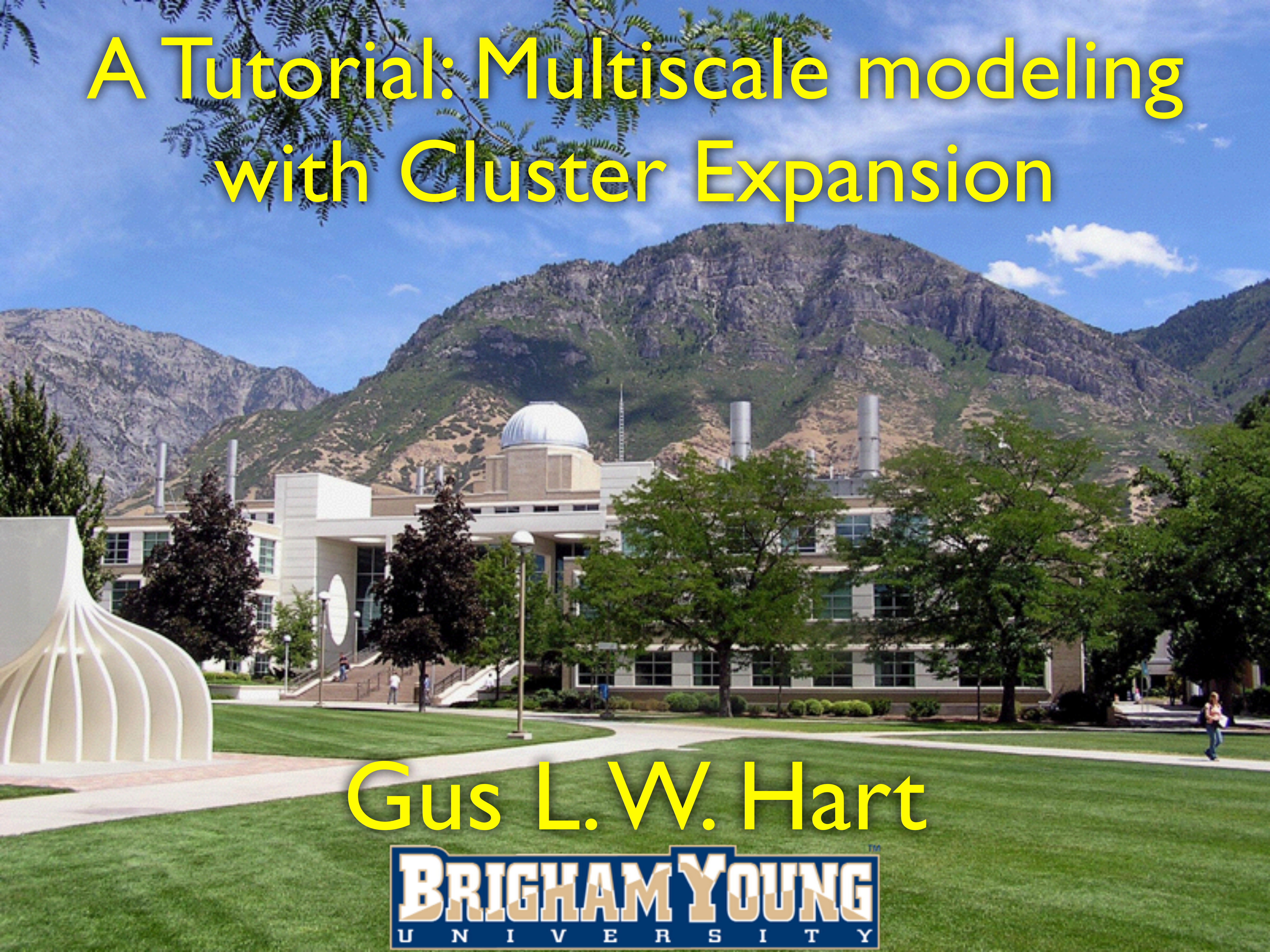
# A Tutorial: Multiscale modeling with Cluster Expansion

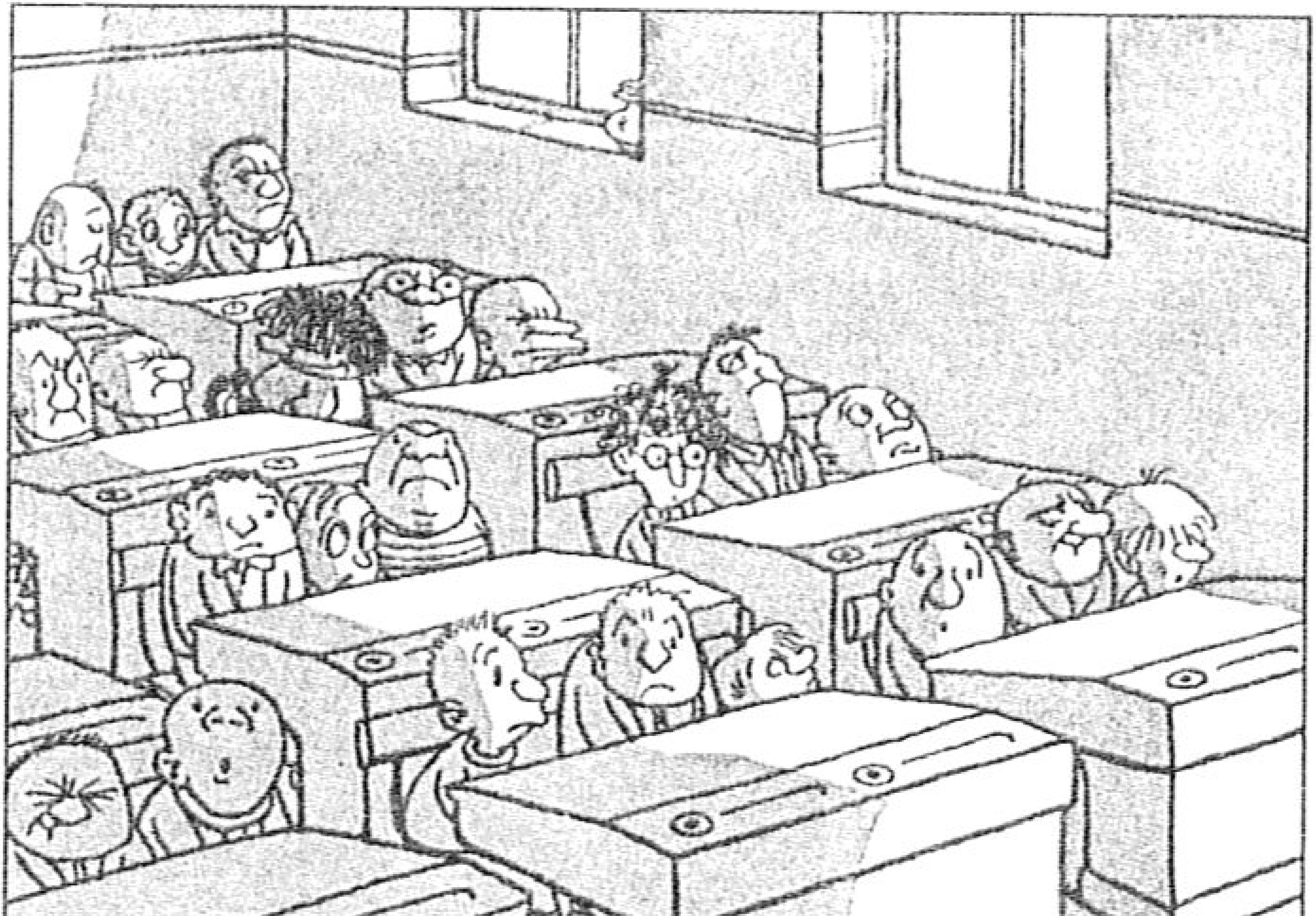


Gus L. W. Hart

Brigham Young University


A Tutorial:

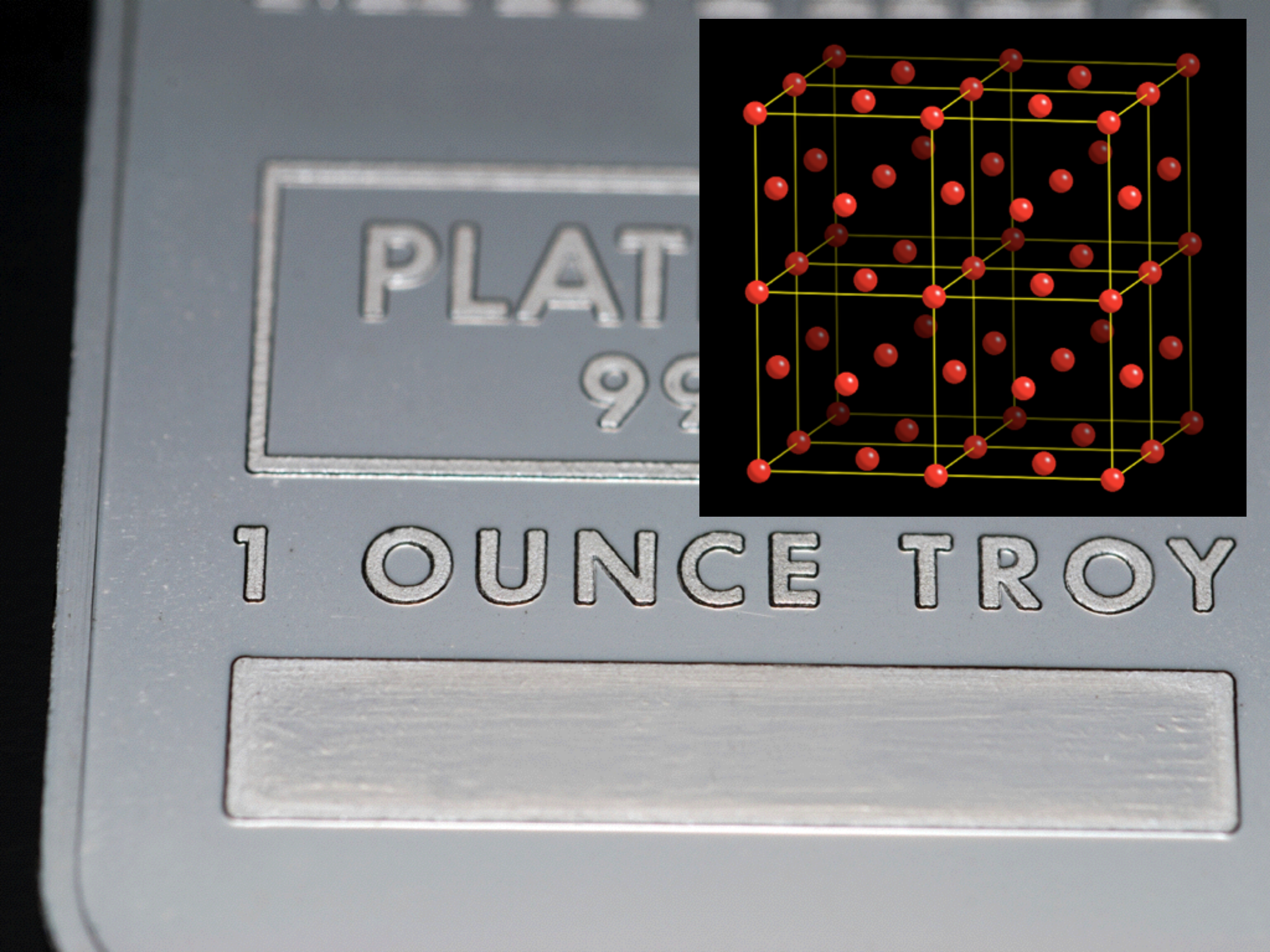
# A Tutorial



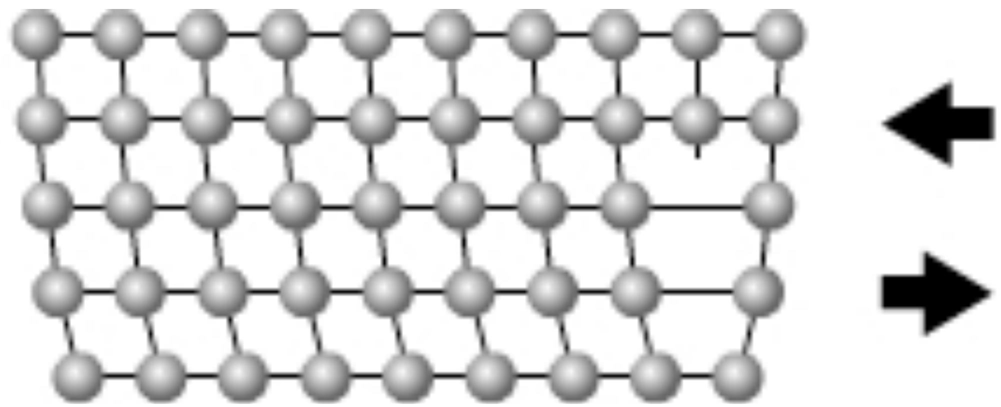
# A Tutorial

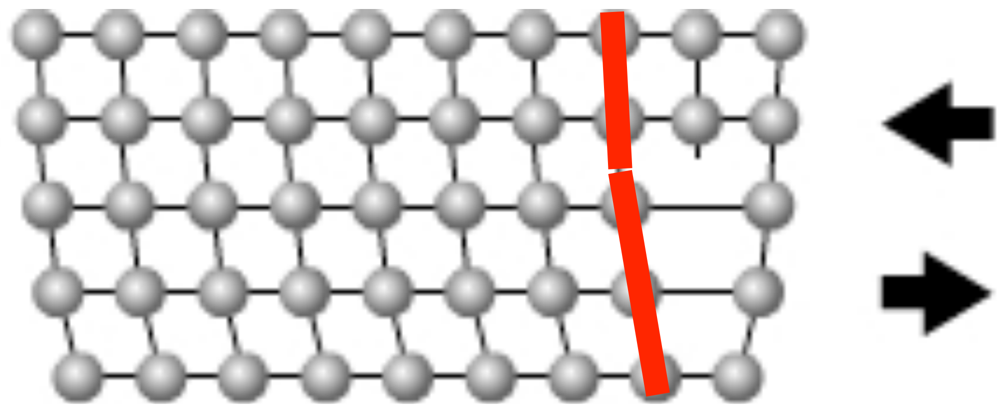

# Interrupt me, please!

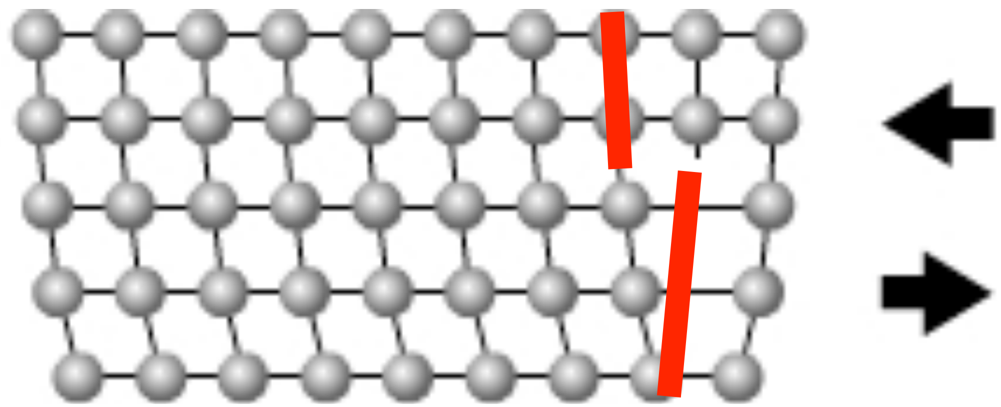

PLATINUM
9995
1 OUNCE TROY

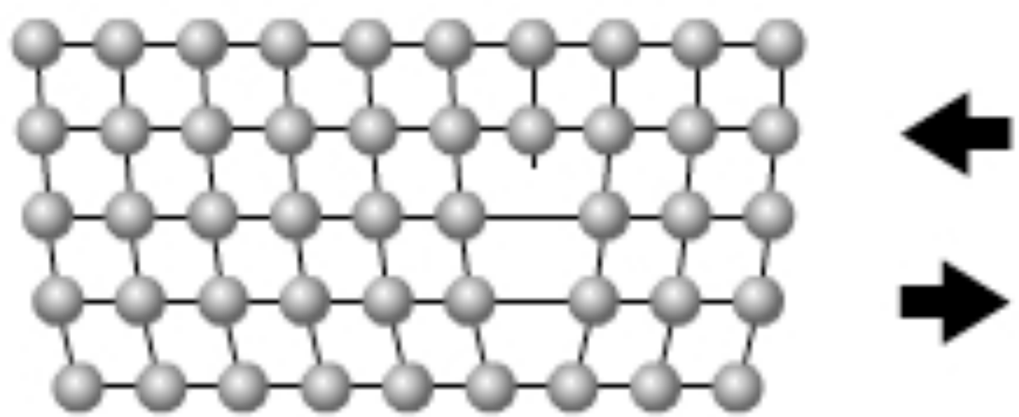

1 OUNCE TROY

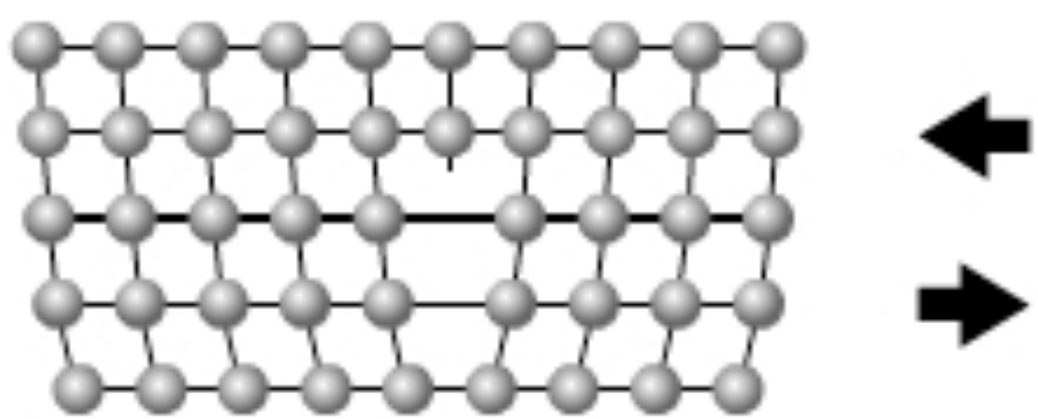
# What makes a metal “soft”?

