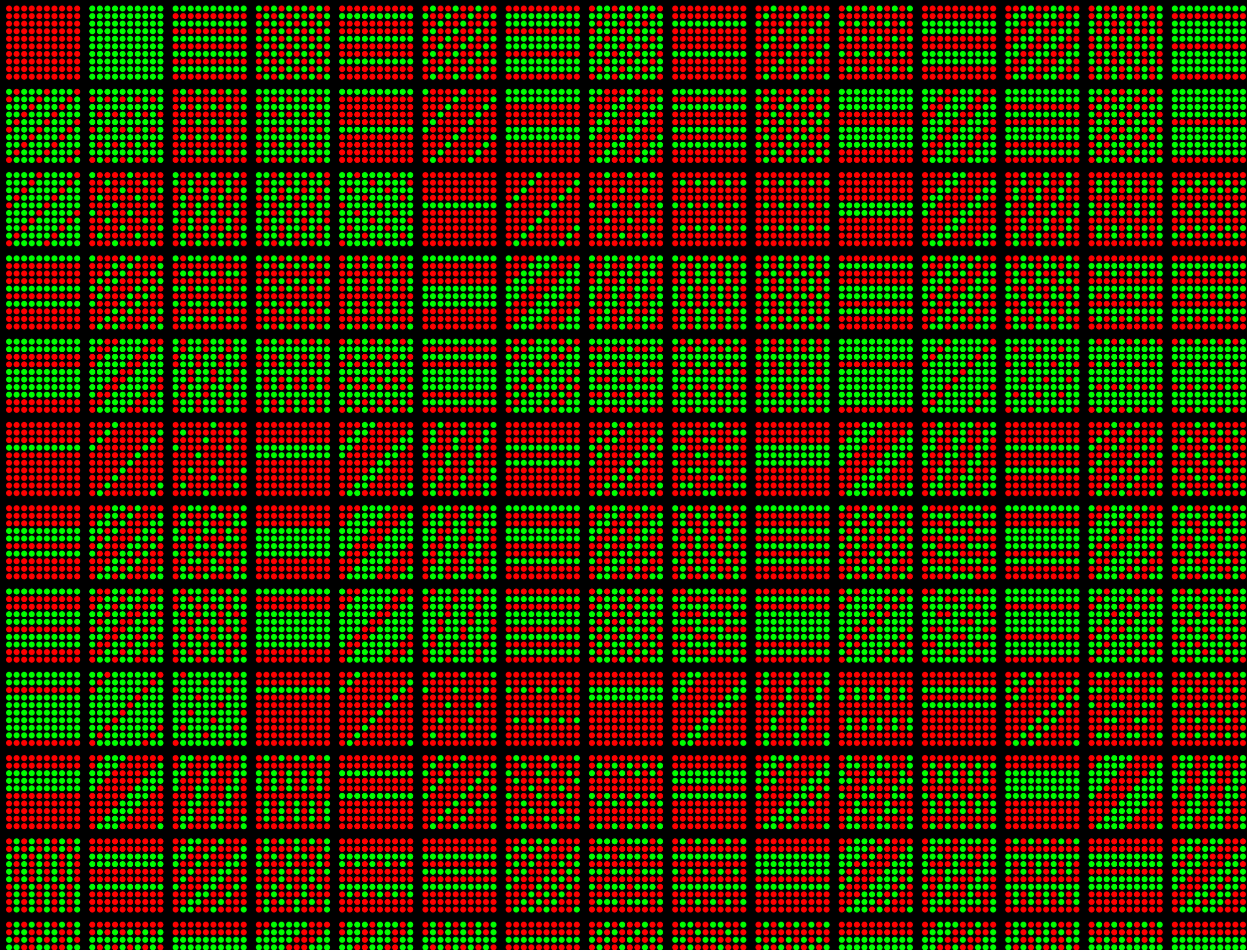
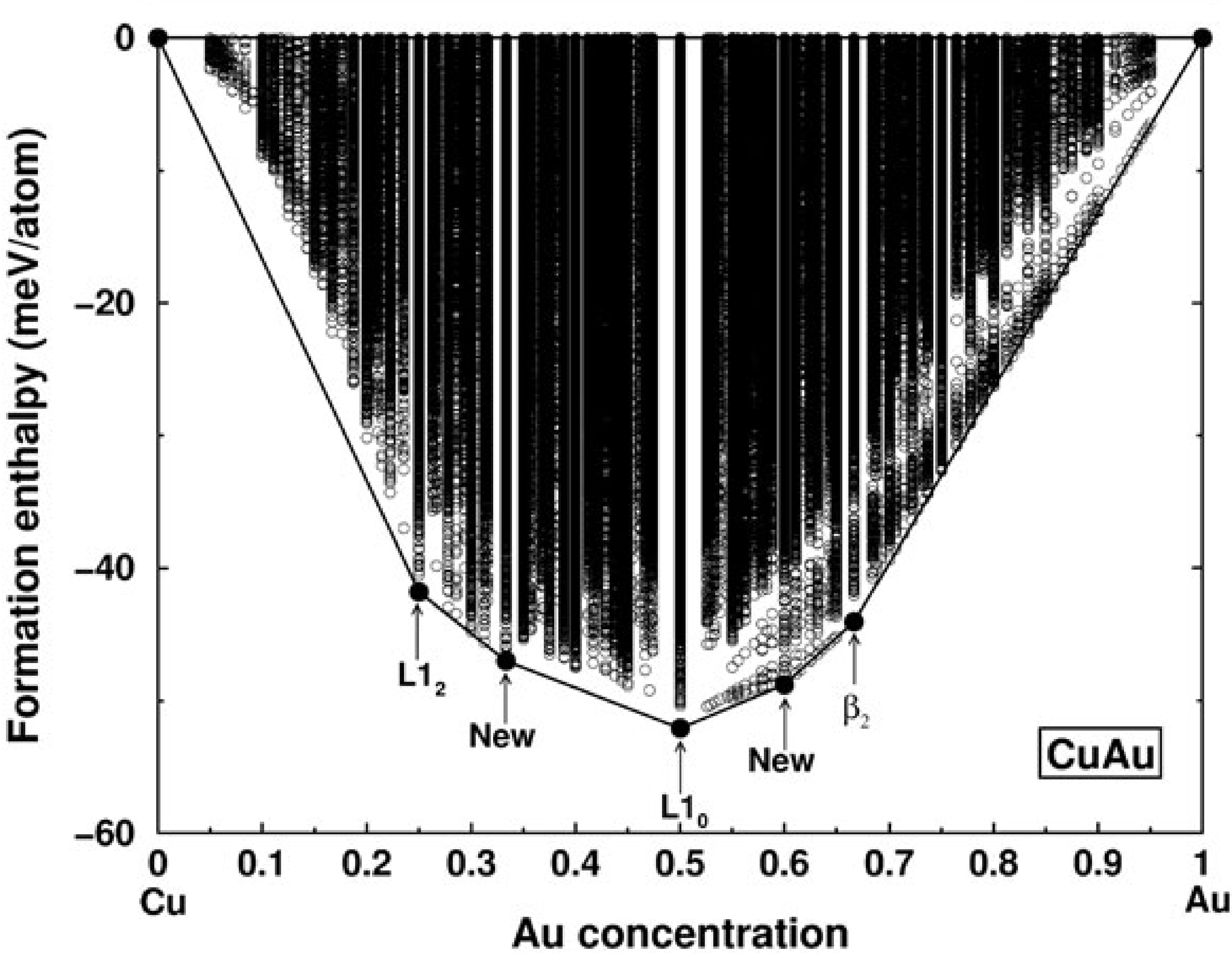
Gus L.W. Hart and Rodney W. Forcade, "Algorithm for enumerating derivative superstructures," Phys. Rev. B **77** 224115 (2008)

Gus L.W. Hart and Rodney W. Forcade, "Generating derivative structures from multilattices: Algorithm and application to hcp alloys," Phys. Rev. B **80** 014120 (2009)