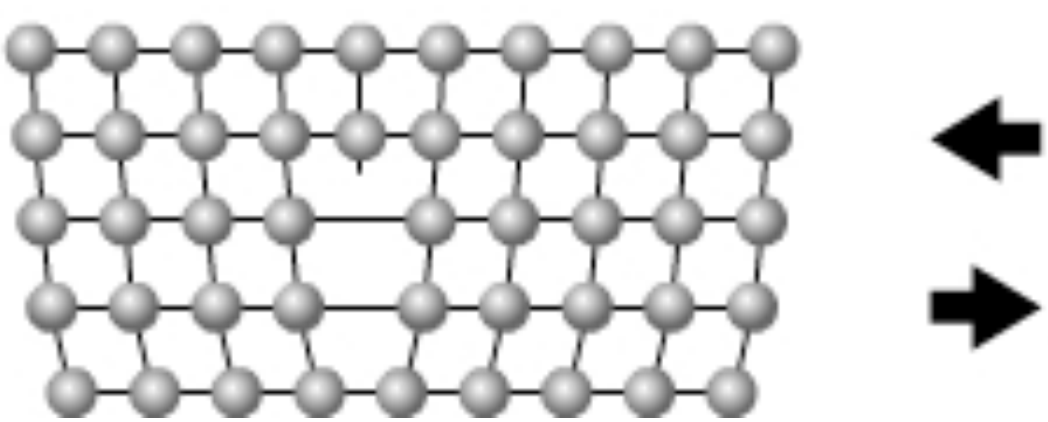


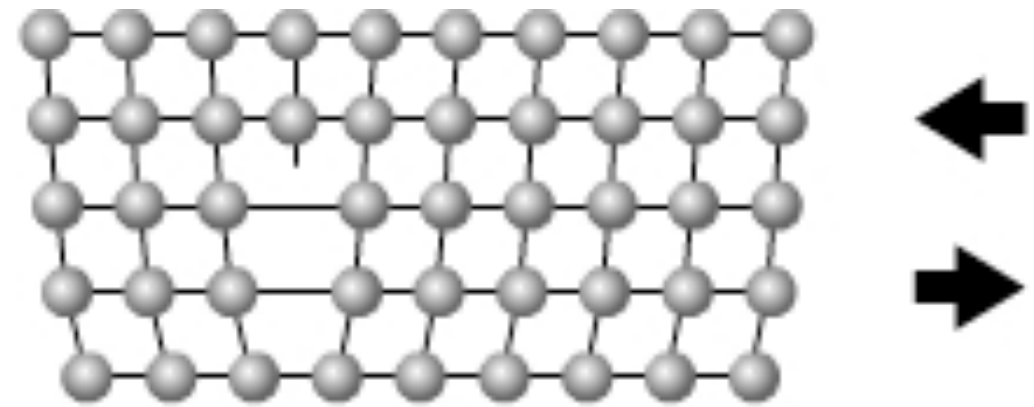


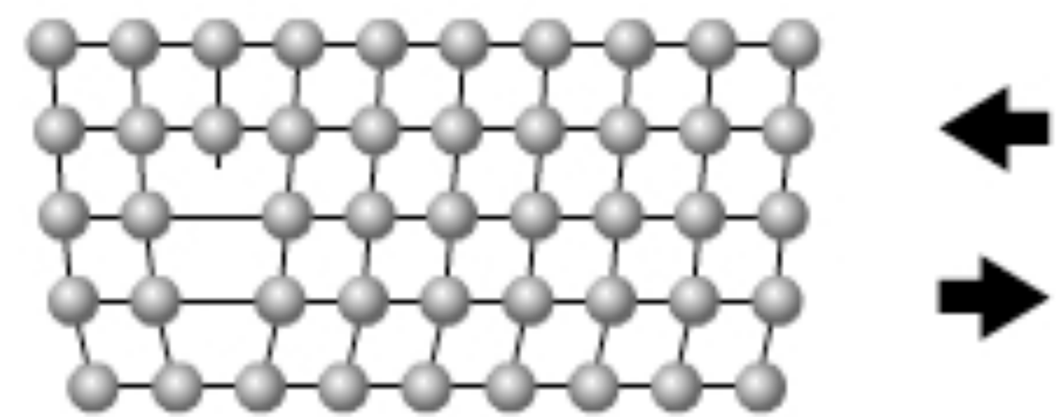


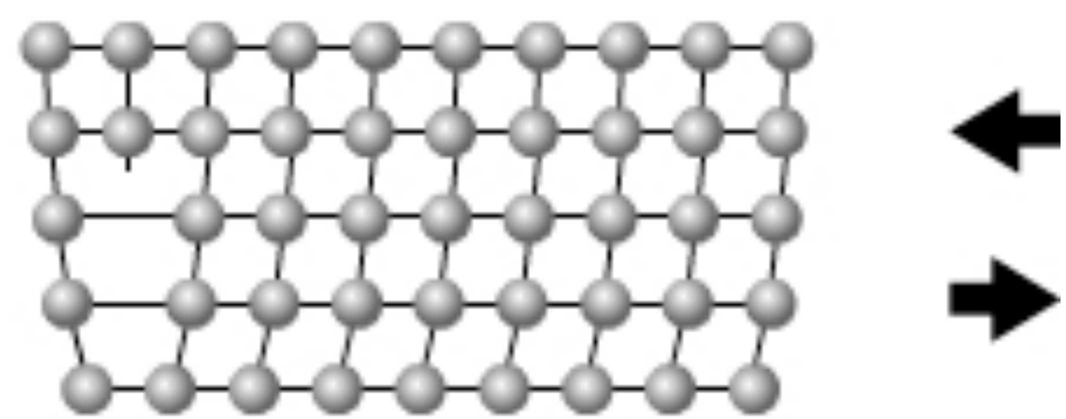


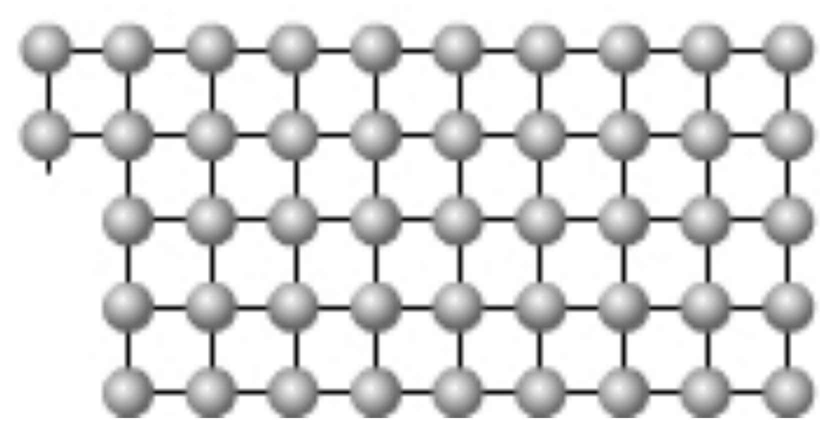




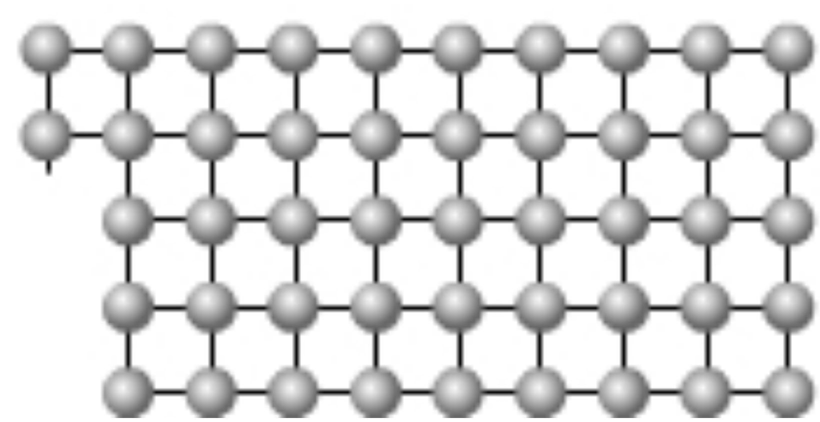




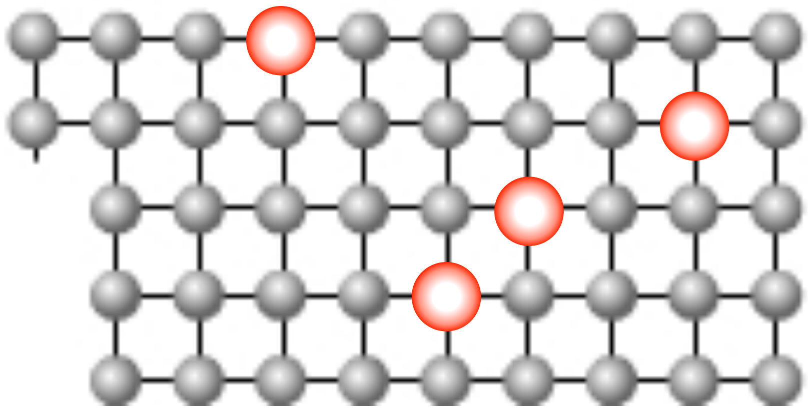




Dislocation motion leads to plastic deformation

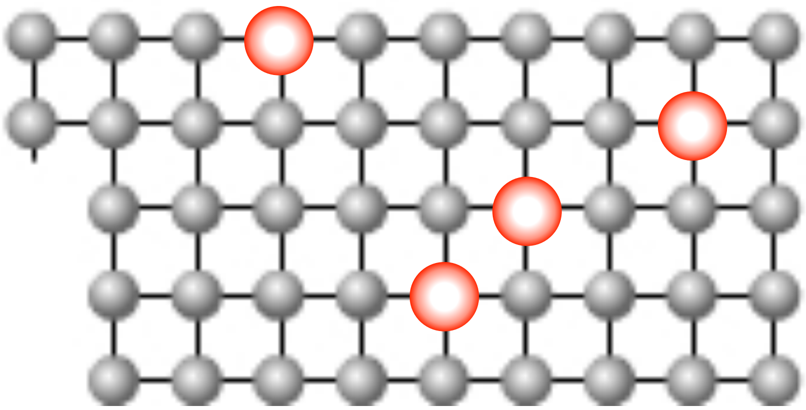


Dislocation motion leads to plastic deformation

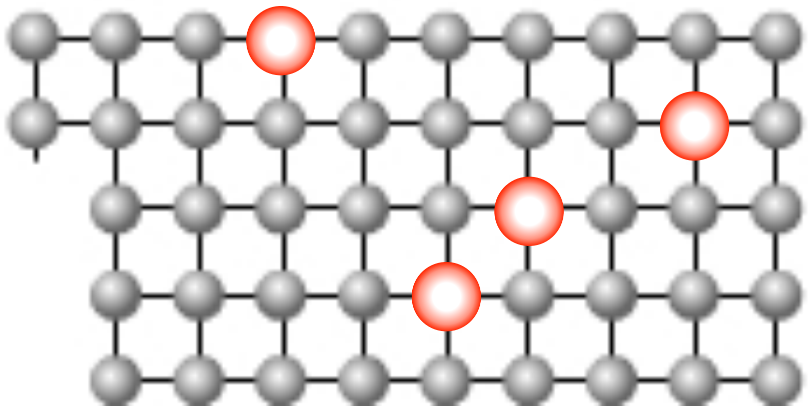


Dislocation motion leads to plastic deformation

Forming a solid solution inhibits dislocations



$$\leq 5\%$$



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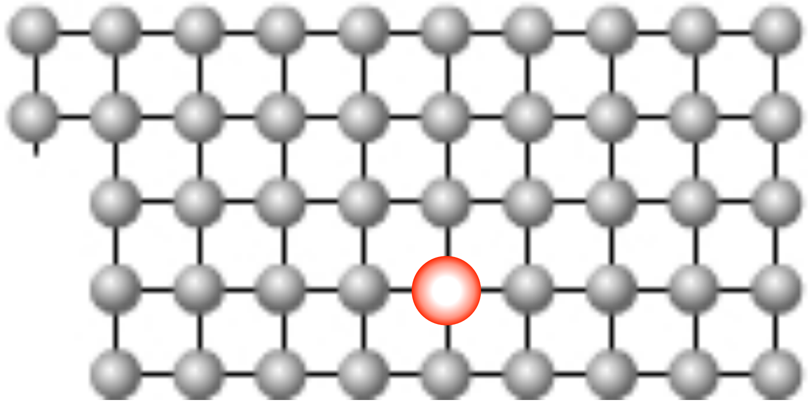
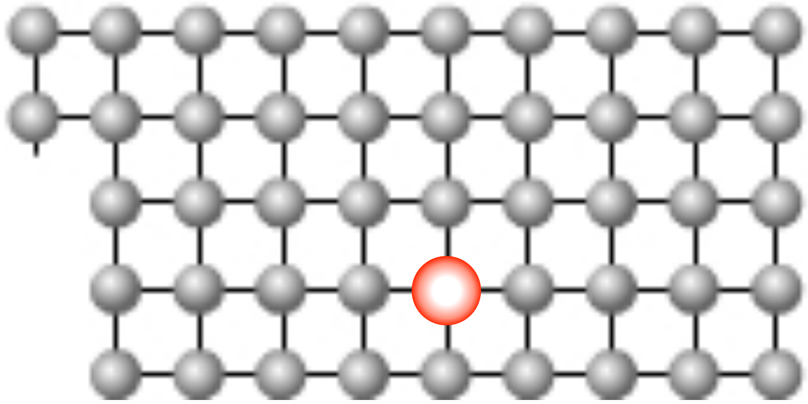
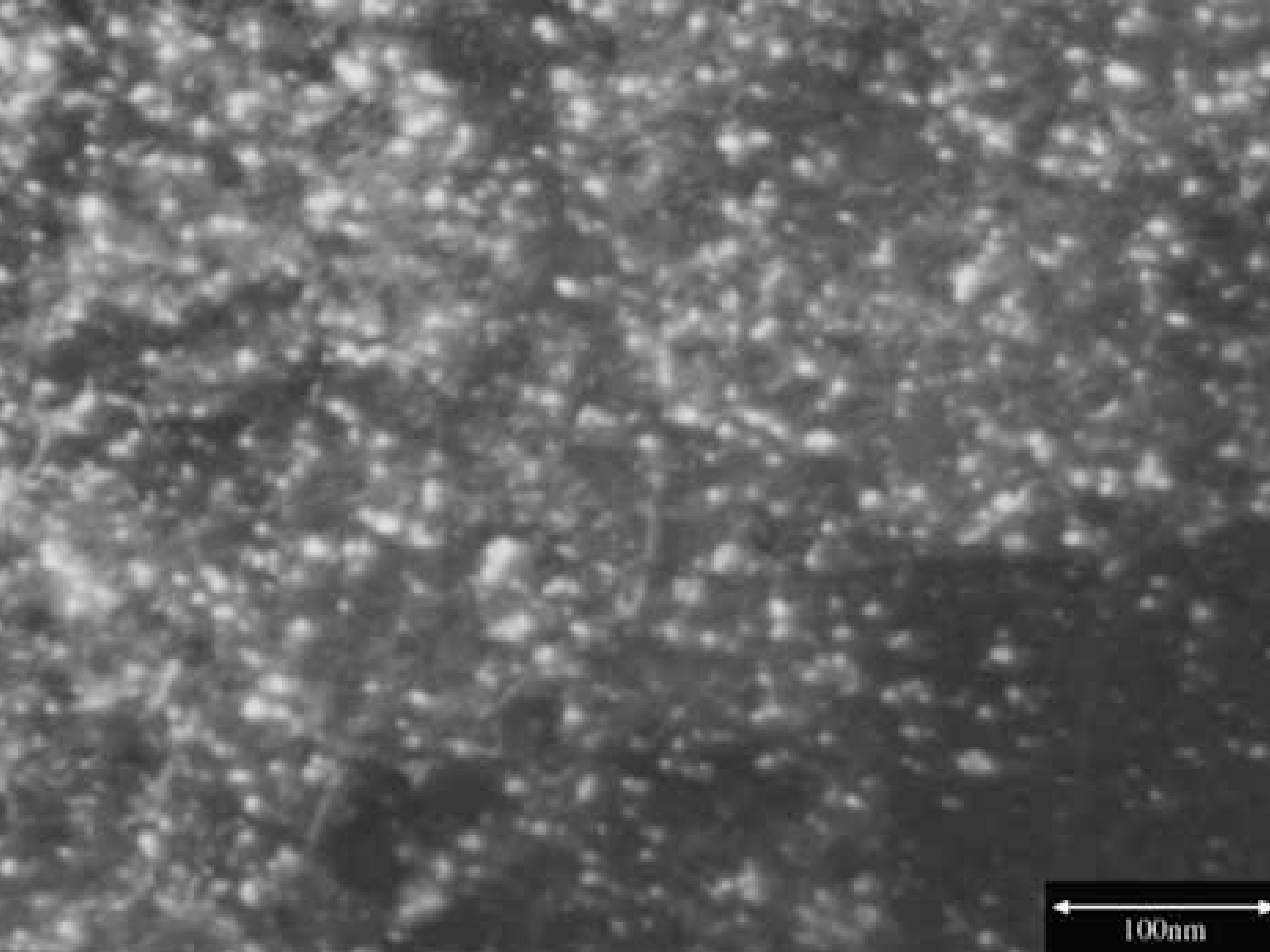
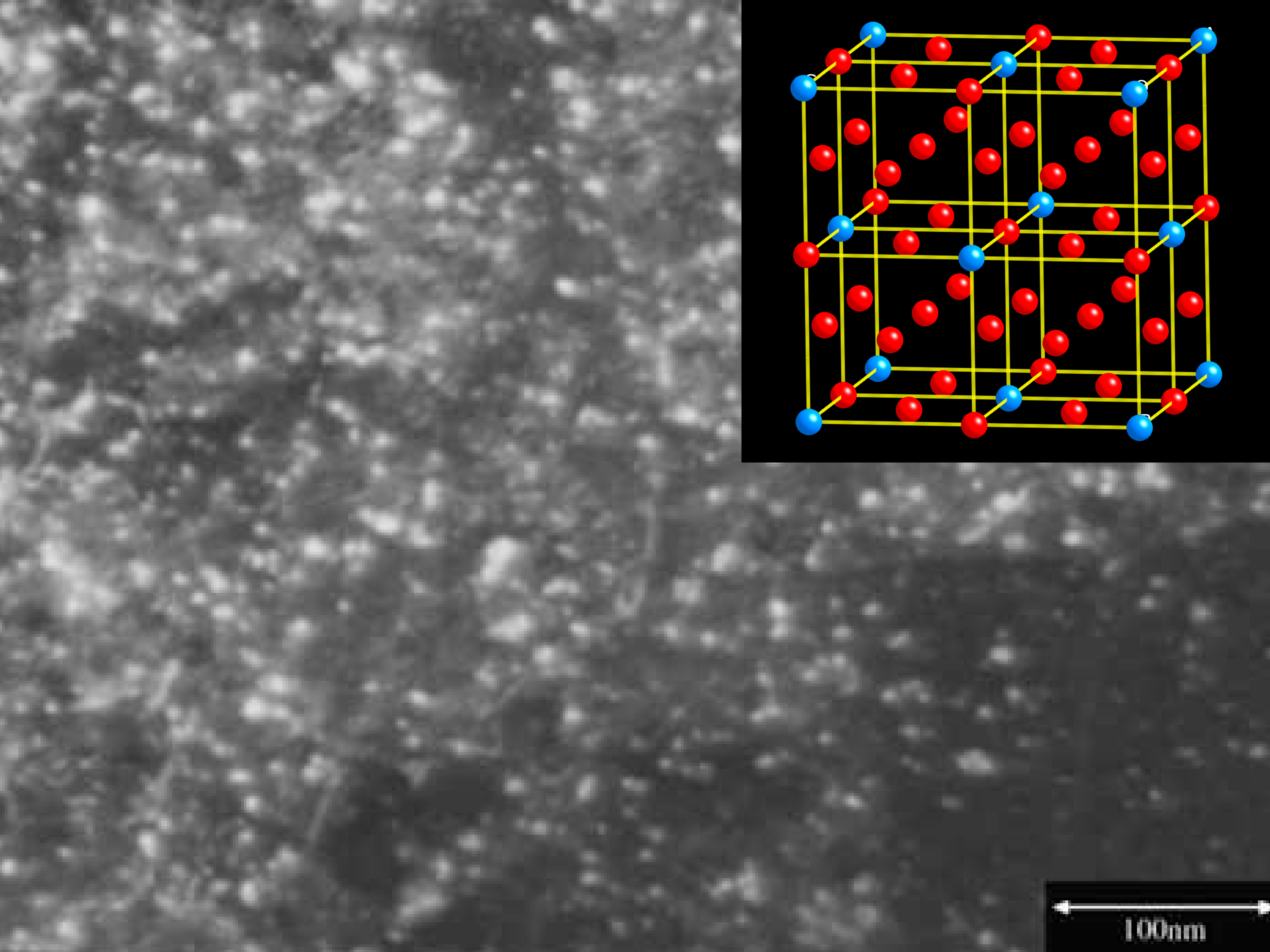


$$\leq 5\%$$

Solid solution hardening is ineffective jewelry alloys




100nm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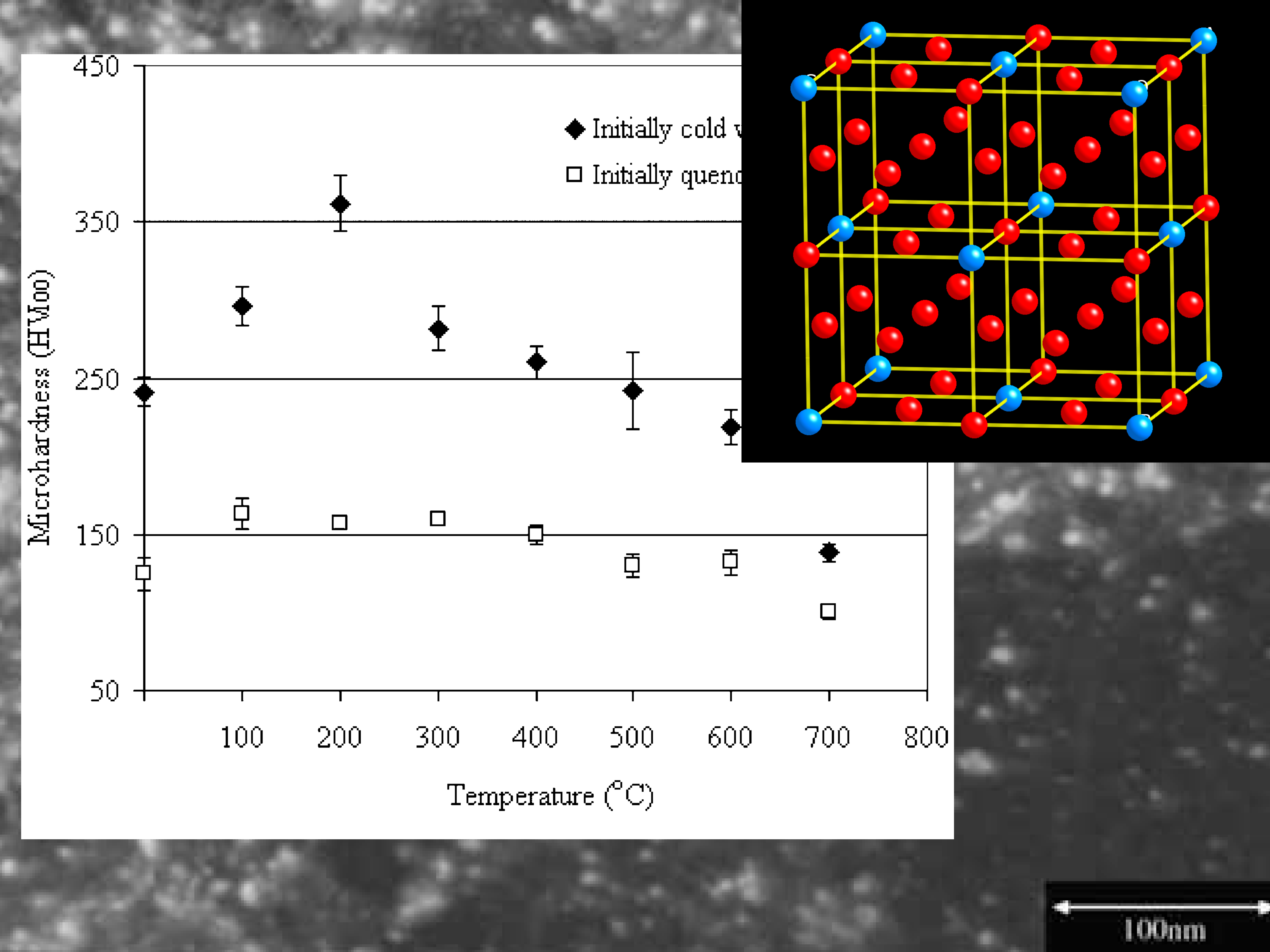
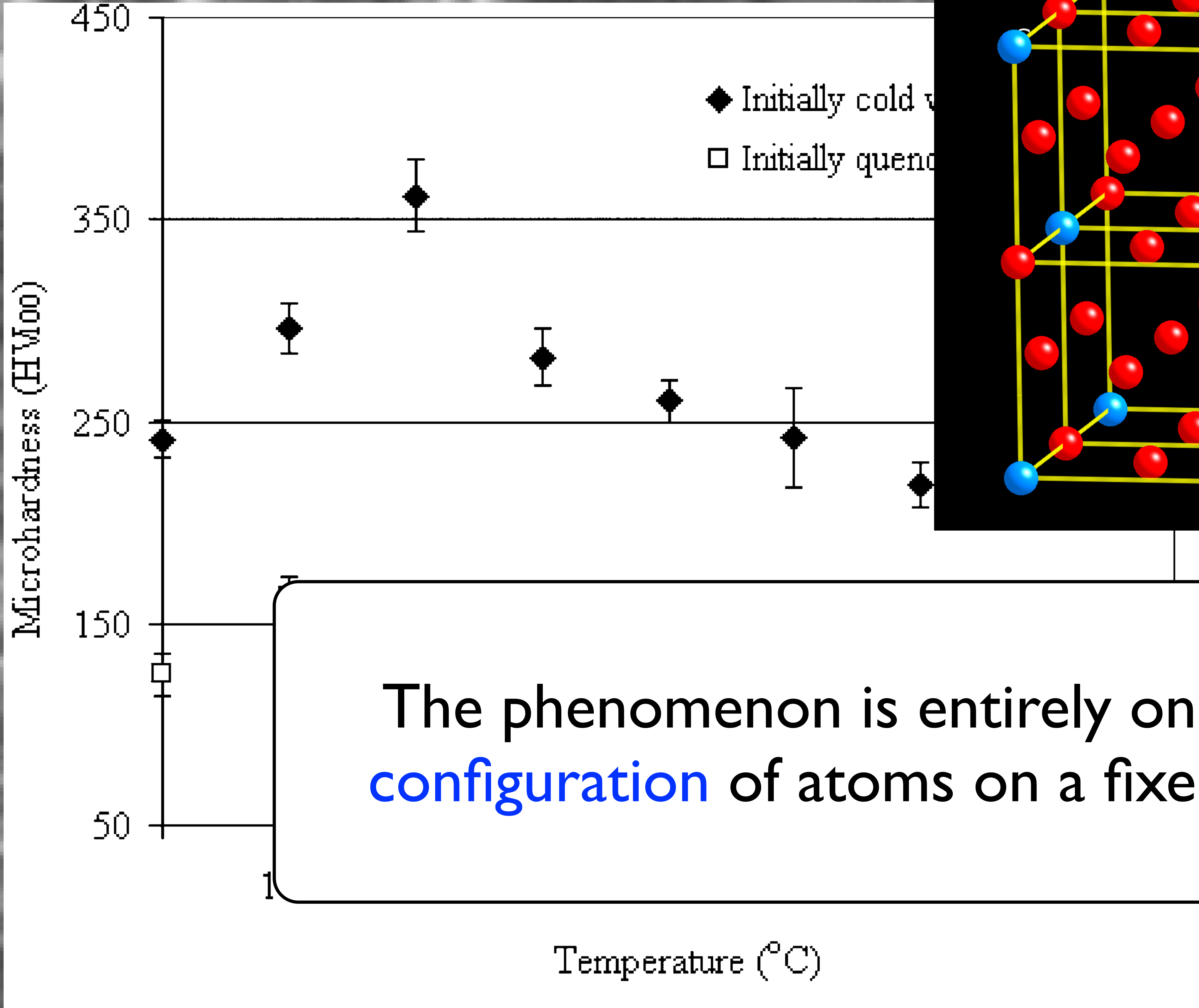
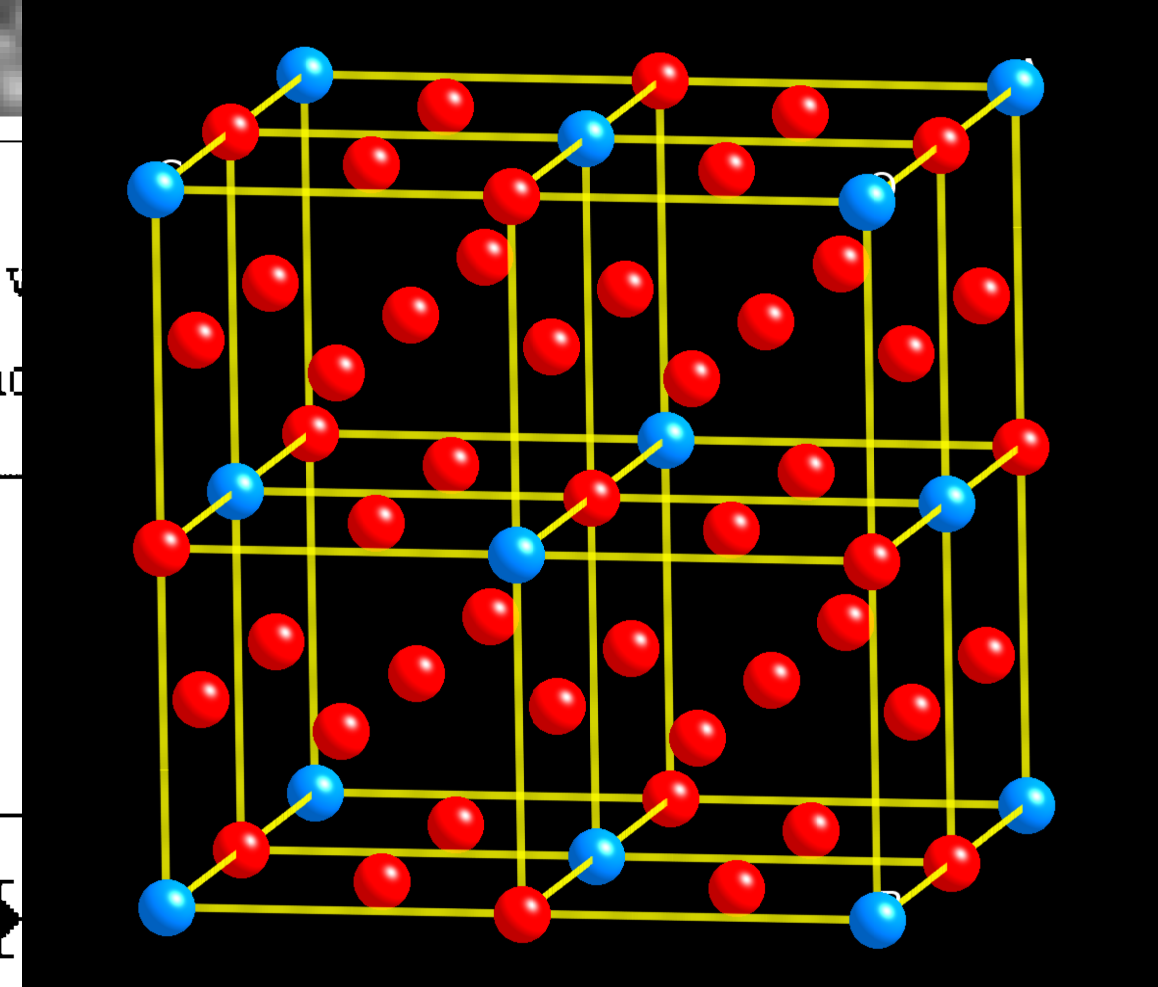
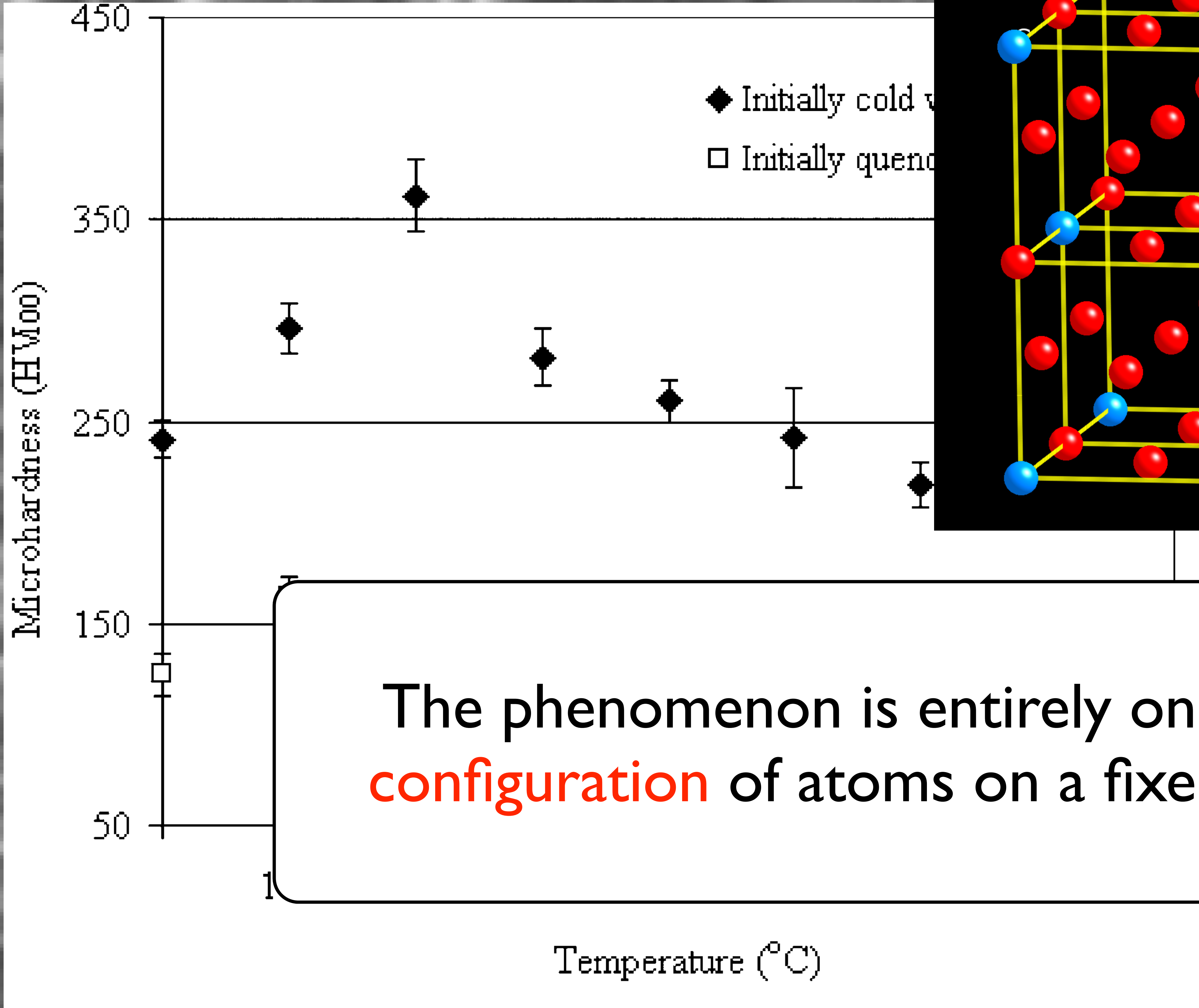