Monday, July 18, 2011

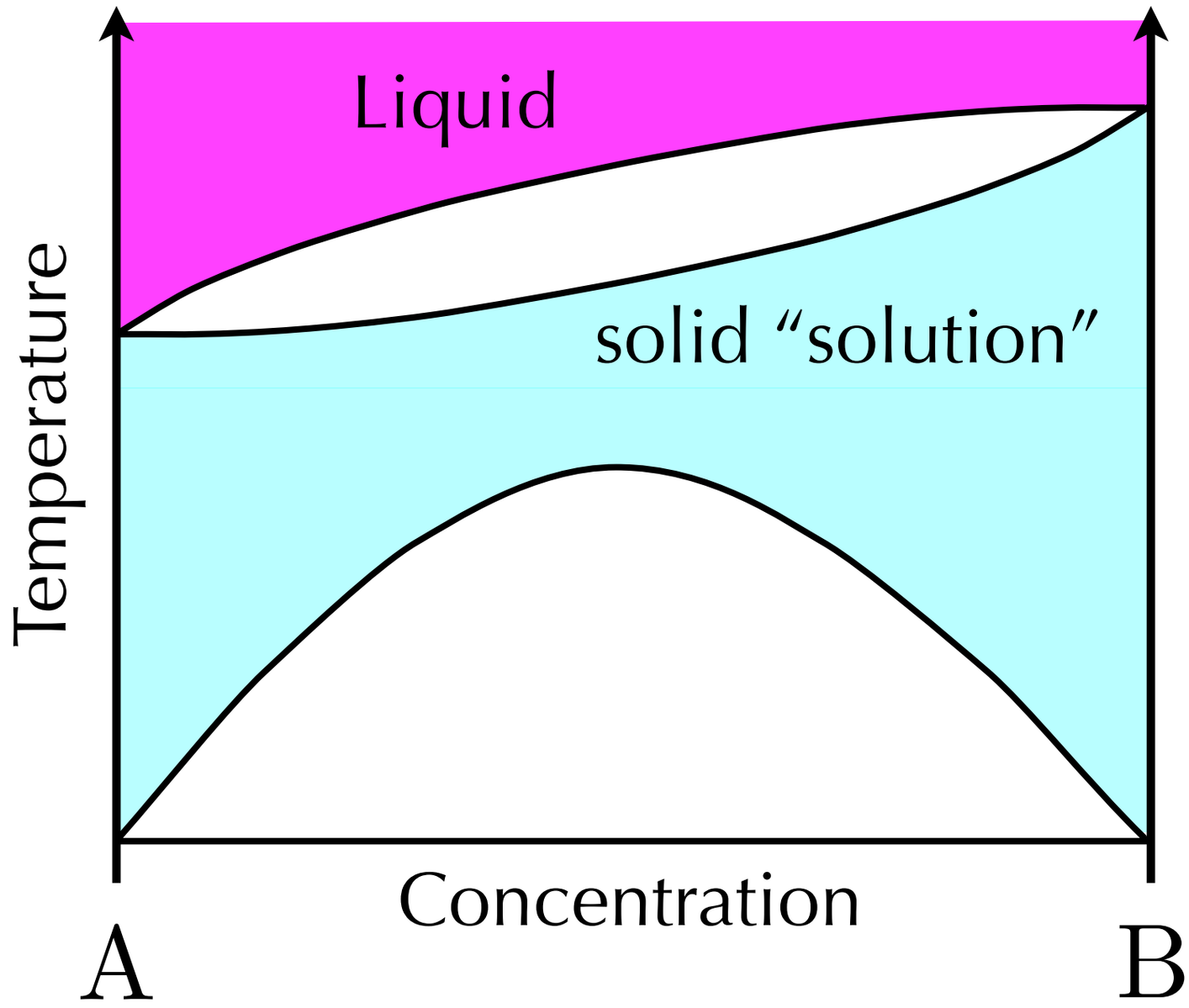

Formation enthalpy (meV/atom)
0
−20
−40
−60
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Cu
Au
Au concentration
L1$_2$
New
L1$_0$
New
β$_2$
CuAu

A ground state search

Tells us which configurations are lowest in energy, but doesn't tell us anything about how the materials behaves as a function of temperature...

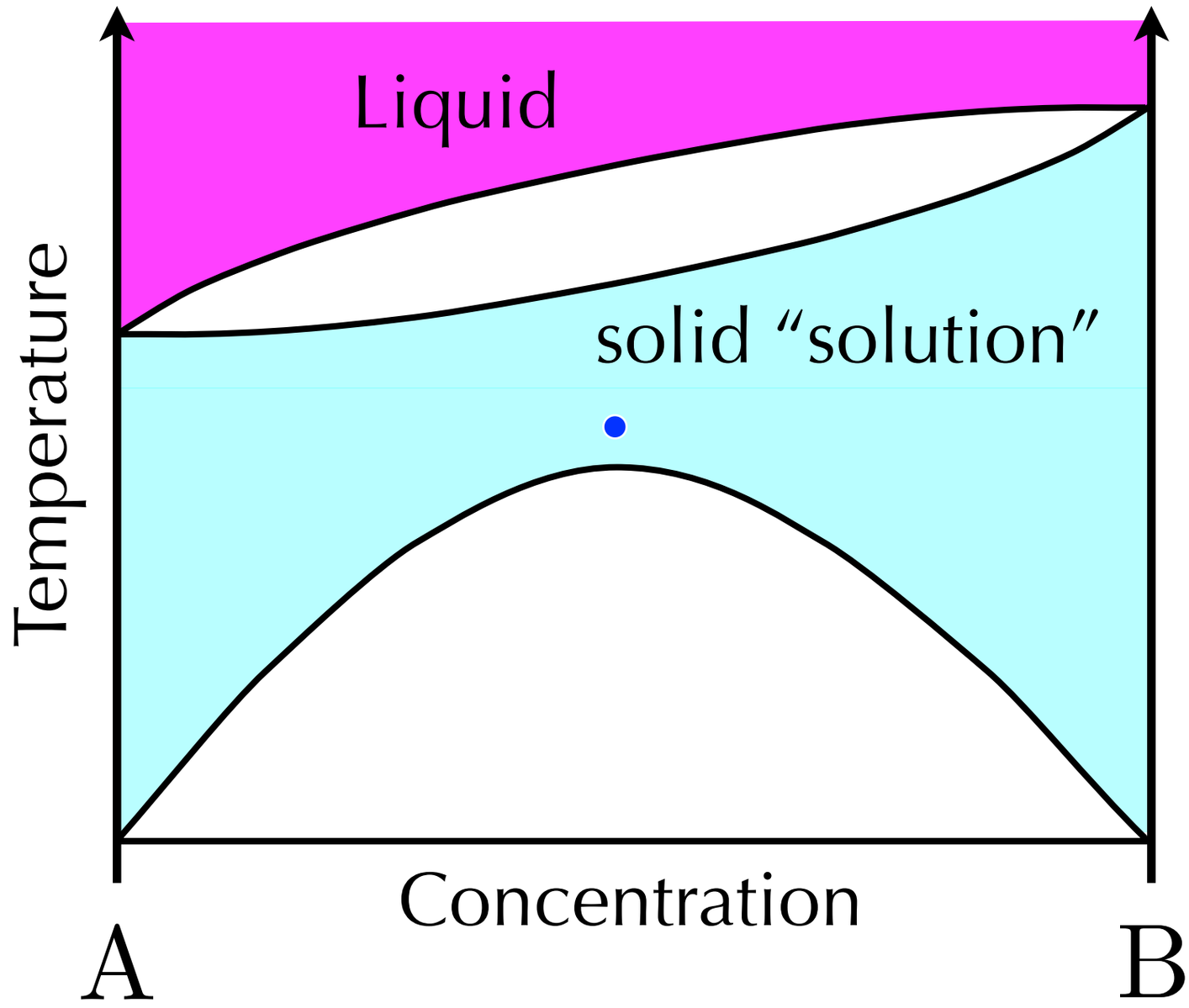
$$F = U - TS$$

Alloy phase diagrams



What happens as it cools?

- Phase diagrams



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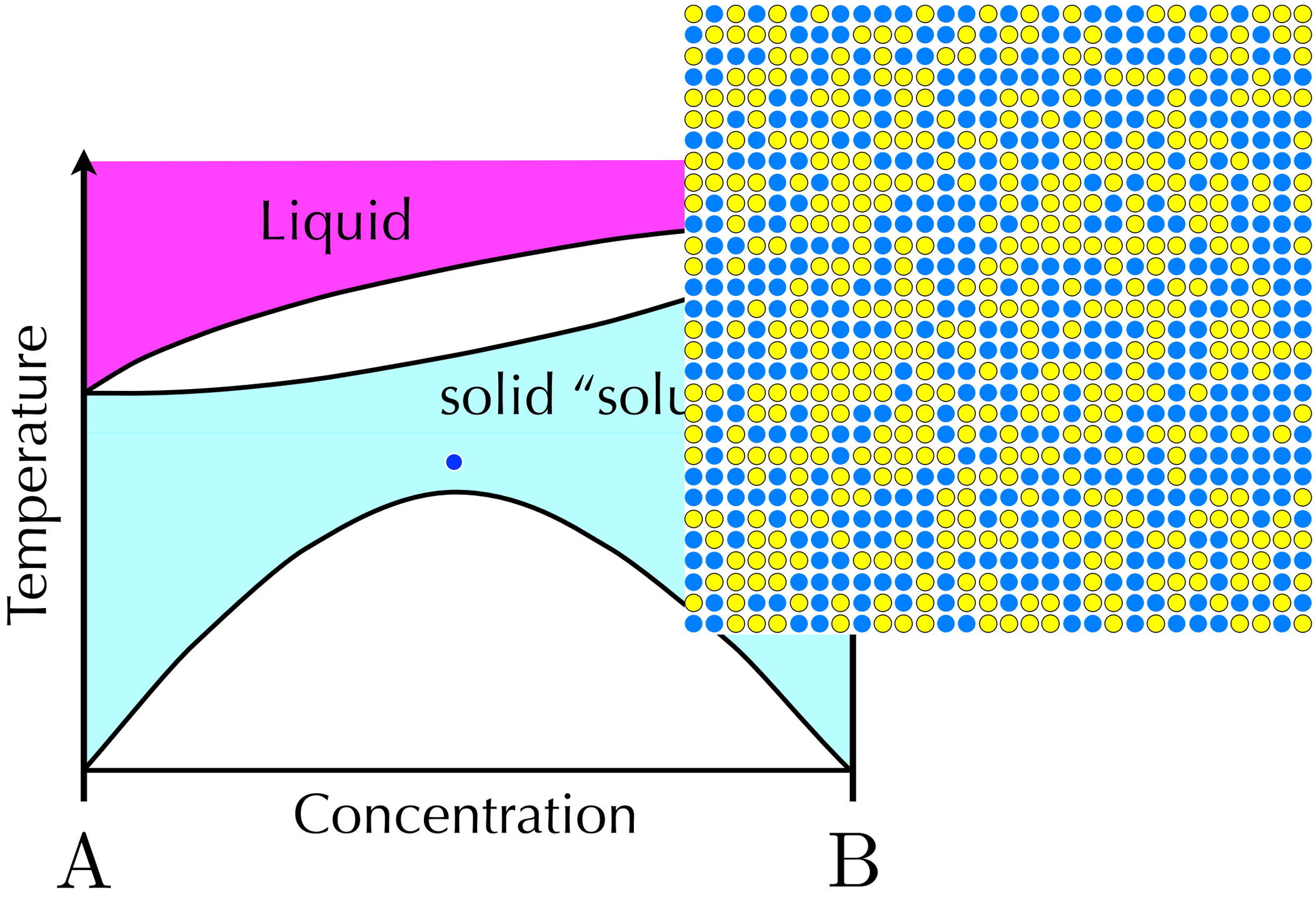

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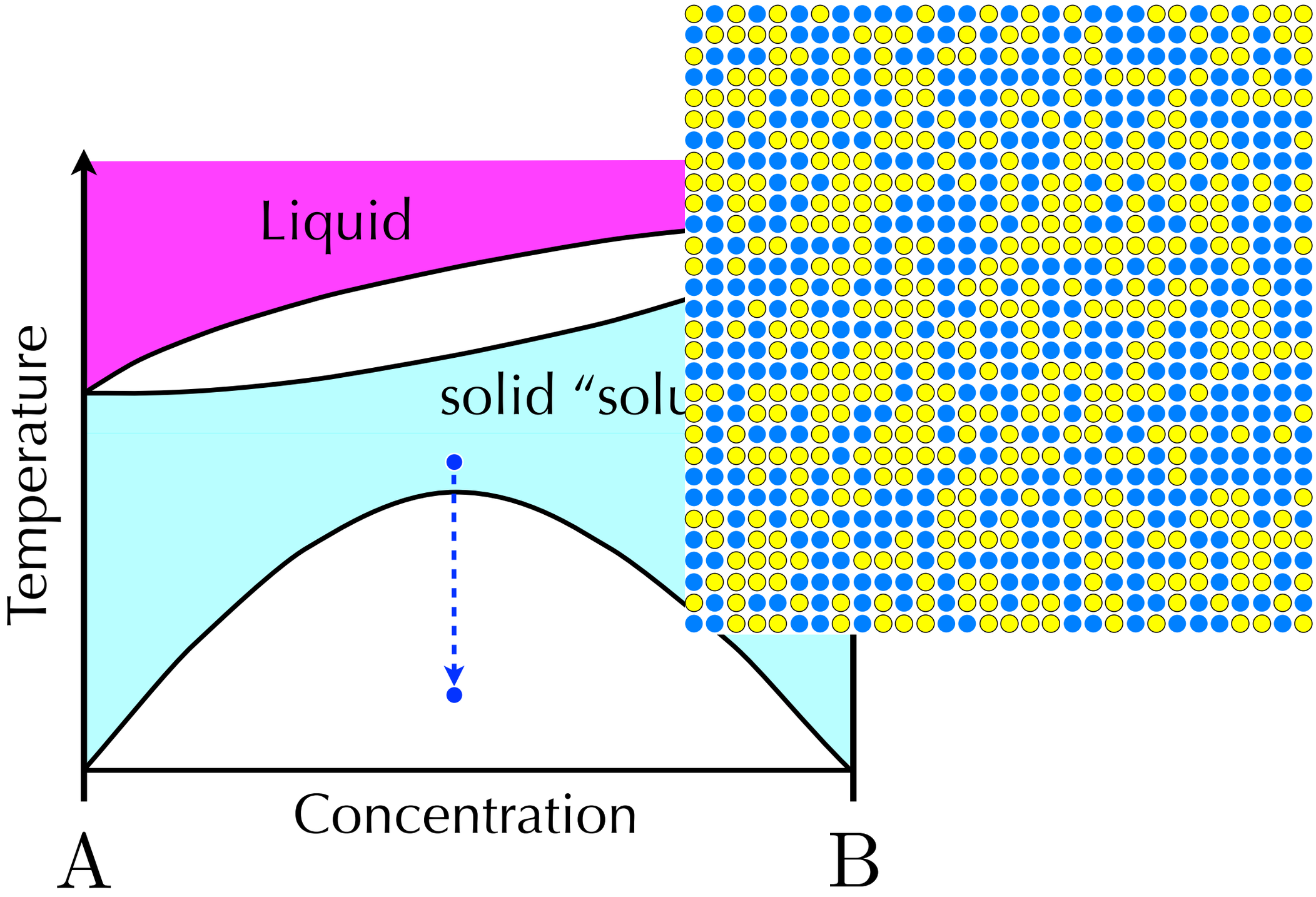