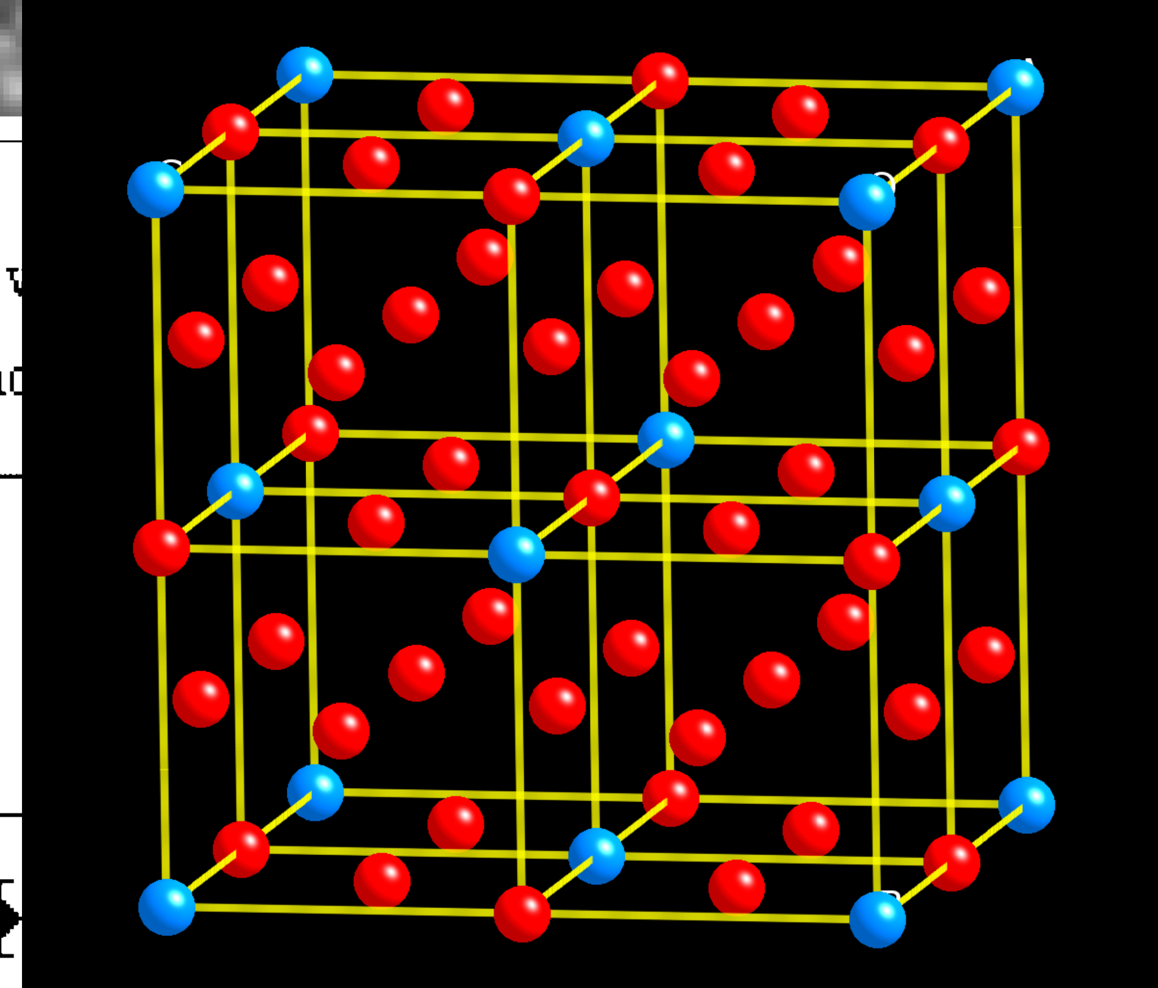
Initially cold w
Initially quenc
Microhardness (HV100)
450
350
250
150
50
100
200
300
400
500
600
700
800
Temperature (°C)
100nm



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



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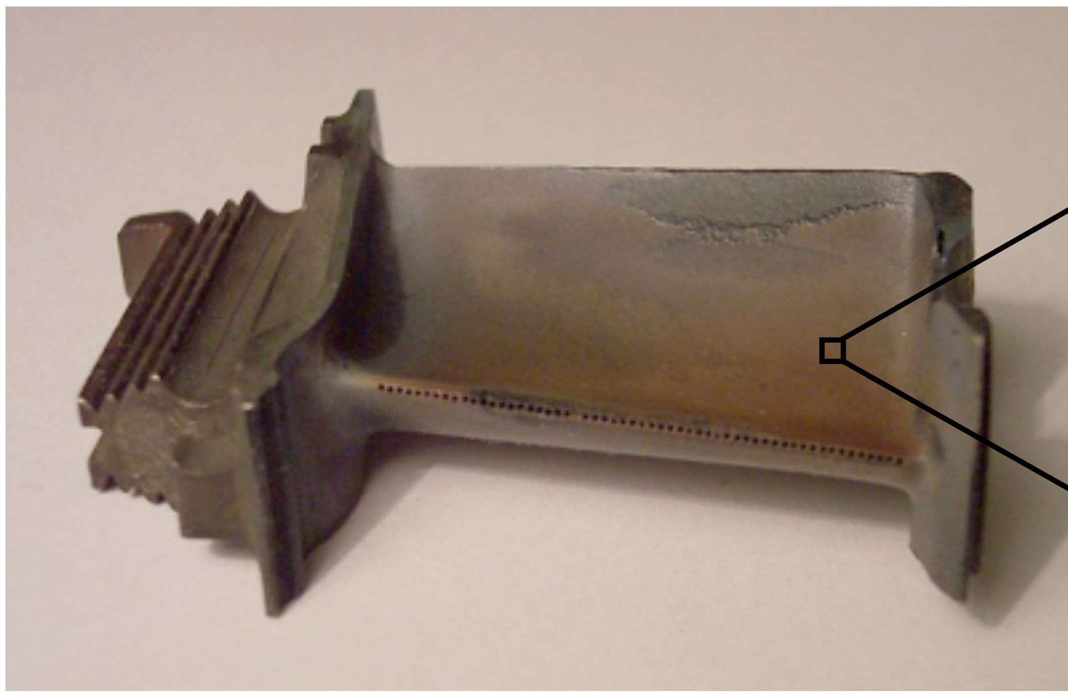
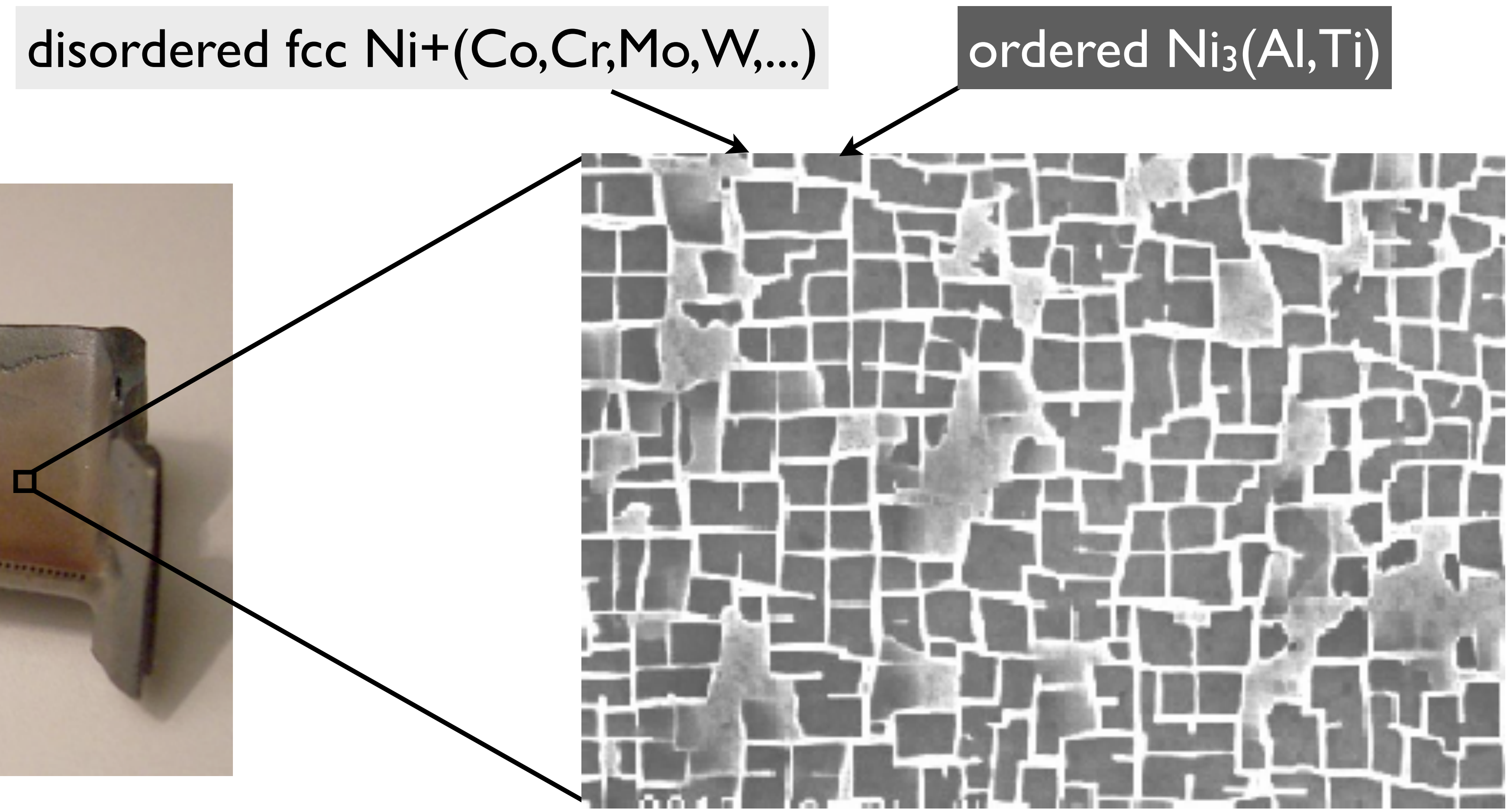
# A second example



Nickel superalloy jet engine turbine blade

http://en.wikipedia.org/wiki/Superalloy




http://www.tms.org/meetings/specialty/superalloys2000/superalloyshistory.html

# 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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1. Search for new phases (step through millions of candidate configurations)

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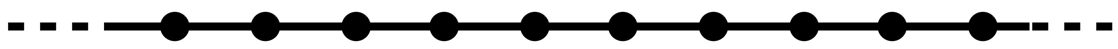
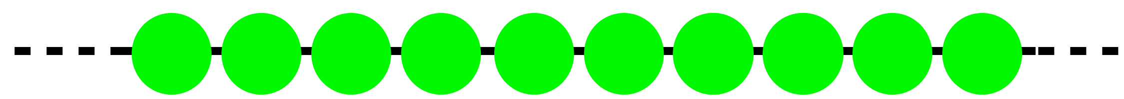
3. Build a kinetic simulation (to model time evolution)

# One-Dim. configurational problem



# One-Dim. configurational problem



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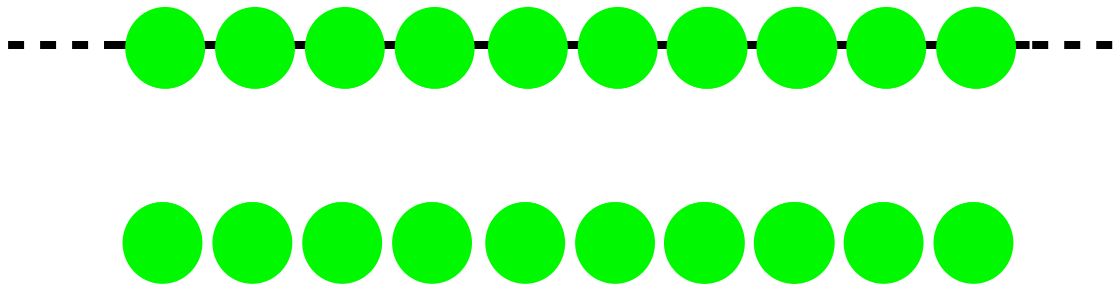

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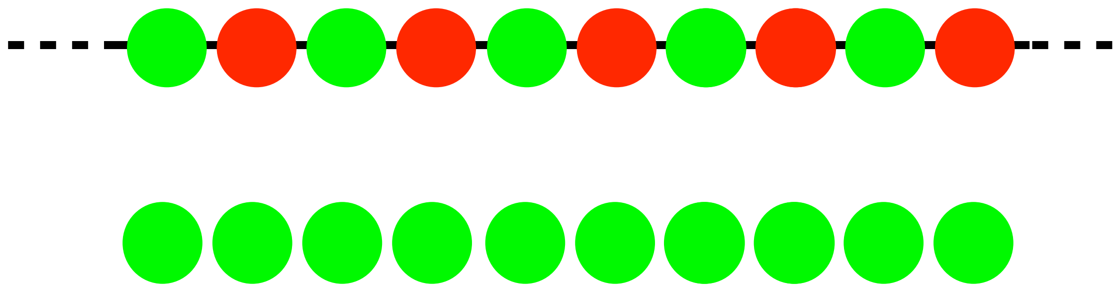

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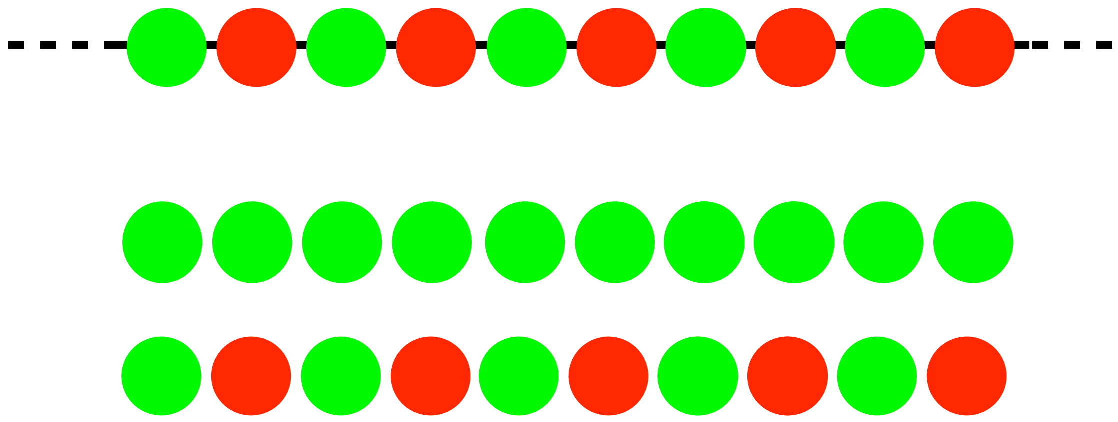

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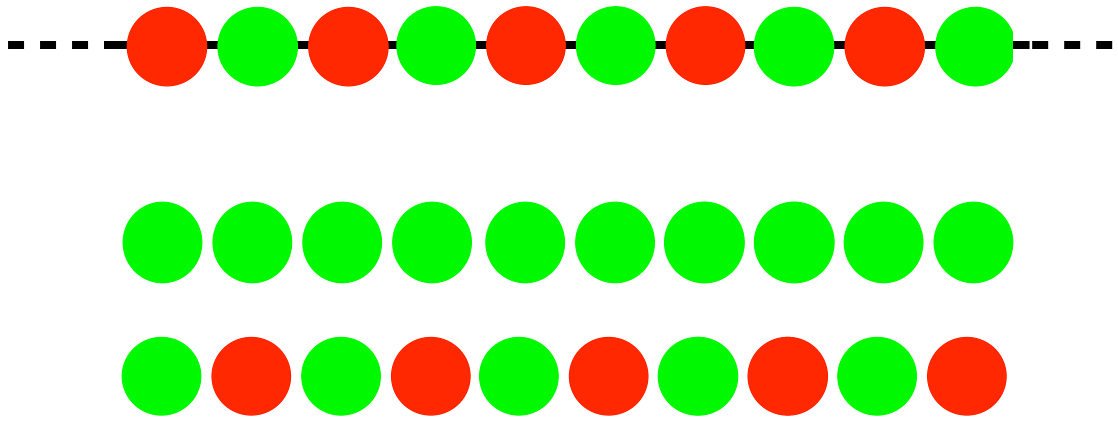