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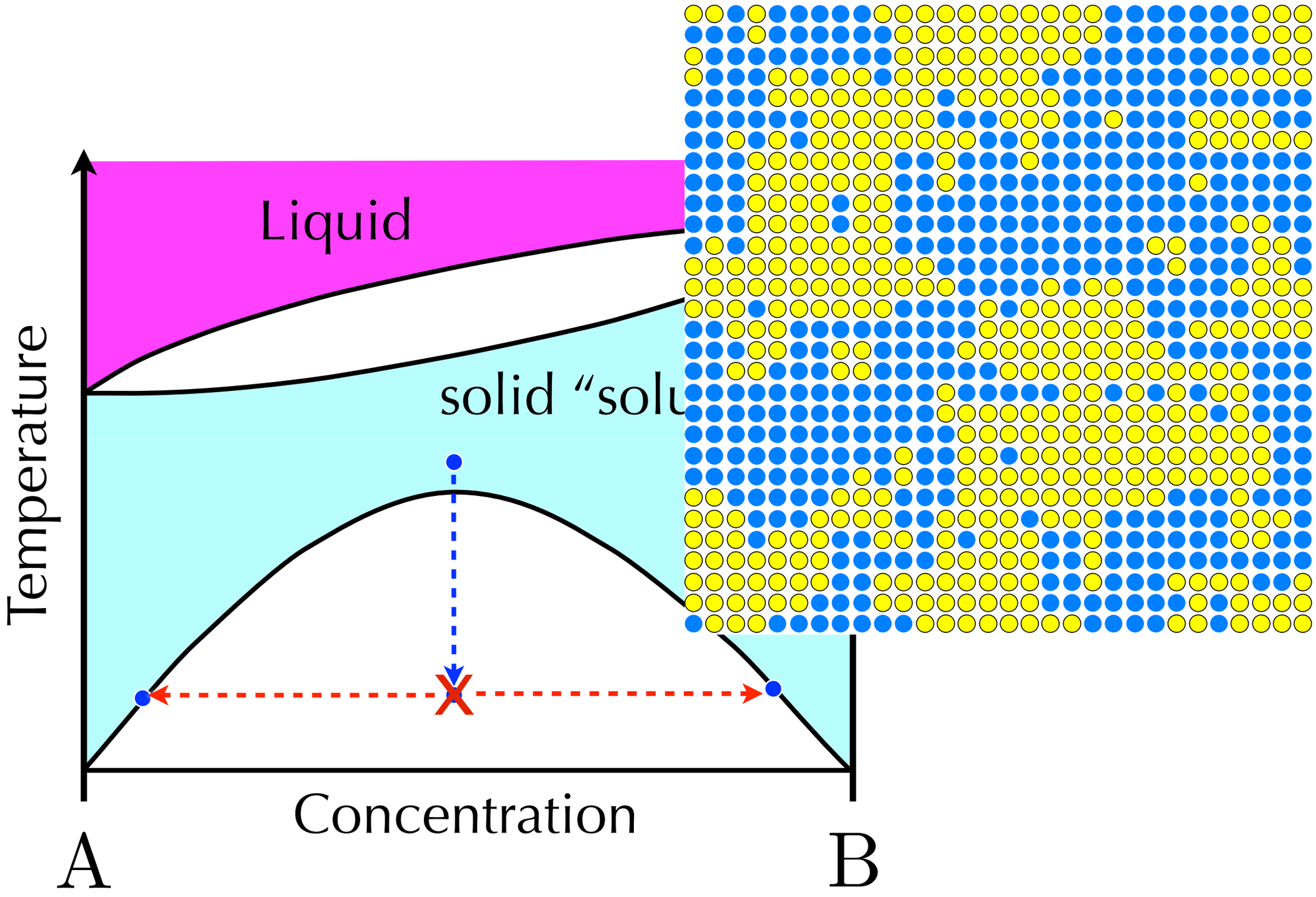
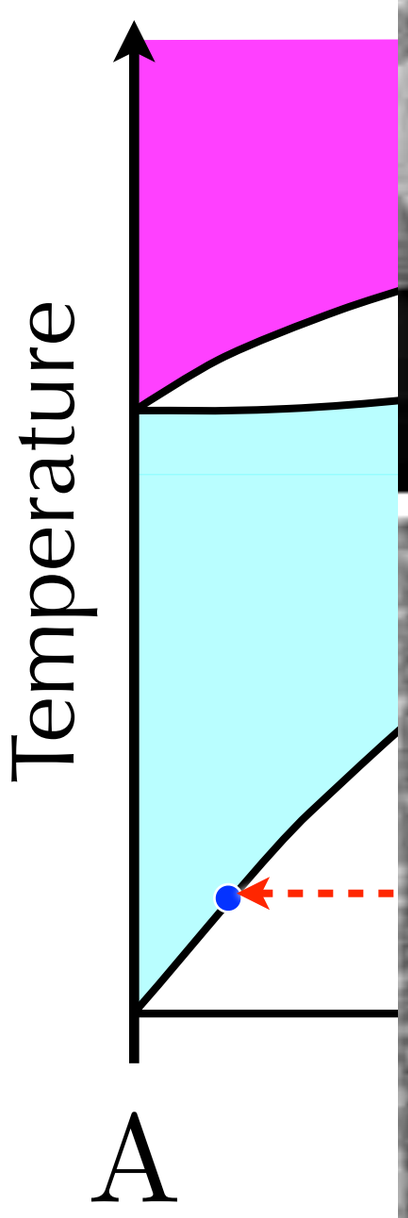
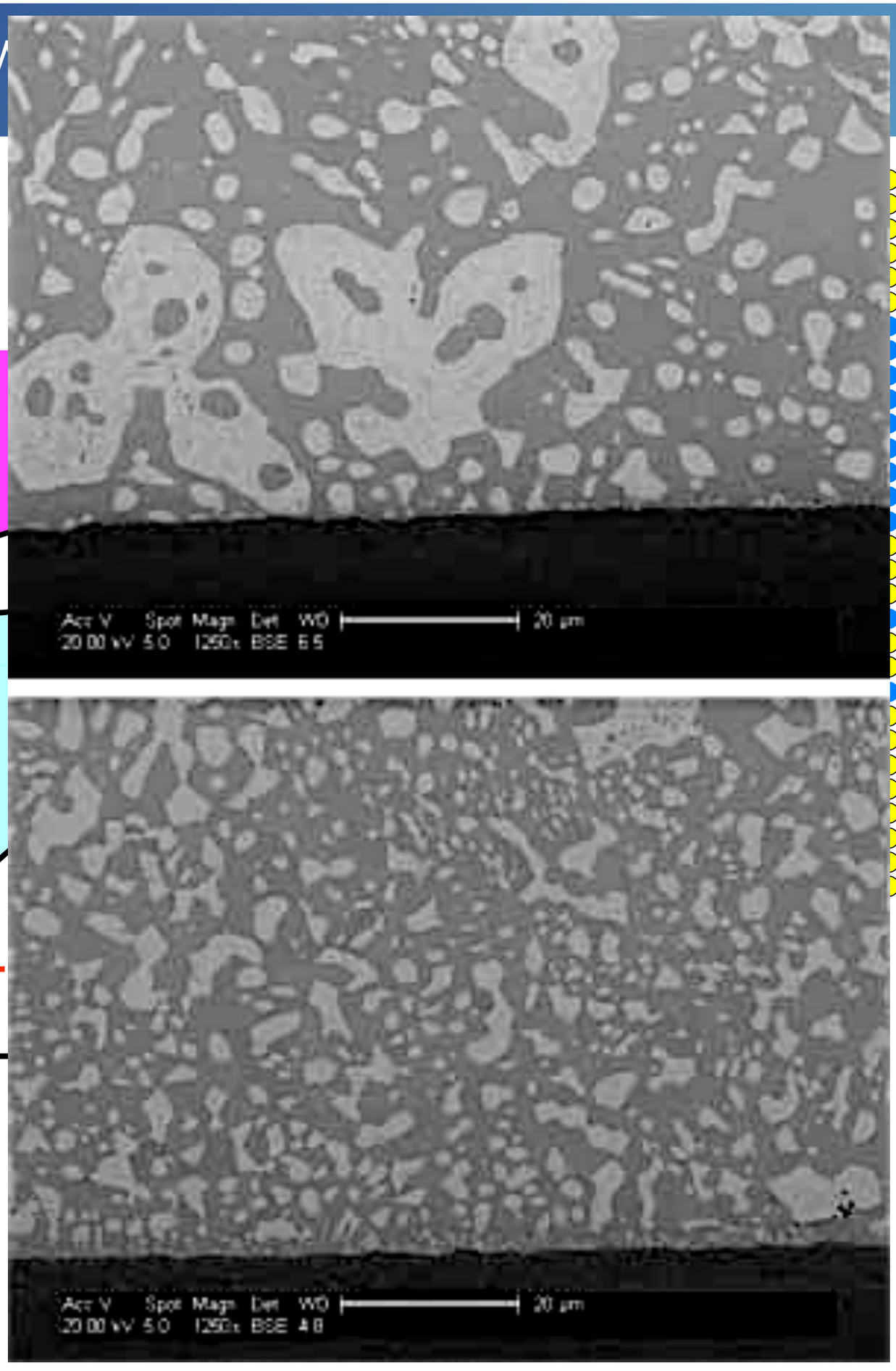
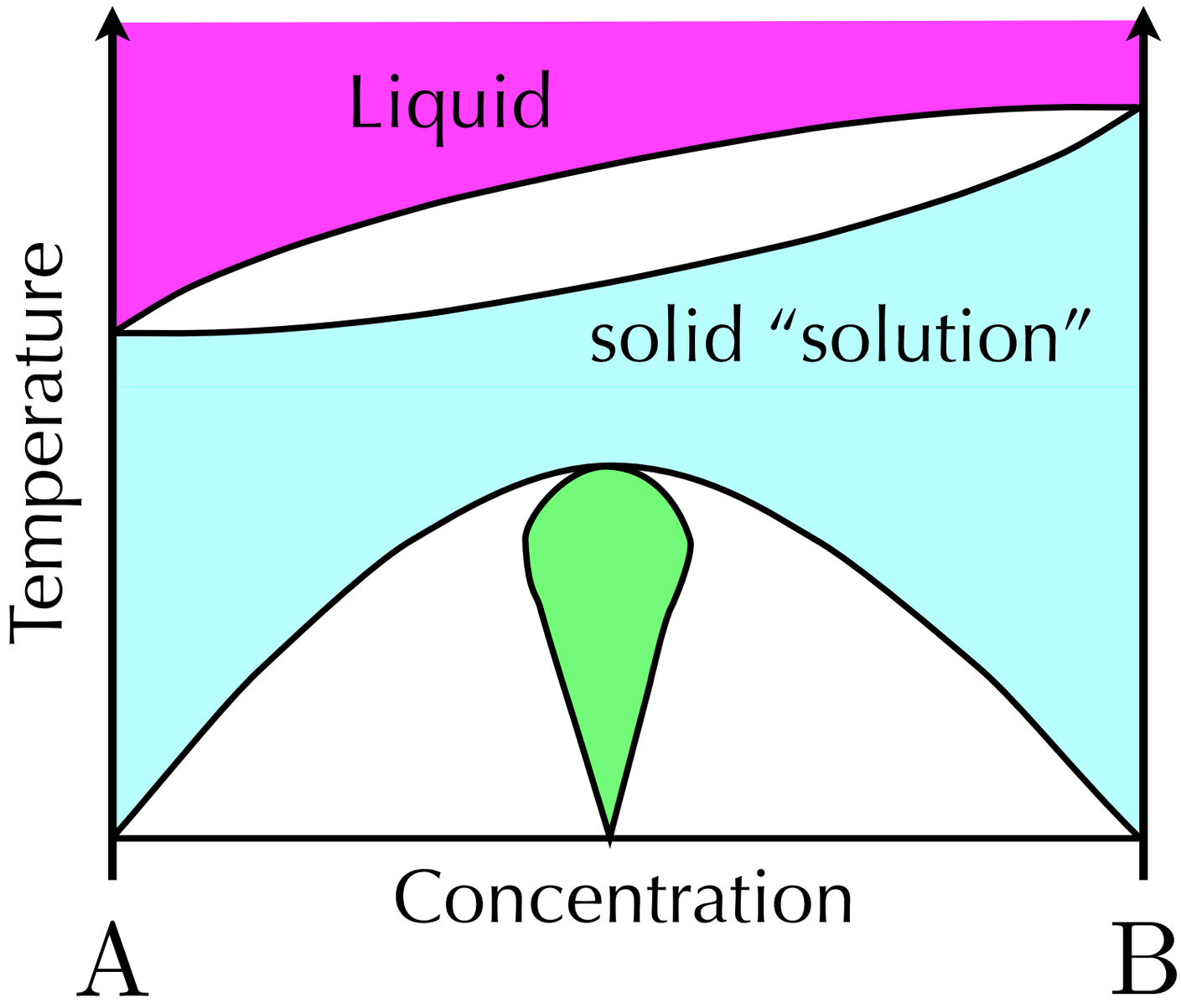


V

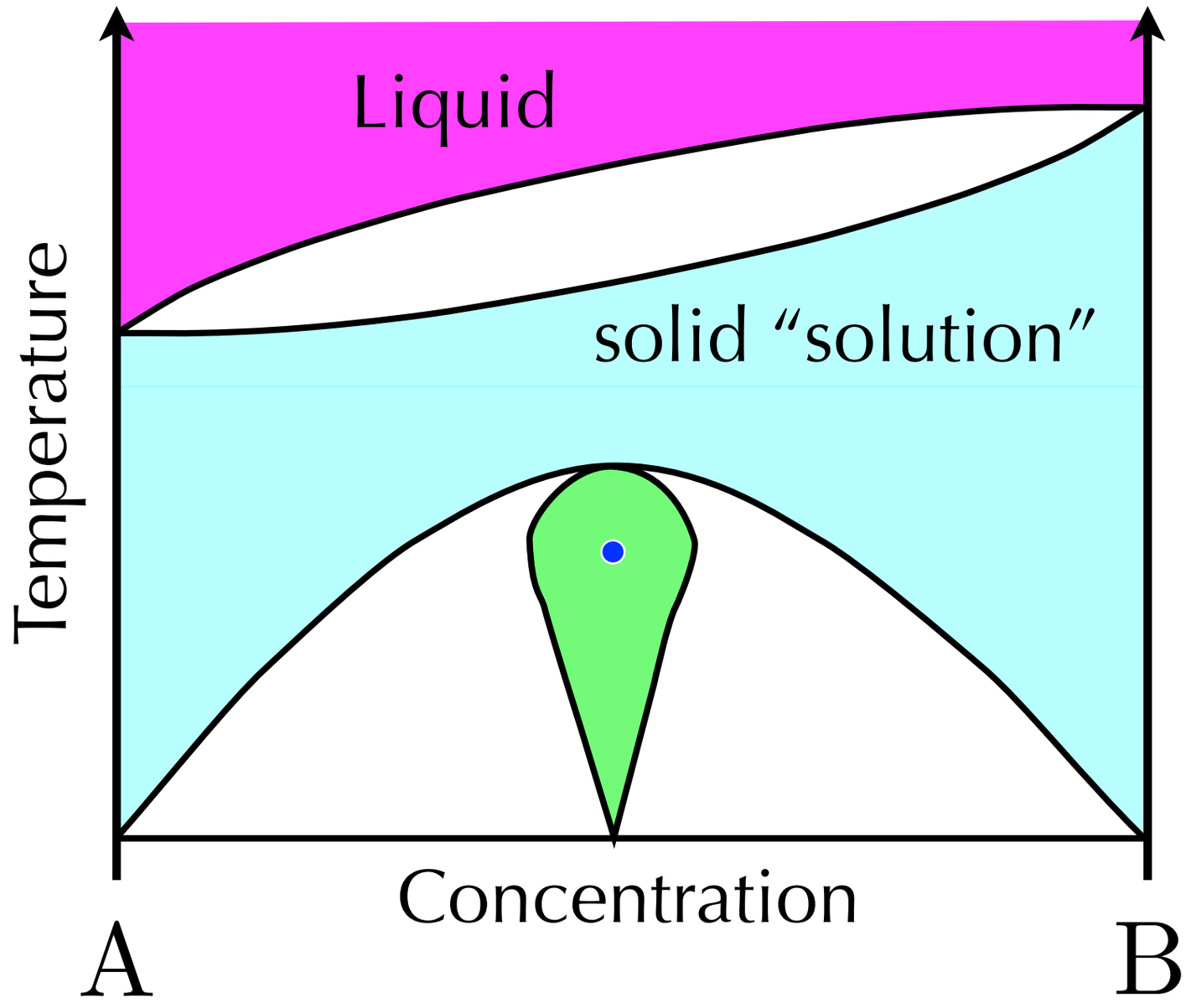

Temperature
A


Acc.V Spot Magn Det WD 20 µm
20.00 kV 5.0 1250x BSE 6.5
Acc.V Spot Magn Det WD 20 µm
20.00 kV 5.0 1250x BSE 4.8