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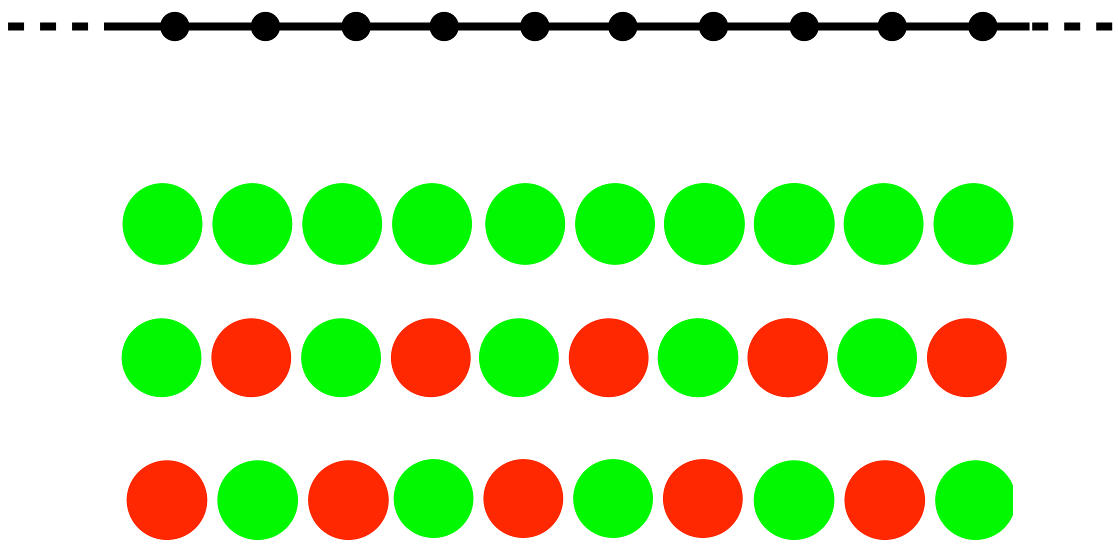

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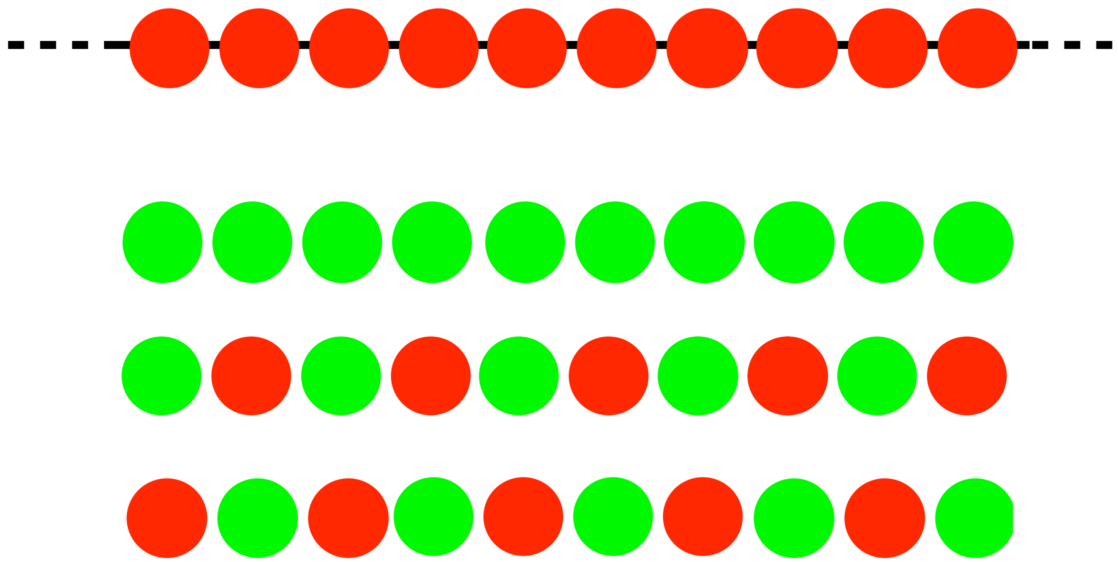

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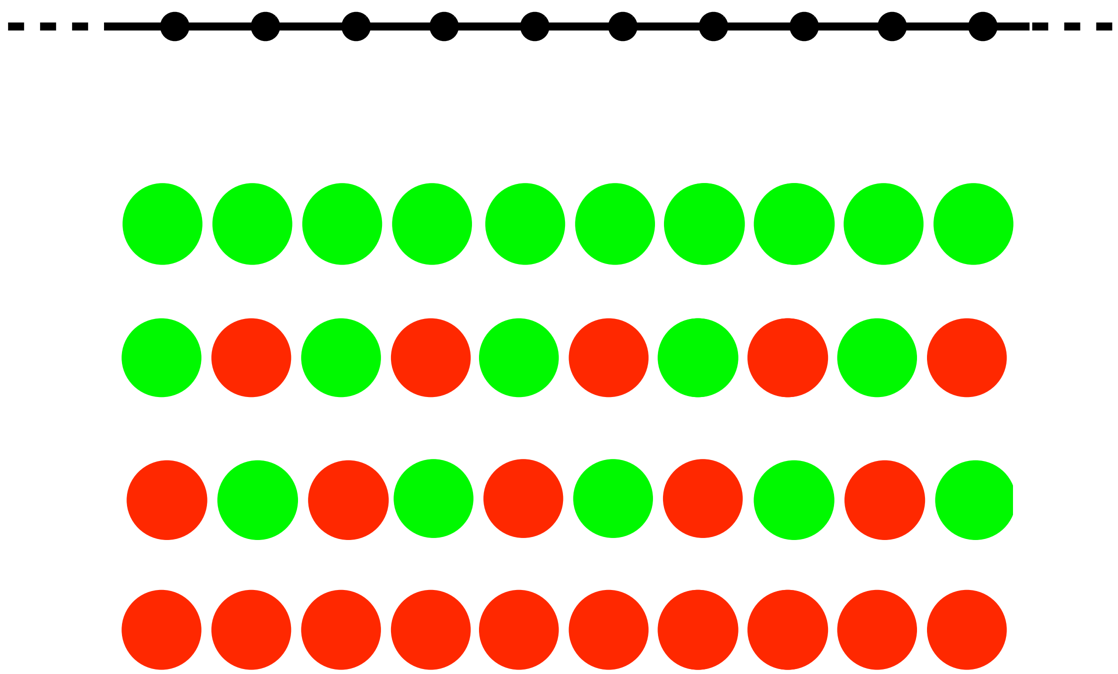

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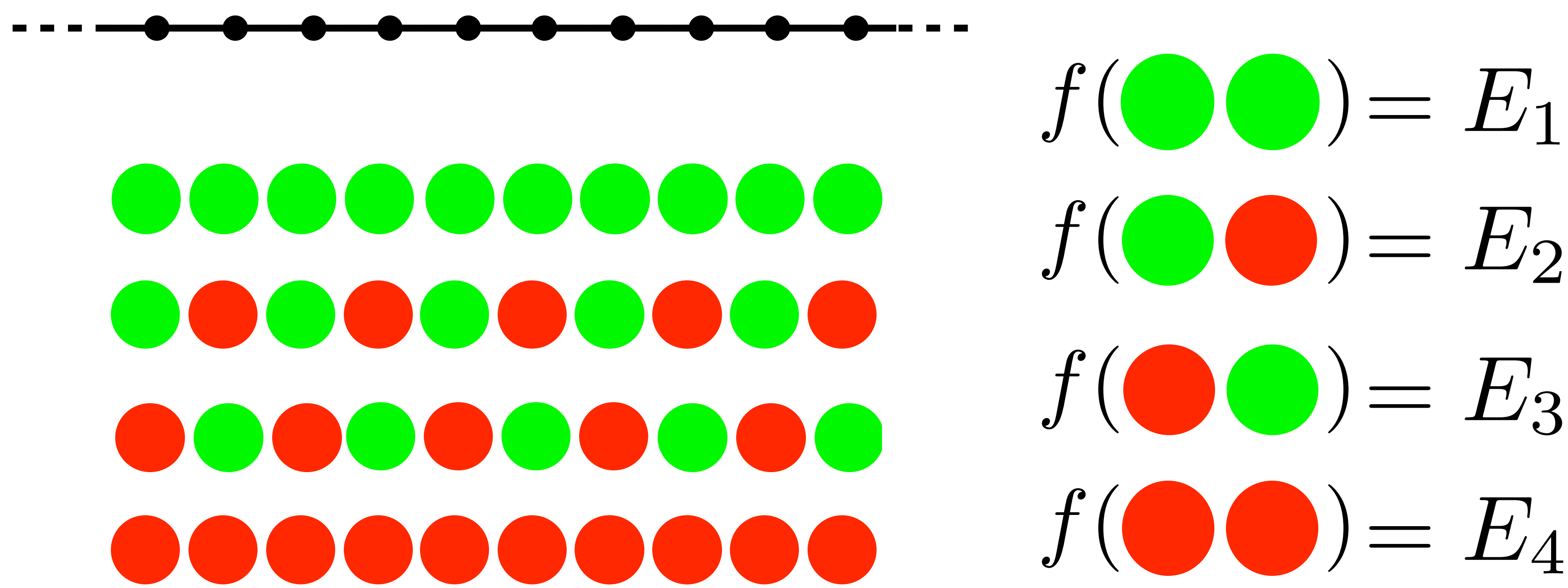
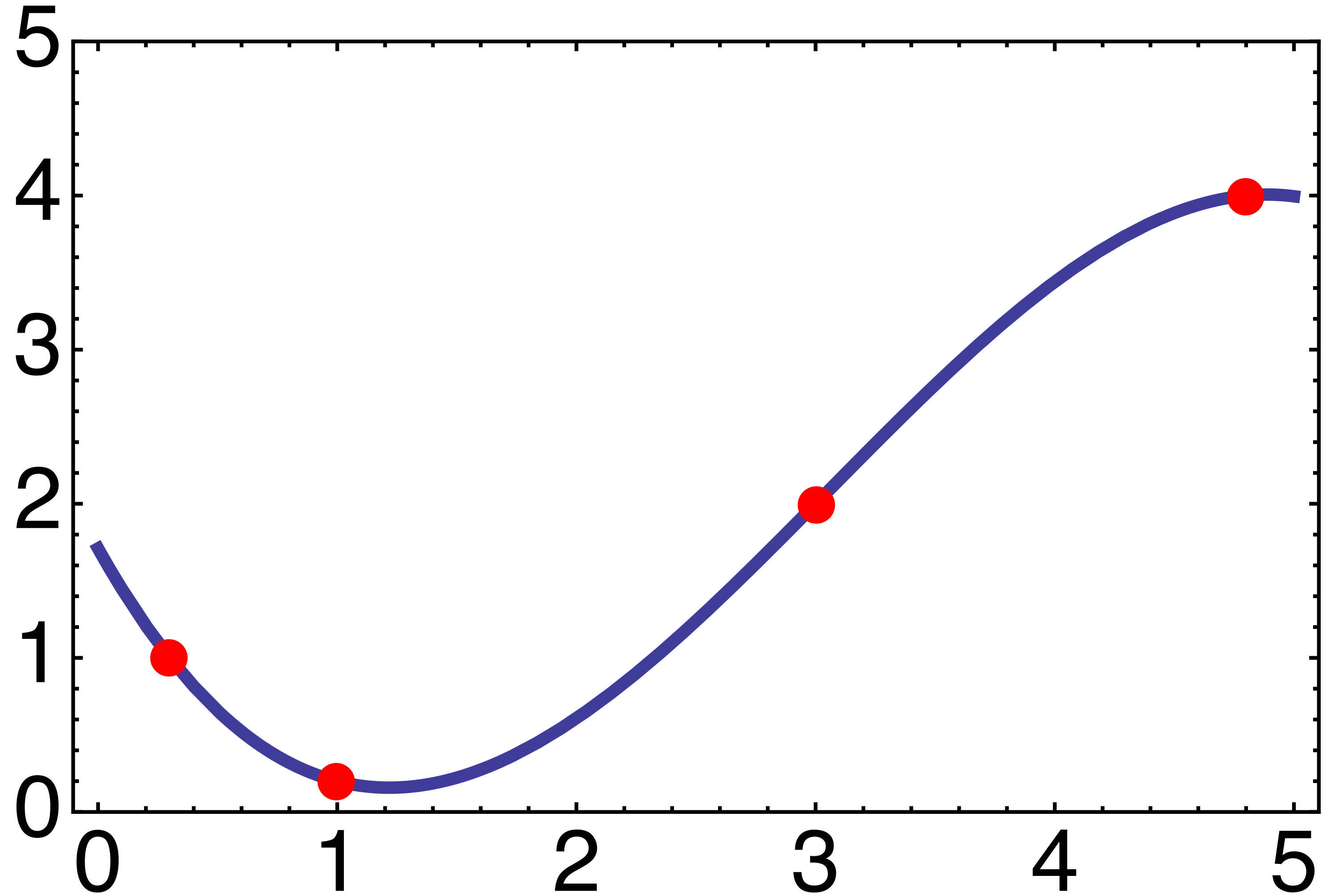