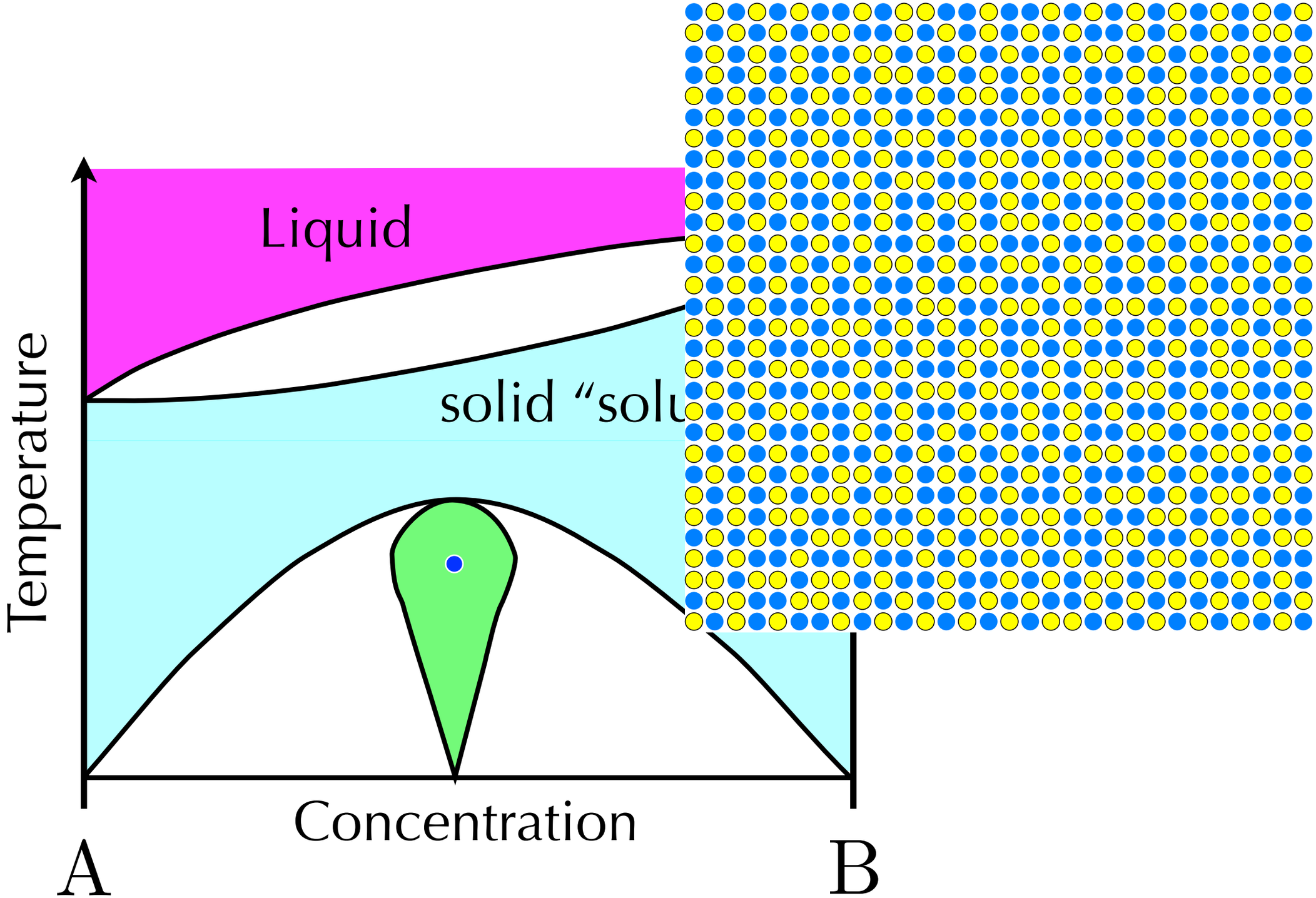
Alloy phase diagrams: Ordering

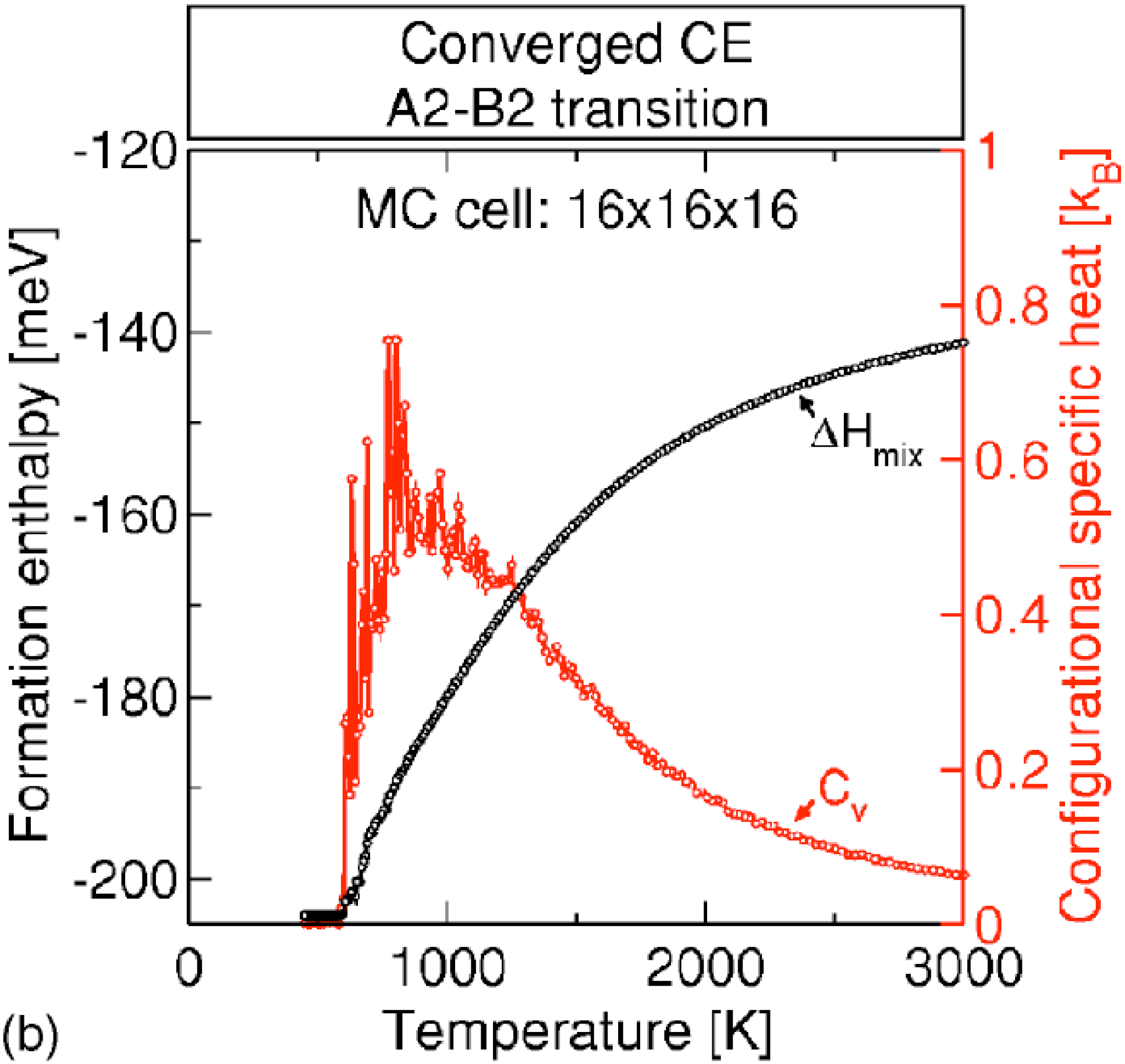


Alloy phase diagrams: Ordering



Alloy phase diagrams: Ordering




Converged CE
A2-B2 transition
MC cell: 16x16x16
Formation enthalpy [meV]
-120
-140
-160
-180
-200
ΔH_mix
C_v
Configurational specific heat [k_B]
1
0.8
0.6
0.4
0.2
0
0
1000
2000
3000
Temperature [K]
(b)

Recap: with a fast lattice Hamiltonian we can...