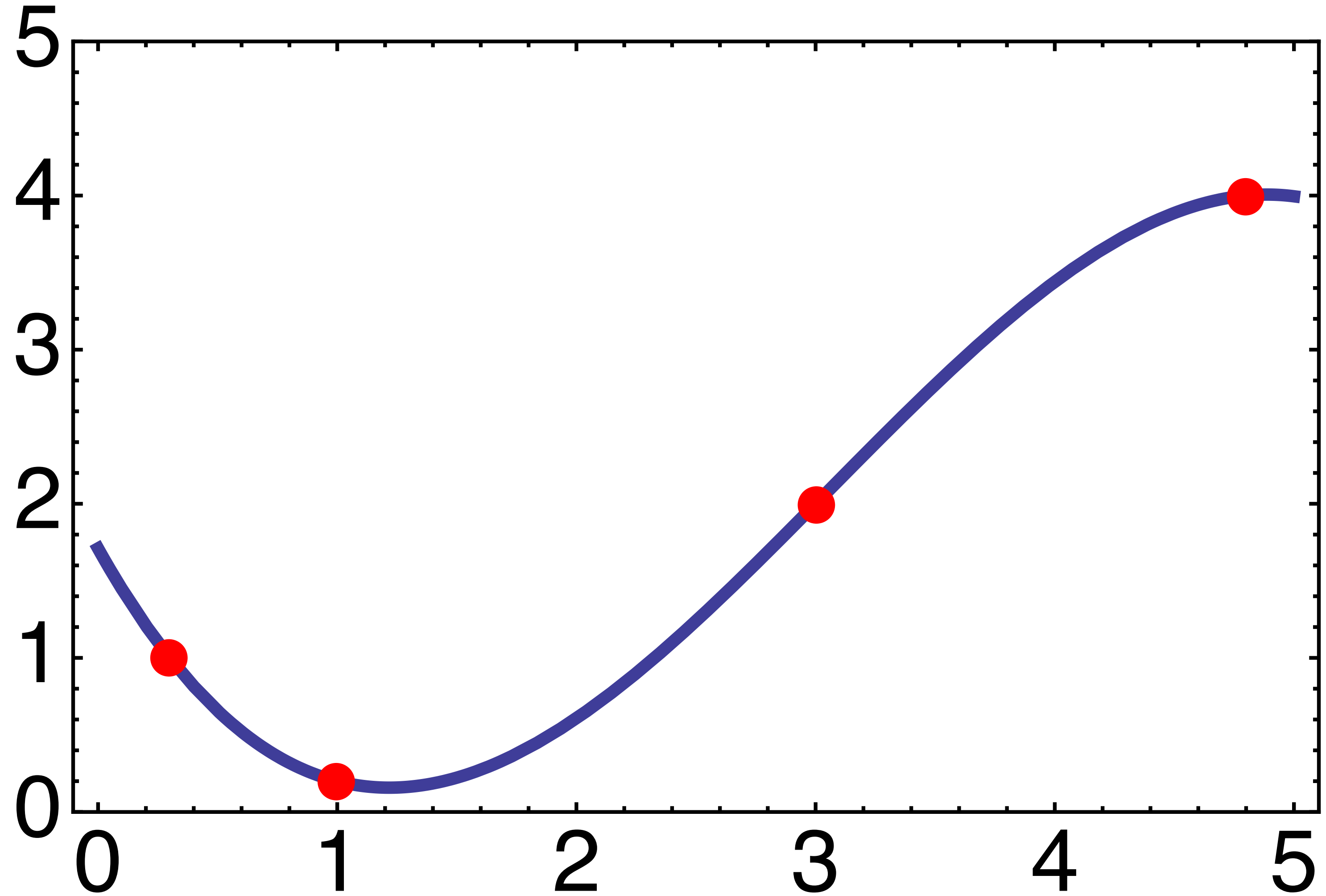
# Expanding in a power series




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

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

# Expanding in a power series

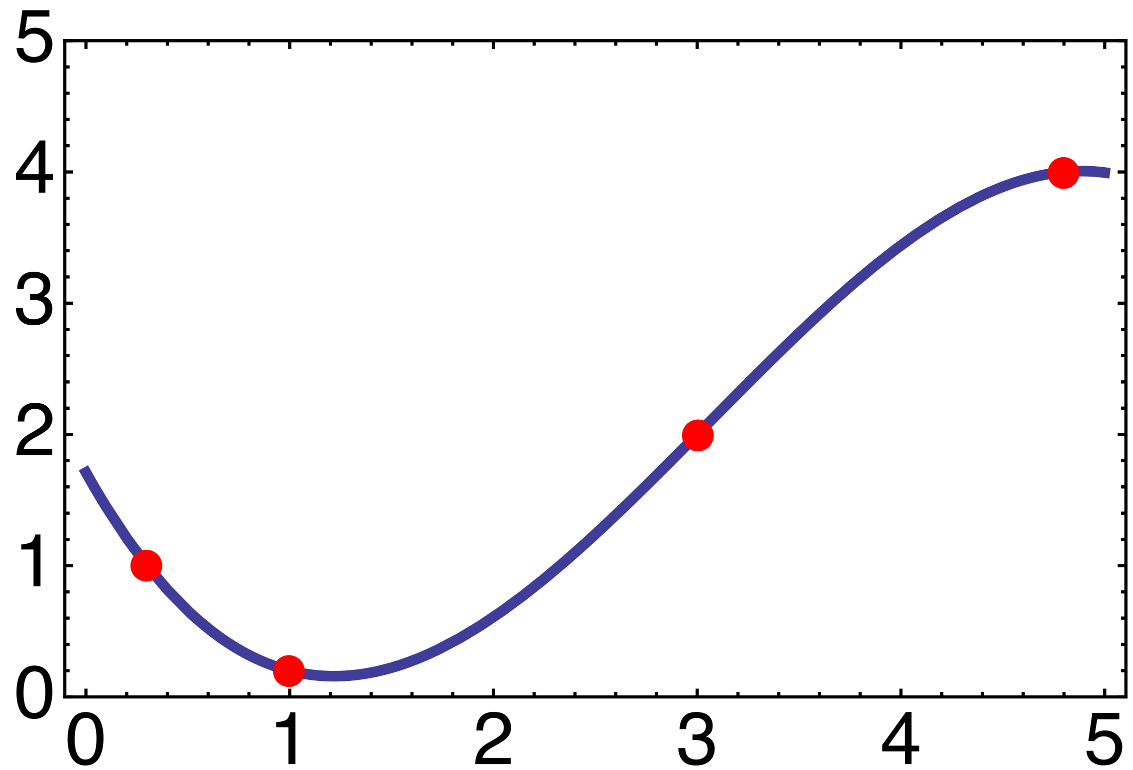



$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

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

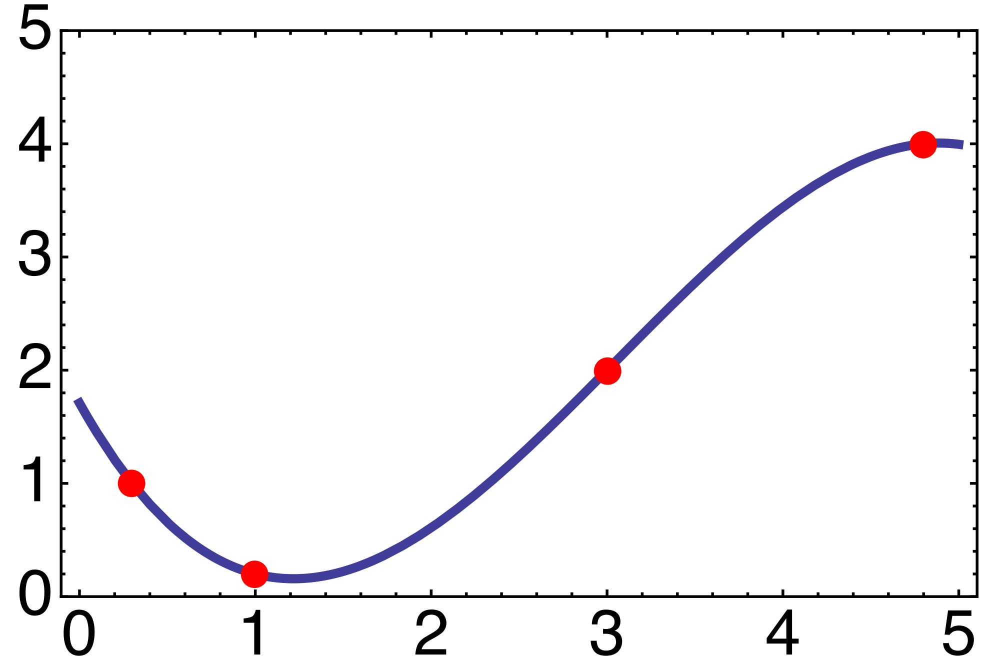
How do we find the coefficients?

# 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




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

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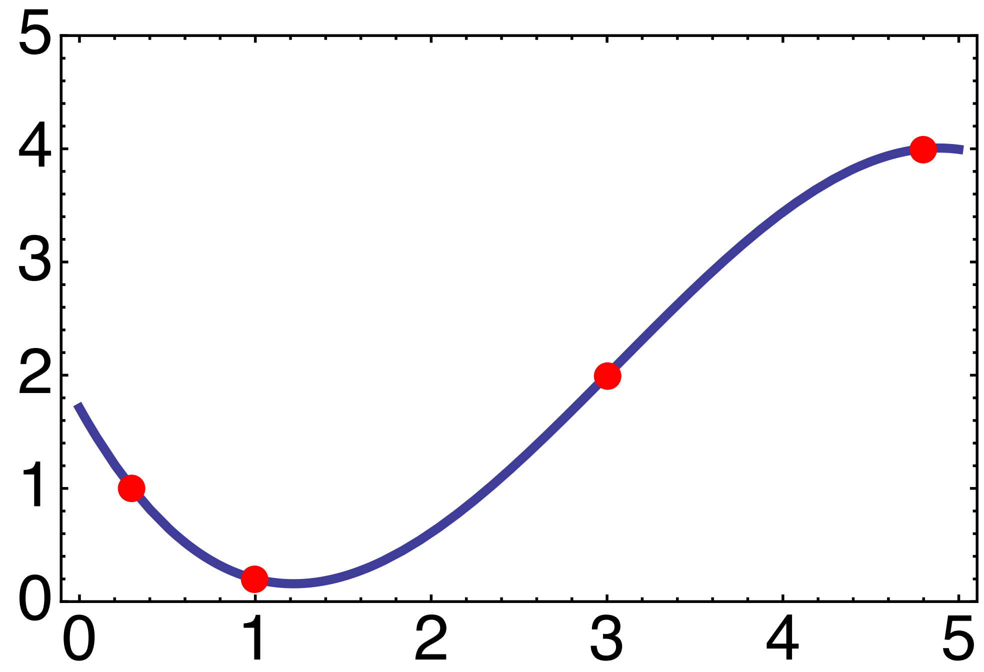


Data

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

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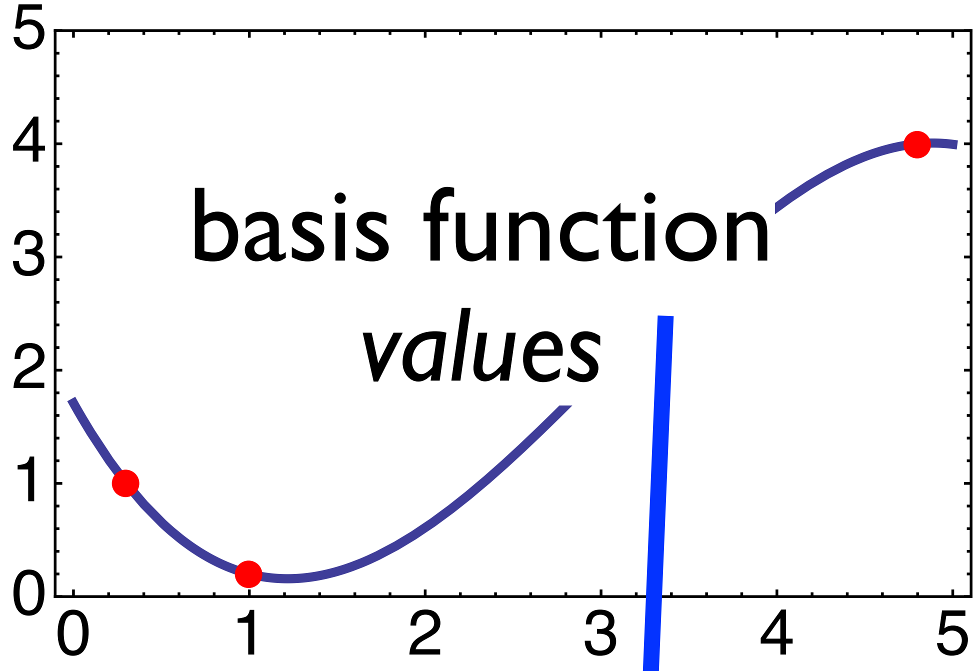


basis function *values*

Data

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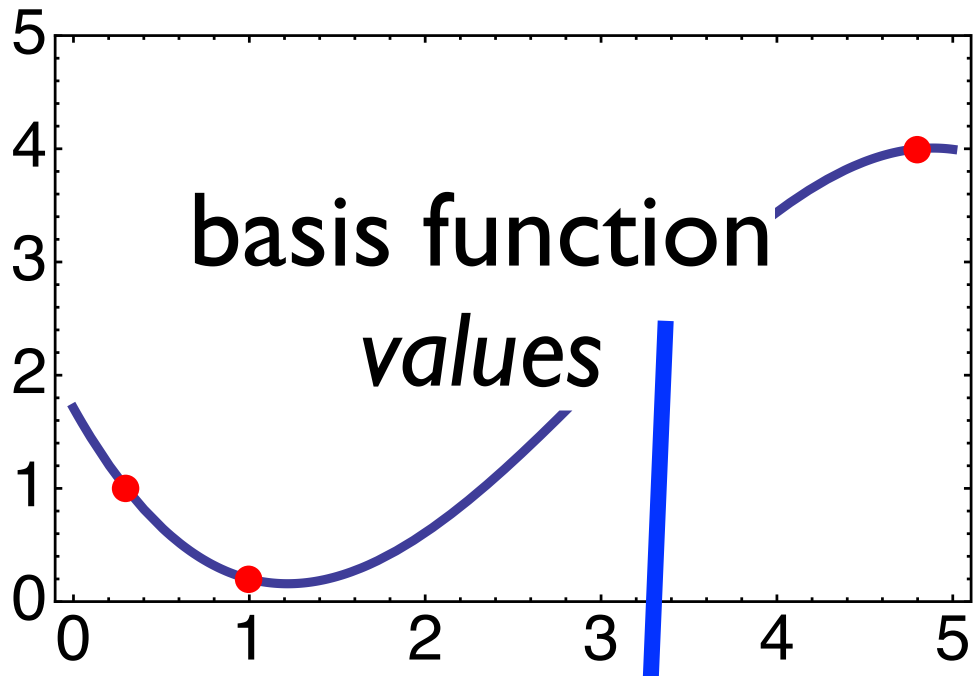


Data

basis function *values*

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

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

$$\begin{aligned}
f(\bigcirc\bigcirc\bigcirc\bigcirc) &= \frac{J_0}{N}\sum_i^{\circ\circ\circ\circ} 1 + J_1 \sum_i^{\circ\circ\circ\circ} \bigcirc_i + J_2 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} + J_3 \sum_i^{\circ\circ\circ\circ} \bigcirc_i \bigcirc_{i+1} \bigcirc_{i+2} + \cdots \\
f(\bigcirc\bigcirc\bigcirc\bigcirc) &= J_0 \quad + \quad J_1 \bar{\Pi}^{\circ} \quad + \quad J_2 \bar{\Pi}^{\circ\circ} \quad + \quad J_3 \bar{\Pi}^{\circ\circ\circ} \quad + \cdots
\end{aligned}$$

# Expanding configurational functions

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

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

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

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

# Expanding configurational functions

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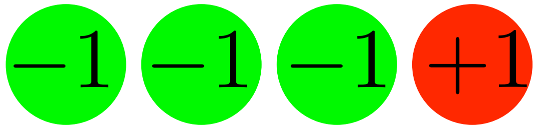


# Expanding configurational functions

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

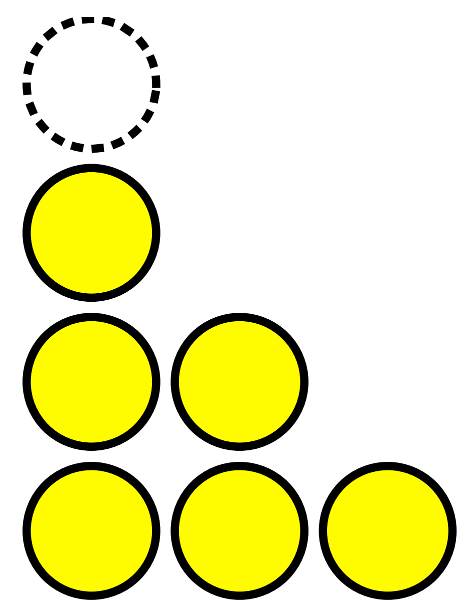
$$f(\bigcirc\bigcirc\bigcirc\bigcirc) = J_0 + J_1 \bar{\Pi}^{\circ} + J_2 \bar{\Pi}^{\circ\circ} + J_3 \bar{\Pi}^{\circ\circ\circ} + \cdots$$

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

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)



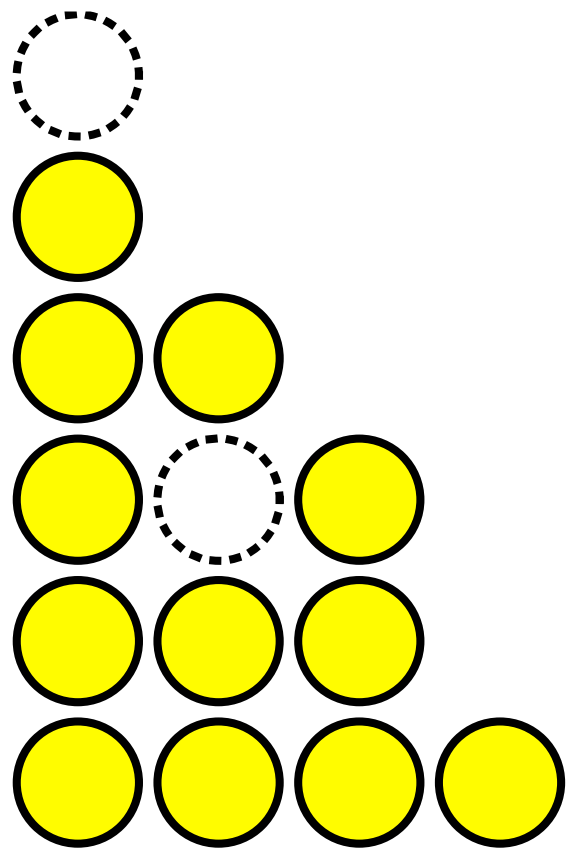
# Cluster Expansion: Example

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

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

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

Calculate the correlations...



# 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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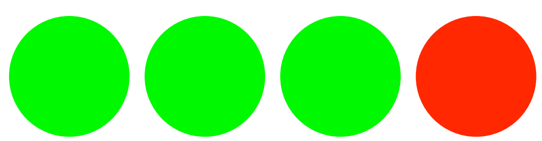

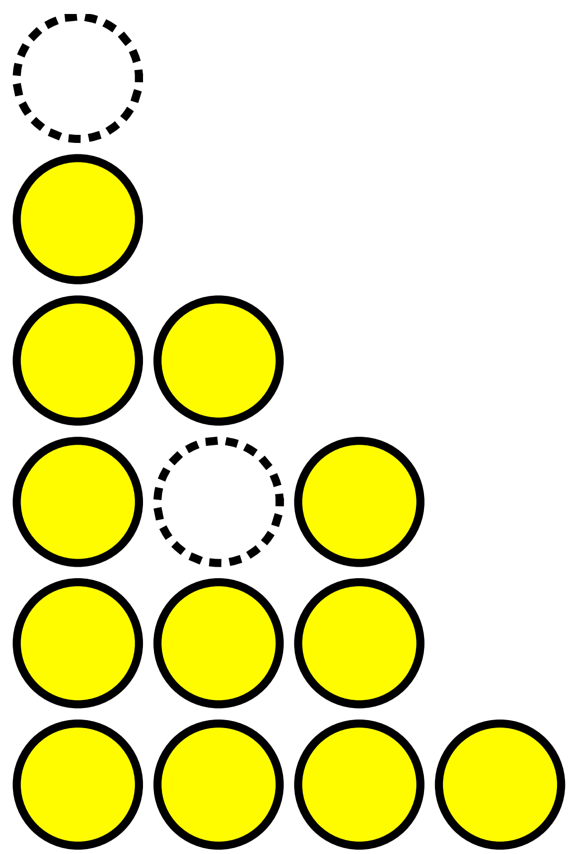

# Cluster Expansion: Example

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

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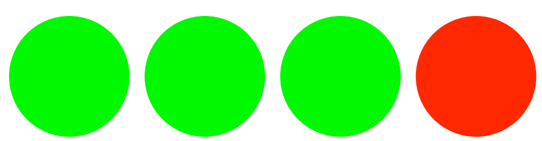

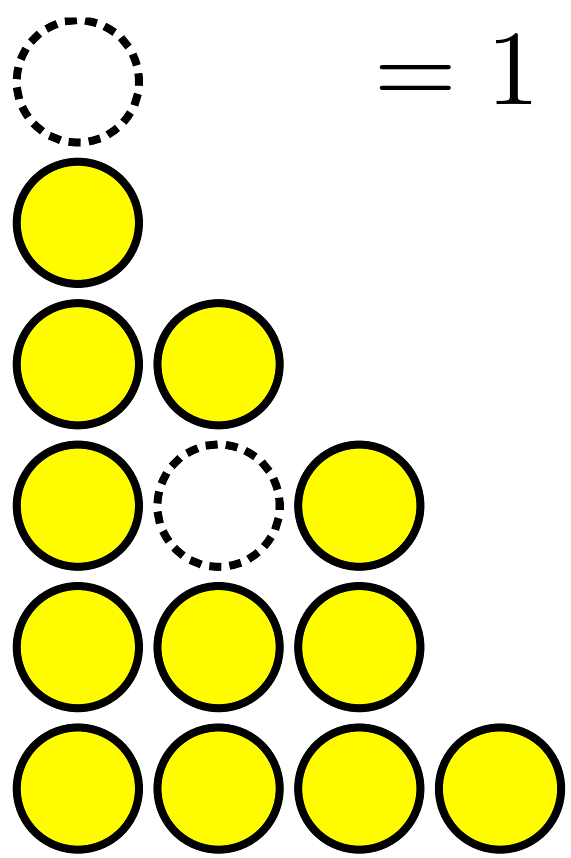

$= 1$

# 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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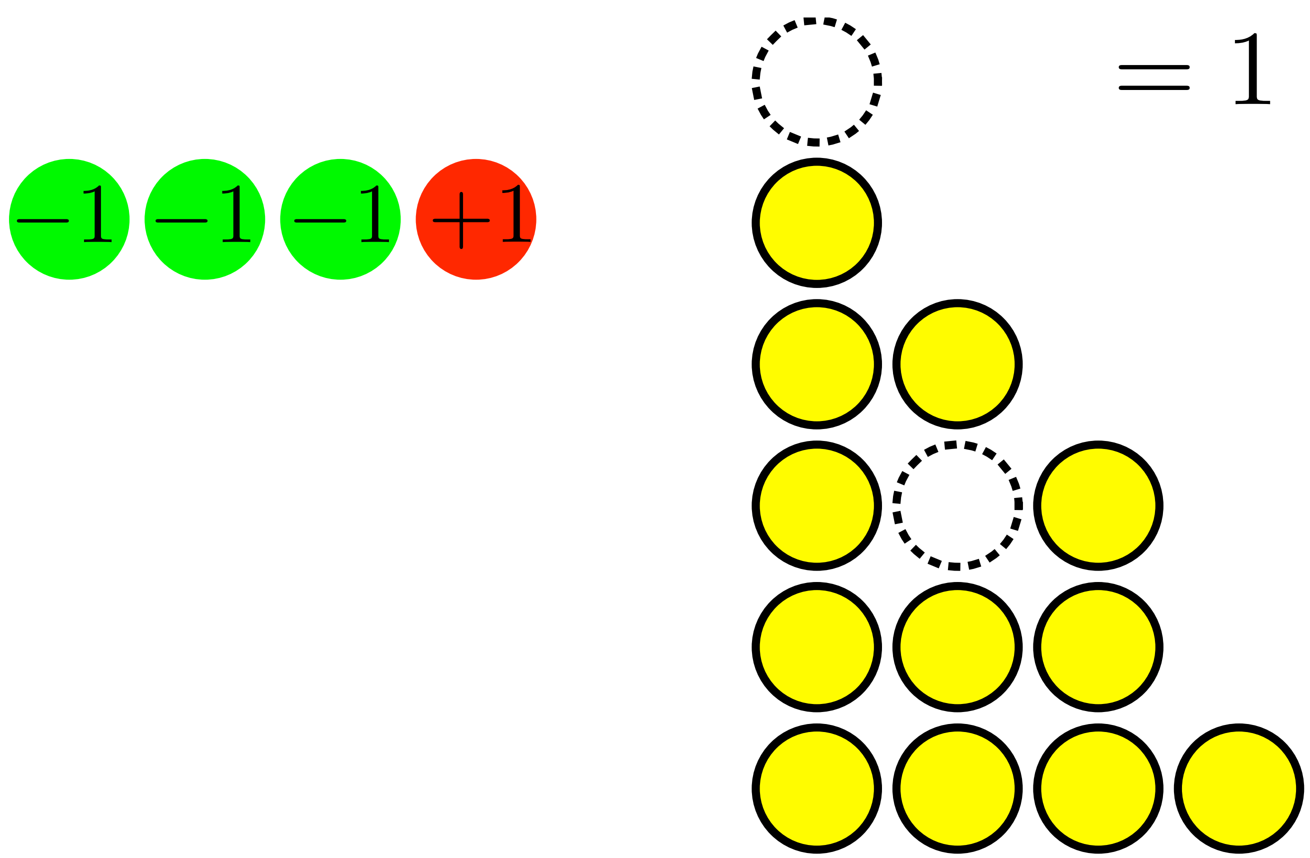

# Cluster Expansion: Example

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

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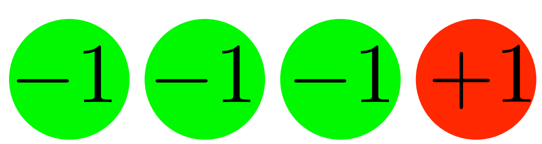


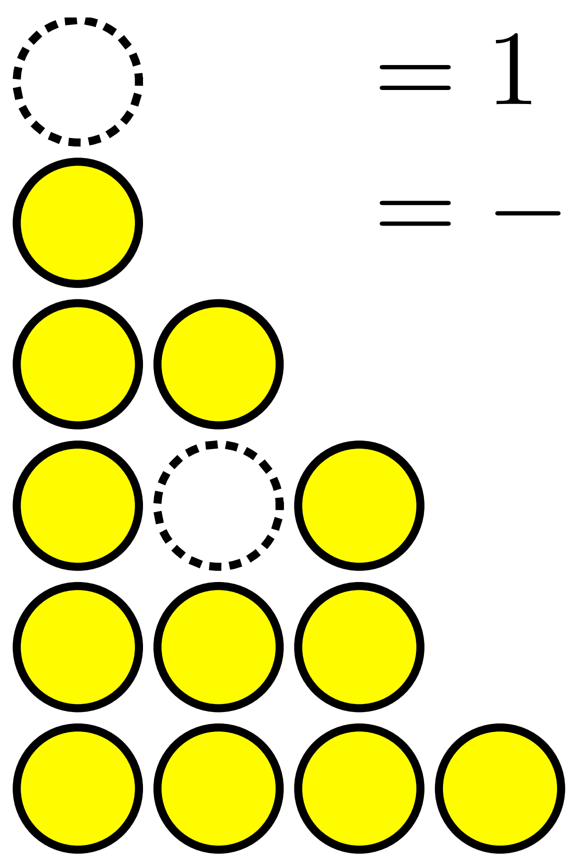

$$= 1$$

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

# 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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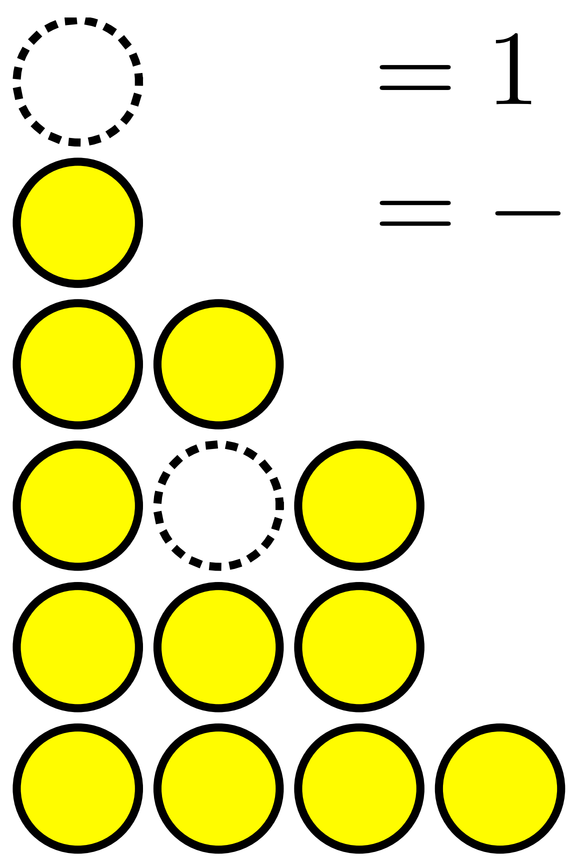

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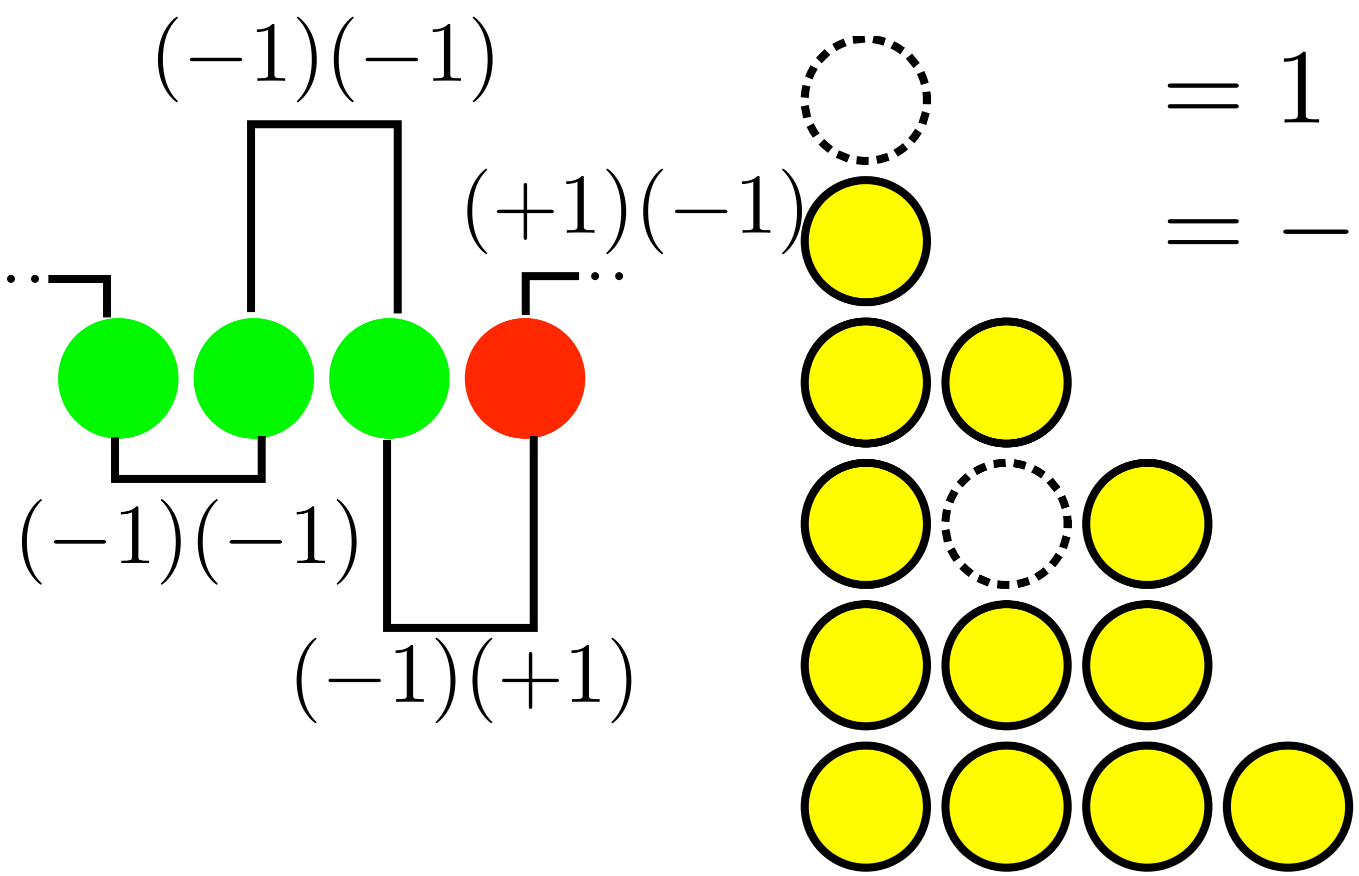


$$= 1$$

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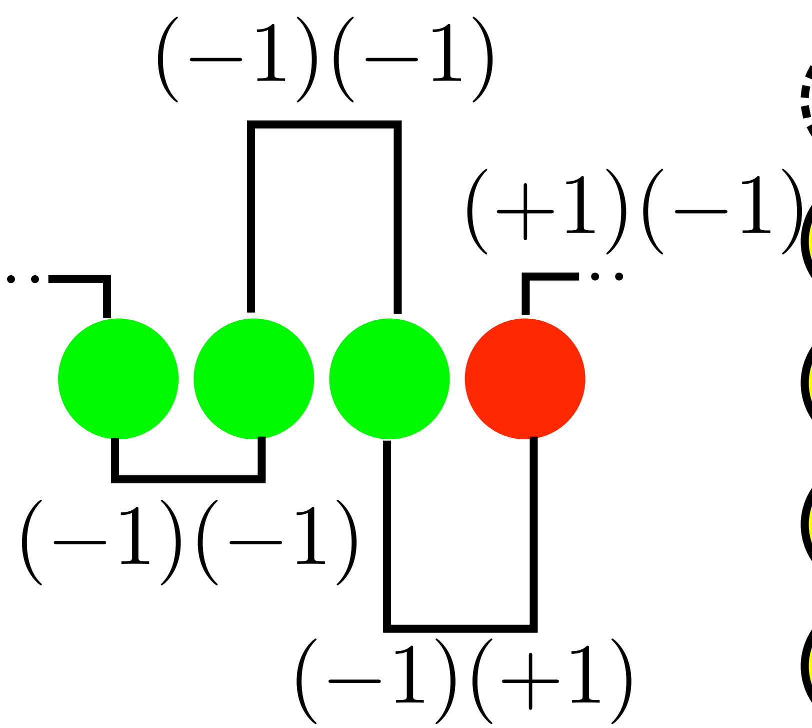


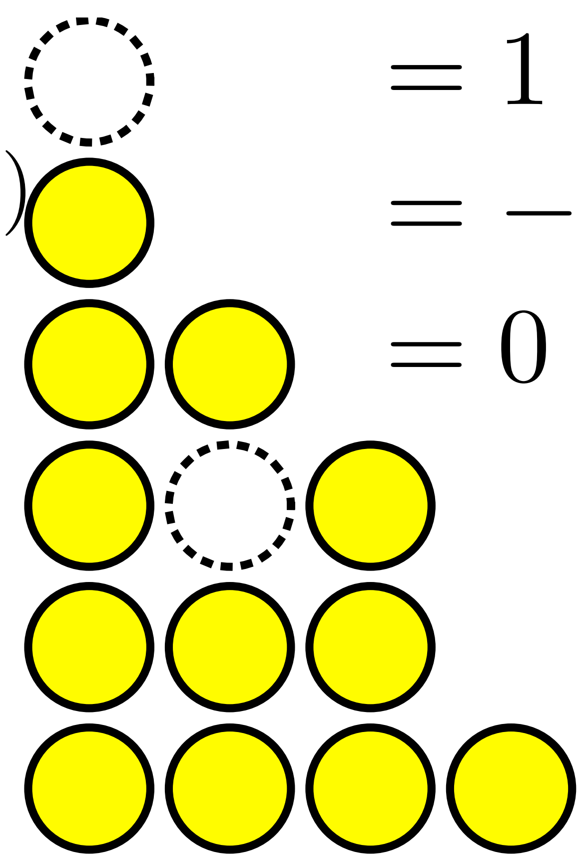

$= 1$

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

$= 0$

# 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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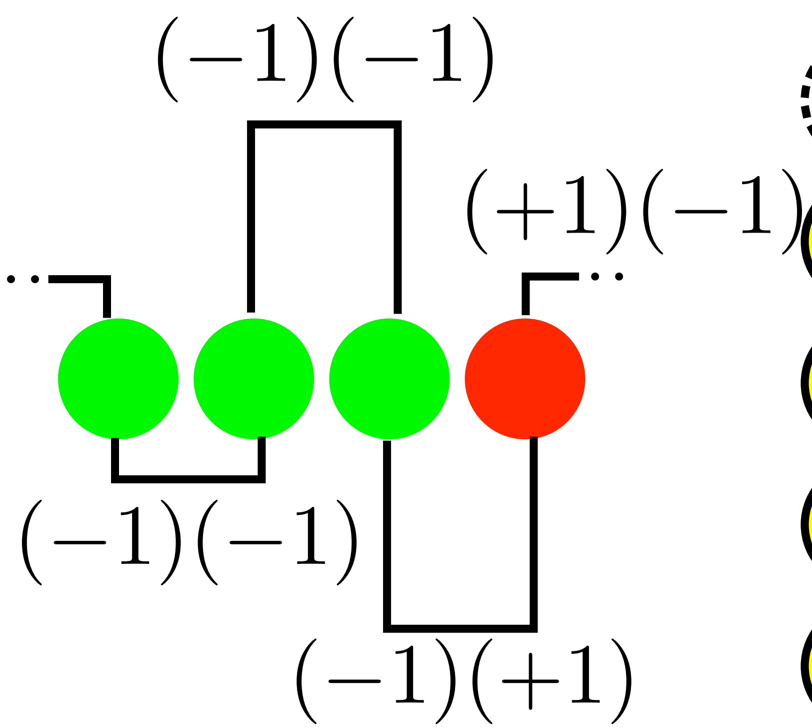