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1. Search for new phases (try millions of trial configurations) **Ground State Search**

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2. Apply thermodynamic modeling (to identify phase transitions) **Monte Carlo**

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1. Search for new phases (try millions of trial configurations) **Ground State Search**

2. Apply thermodynamic modeling (to identify phase transitions) **Monte Carlo**

3. Build a kinetic simulation (to model time evolution) **Kinetic MC**

PAULING FILE

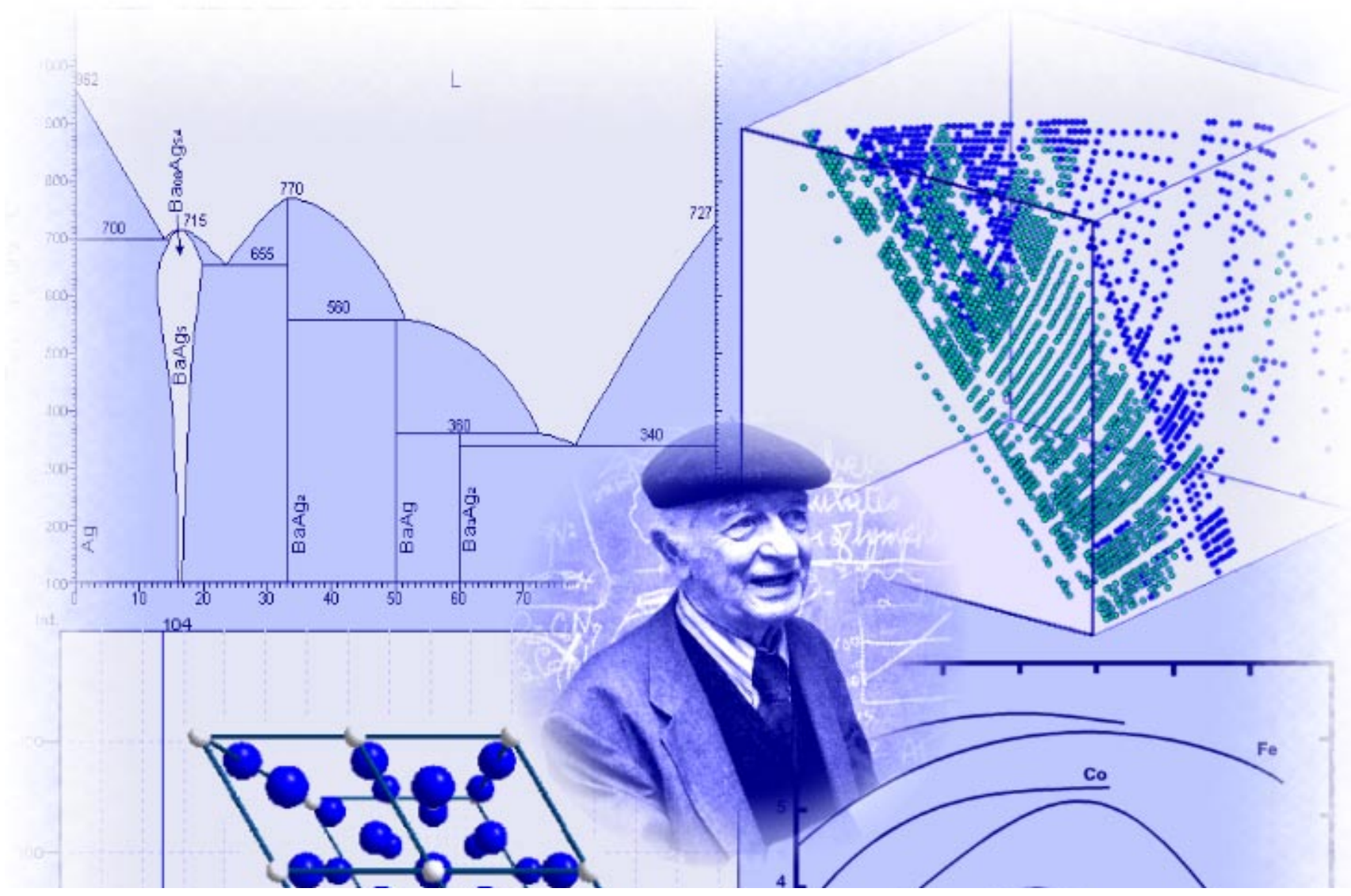
Inorganic Materials Database and Design System

Editor-in-chief: P. Villars

Section editors: K. Cenzual, J.L.C. Daams, F. Hulliger, T.B. Massalski, H. Okamoto, K. Osaki, A. Prince†

Project coordinator: S. Iwata

Software development: Crystal Impact



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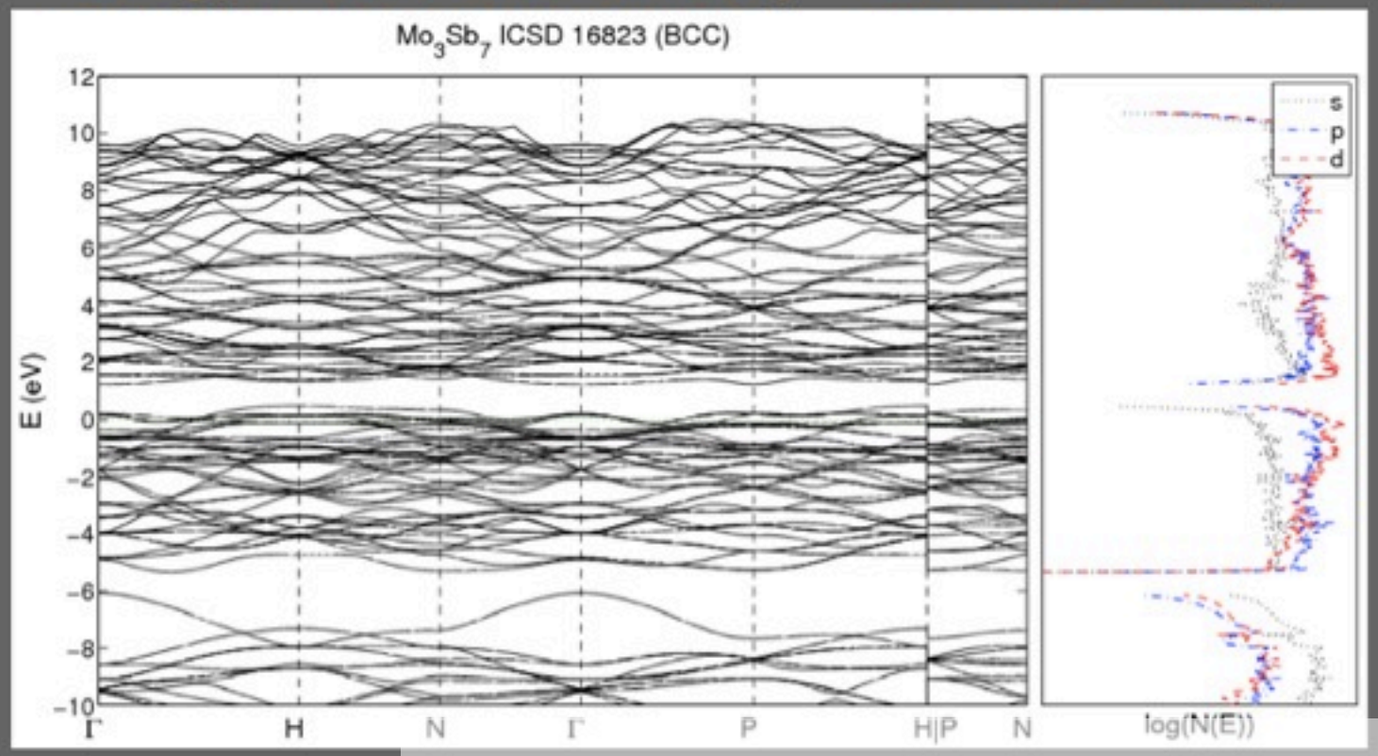
700 binary x ~200 structures
~20 million cpu hours

Energy Materials Laboratory - Curtarolo Group



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S. Curtarolo W. Setyawan S. Wang K. Taylor J. Xue O. Levy

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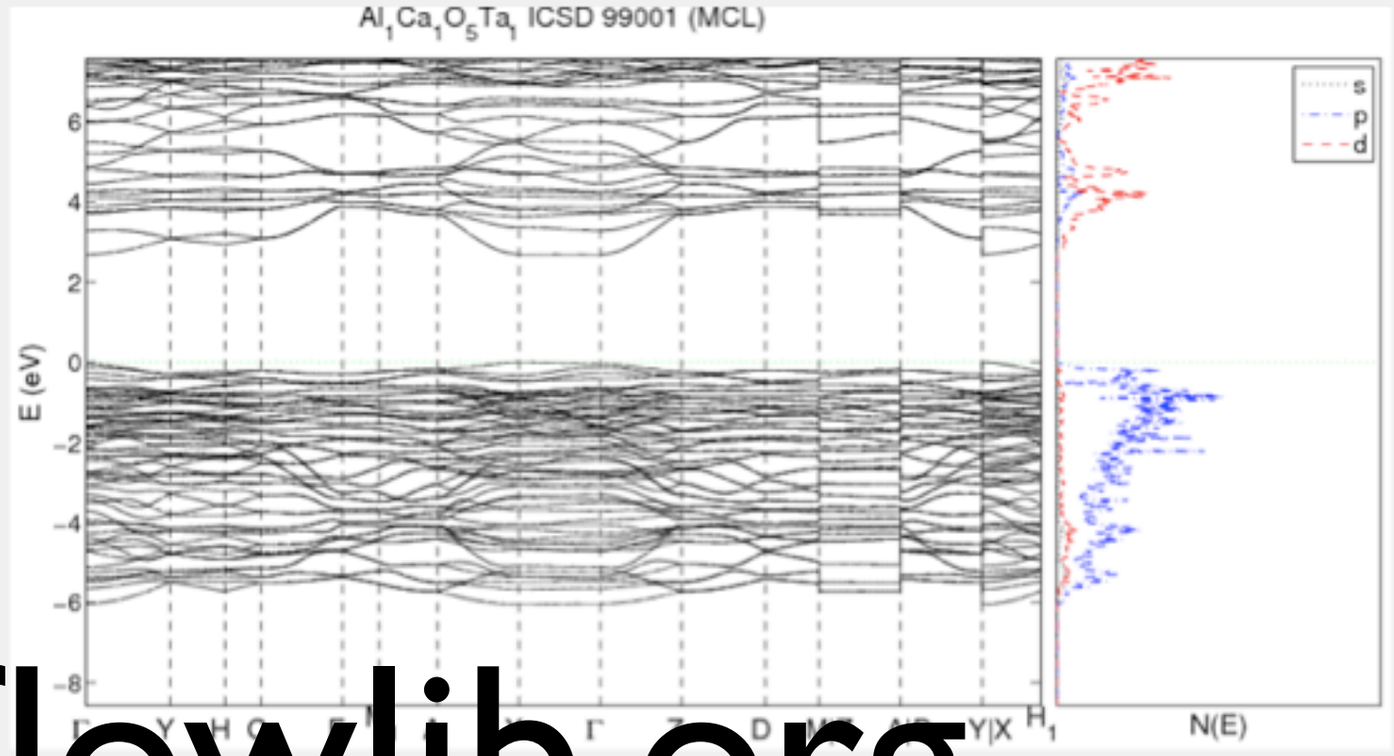
CHOOSE DATABASES

☑ Structure Properties ☐ *Electronic Properties* ☐ *Thermoelectric Properties* ☐ *Scintillator Database* ☐ *Magnetic Properties*

SEARCH AFLOWLIB (9000 COMPOUNDS)

Index	▲Name	ICSD Number	Bravais Lattice	Atom Number	Space Group Number	Pearson Symbol	Band Gap (eV)	Fit Band Gap (eV)	m_e (m_0)	m^{min}_e (m_0)	m_h (m_0)	m^{min}_h (m_0)	Mass ratio	Valence Band Width (eV)	Core Valence Gap (eV)	Density (g/cm^3)	Proto Name
1	$Al_1Ca_1O_5Ta_1$	99001	MCL (Monoclinic)	32	14 (P121/n1)	mP32	2.68 (I)	4.53	6.66	0.41	2.85	0.96	2.33	6.05	9.11	5.45	Al1Ca1O5Ta1_ICSD_99001



Lattices: a = 7.40Å b = 7.97Å c = 7.71Å
α = 68.69° β = 90.00° γ = 90.00°

Volume: 423.76Å^3

Unit Cell Atom Number: 32

Space Group Number: 14
Pearson Symbol: mP32
Lattice Primitive: MCL
Lattice Variation: MCL
Crystal Family: Monoclinic
Crystal System: Monoclinic
Crystal Class: Monoclinic-prismatic

Point Group (Hermann Mauguin): 2/m
Point Group (Schoenflies): C$_{2h}$
Point Group Orbifold: 2*
Point Group Type: centrosymmetric
Point Group Order: 4
Point Group Structure: 2 X Cyclic

Superlattice Primitive unit cell: MCL
Superlattice Variation: MCL
Pearson Symbol Superlattice: monoclinic

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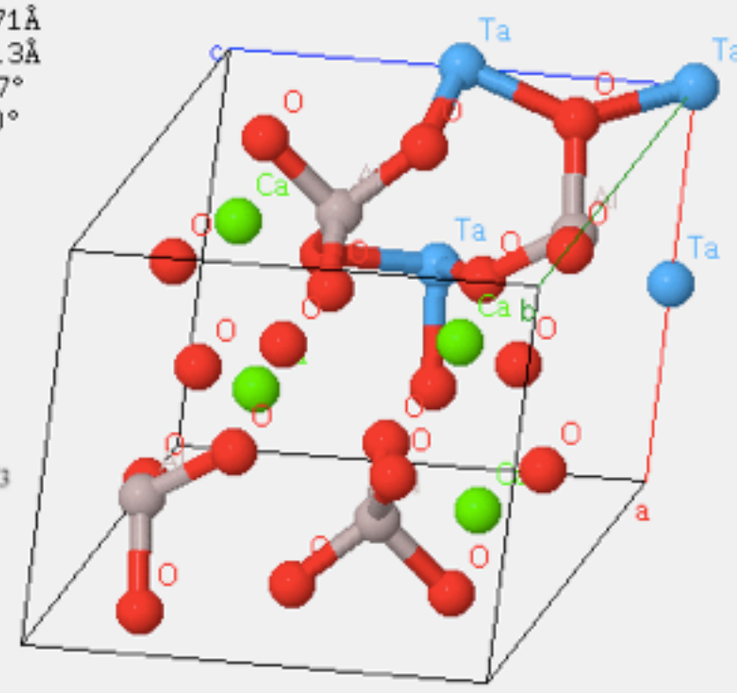
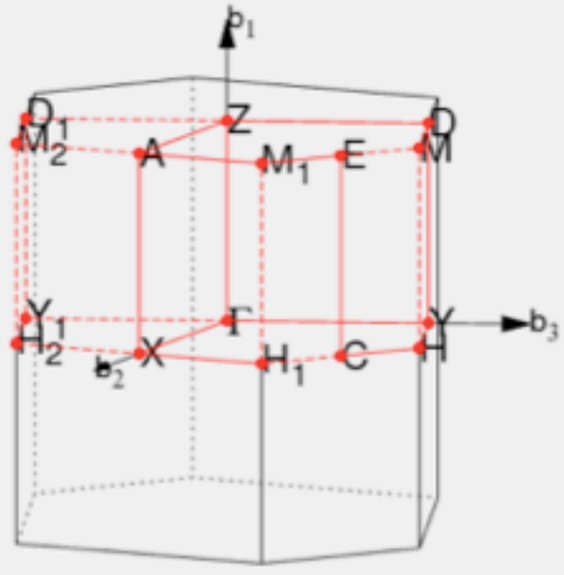
a=7.399Å
b=7.971Å
c=7.713Å
α=68.7°
β=90.0°



Reciprocal Space Lattices

Reciprocal Lattices: a = 0.85Å b = 0.85Å c = 0.87Å
α = 111.31° β = 90.00° γ = 90.00°

Volume: 0.59 Å^{-3}
Lattice Primitive: MCL
Lattice Variation: MCL



MCL path: Γ-Y-H-C-E-M_1-A-X-Γ-Z-D-M|Z-A|D-Y|X-H_1