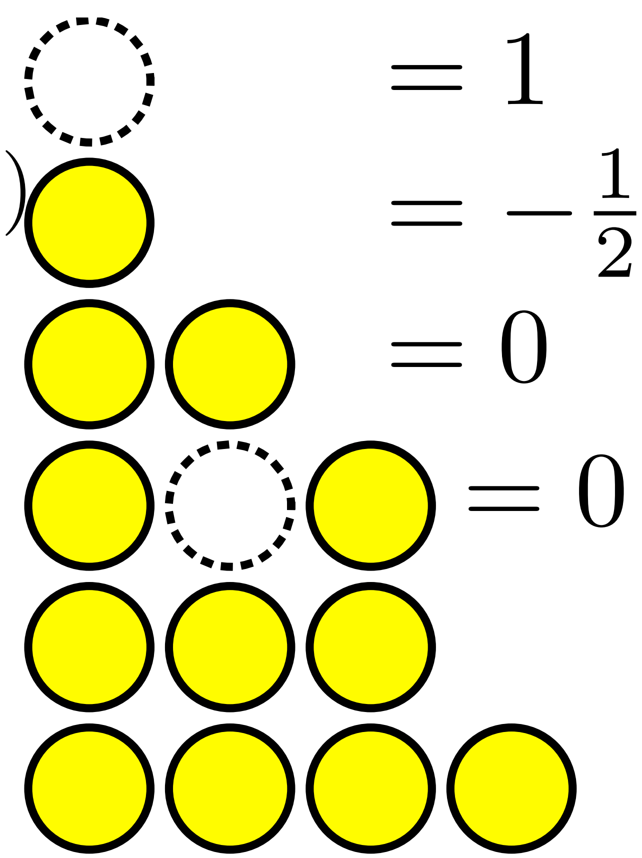

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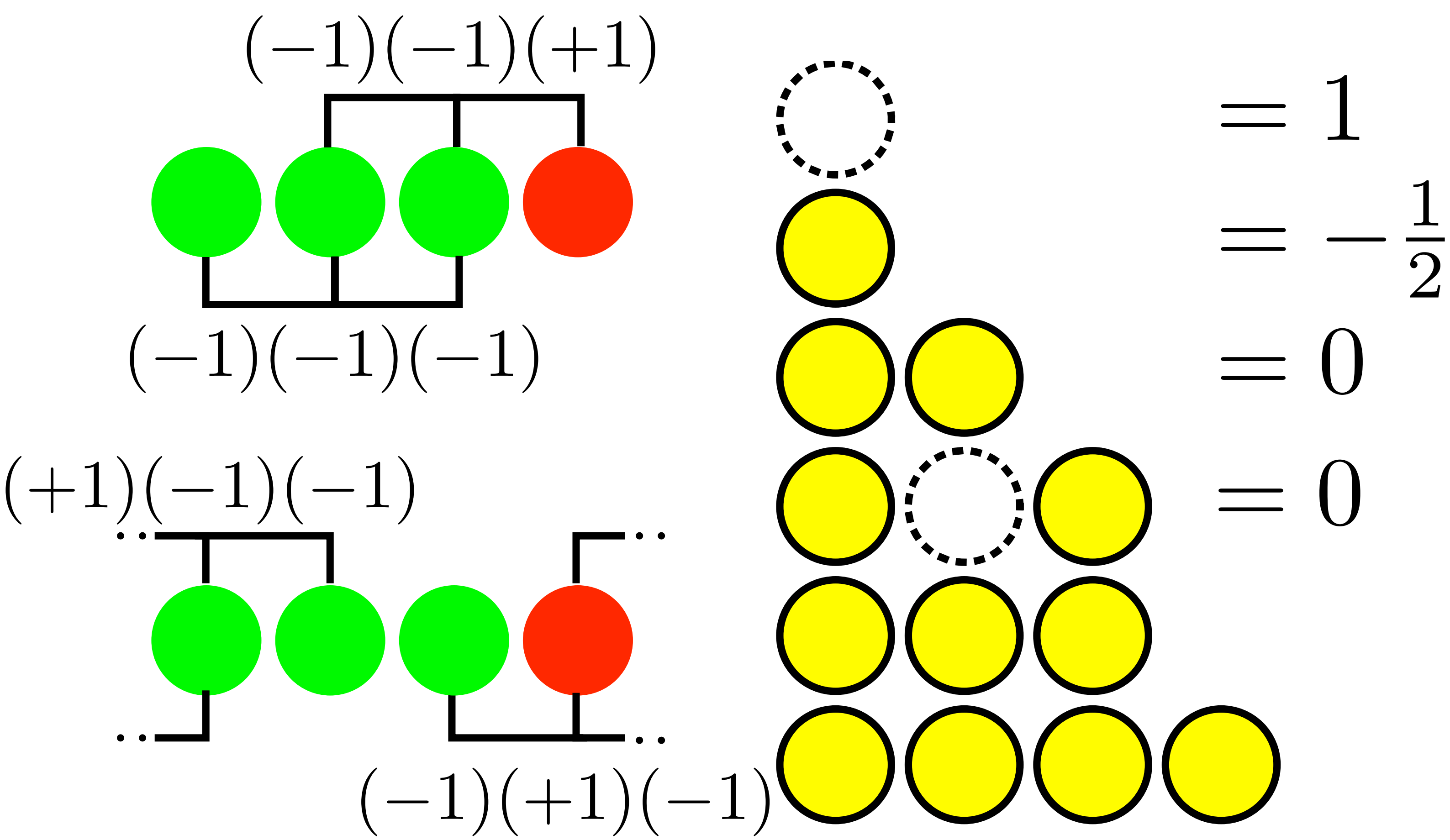

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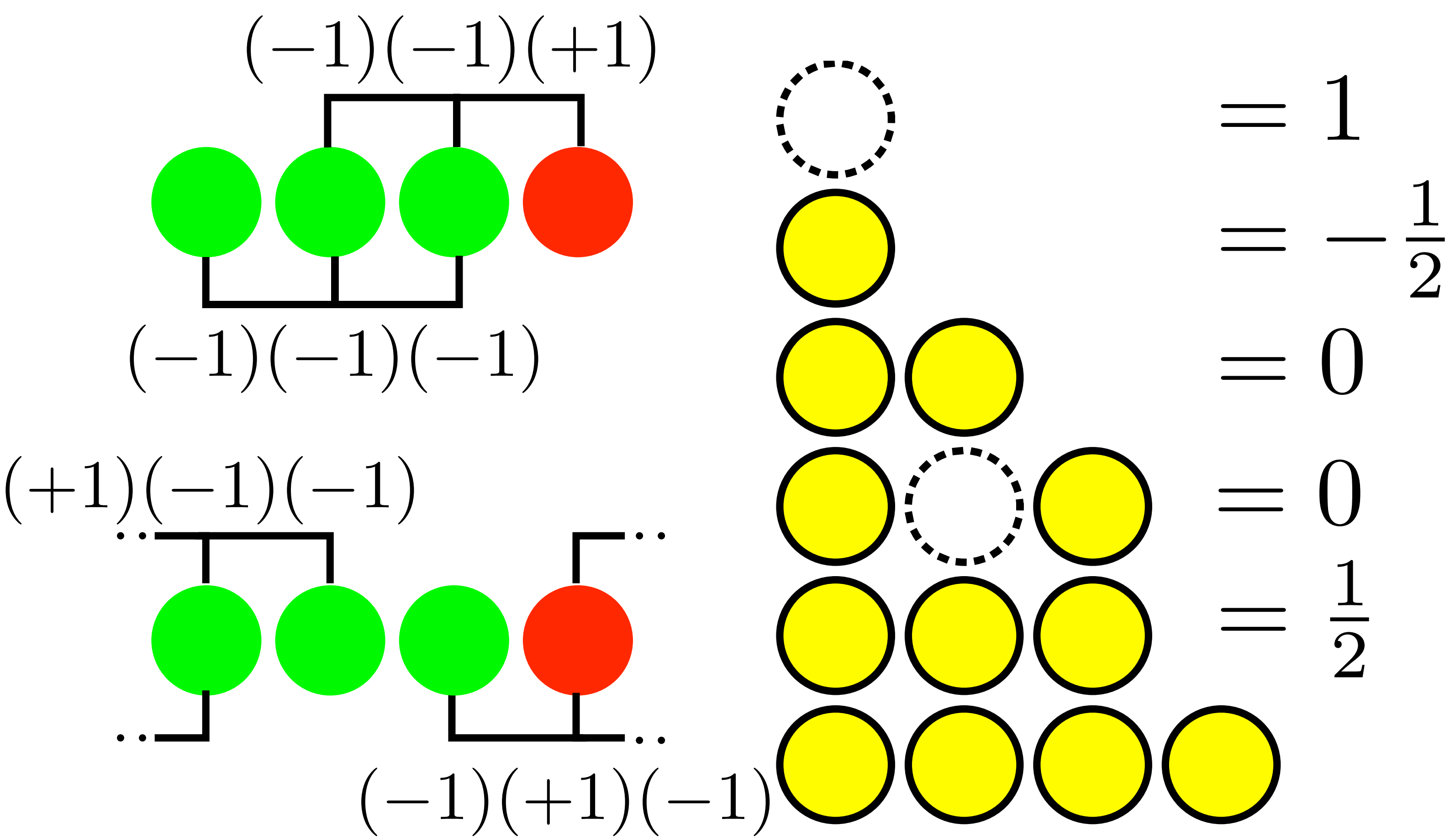

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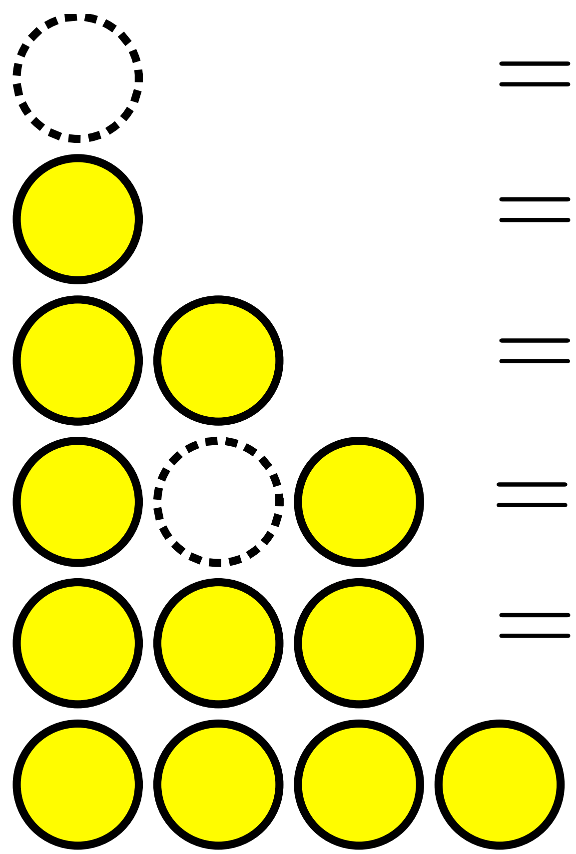

$$= 1$$

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

$$= 0$$

$$= 0$$

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

$$= -1$$

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

$$\bigcirc = 1$$

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

$$\bullet\bullet = 0$$

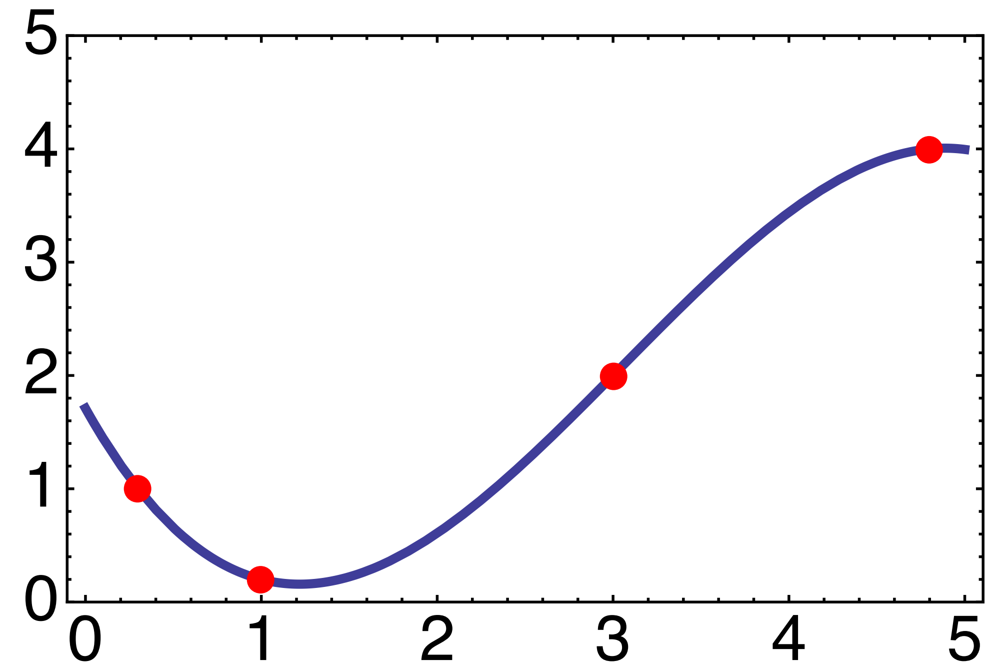
$$\bullet\bigcirc\bullet = 0$$

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

$$\bullet\bullet\bullet\bullet = -1$$

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

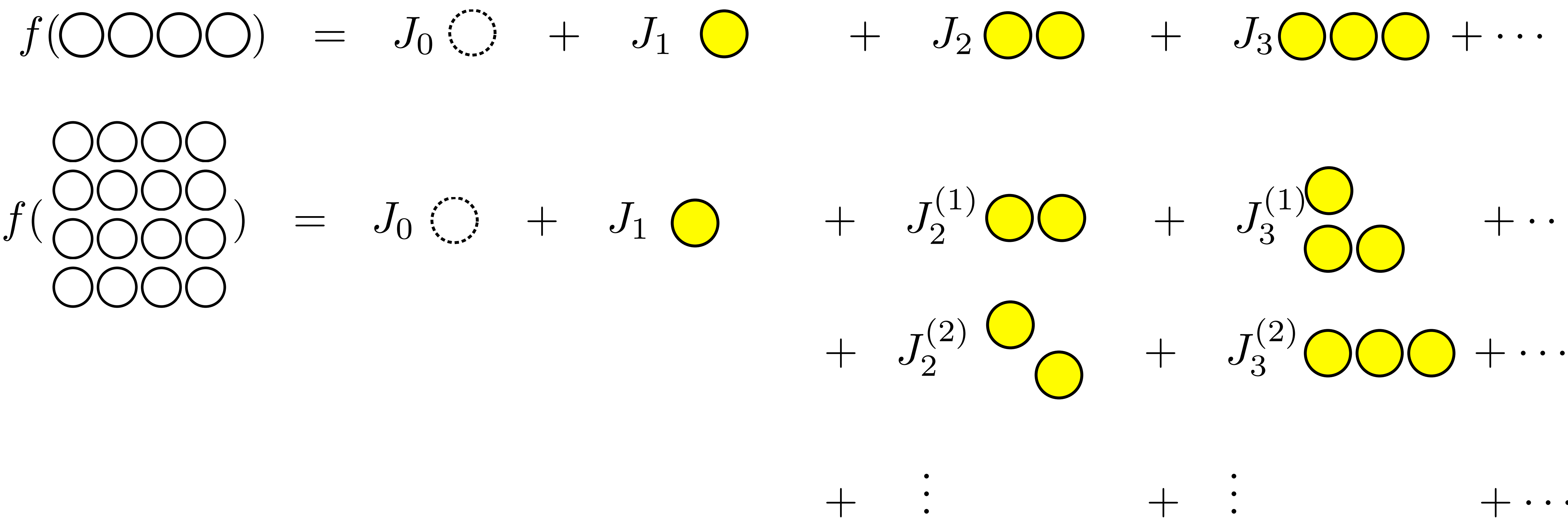
# Expanding in a power series




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

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

# In more than one dimension...



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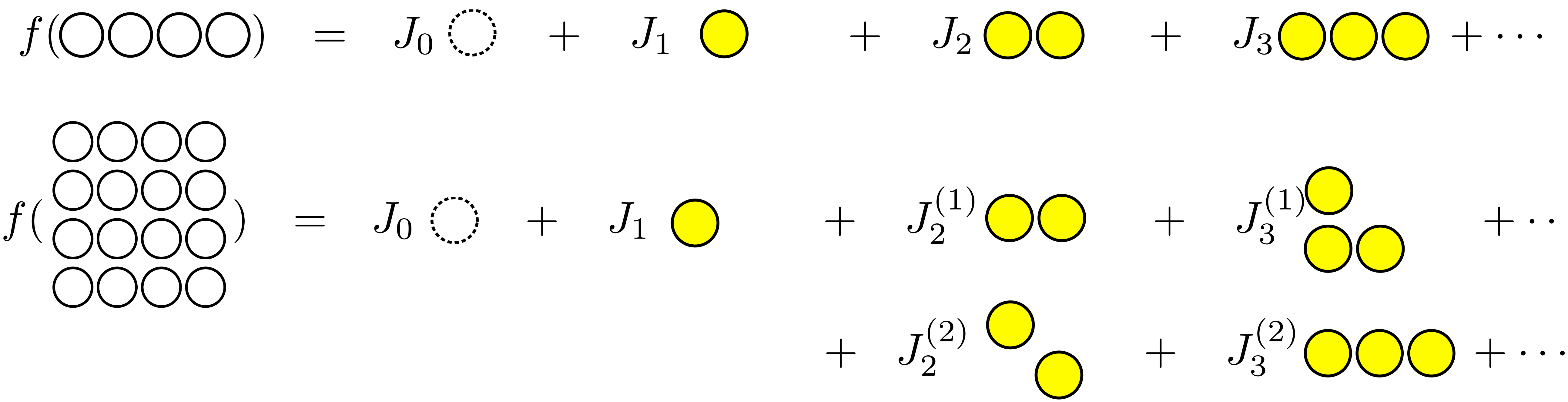
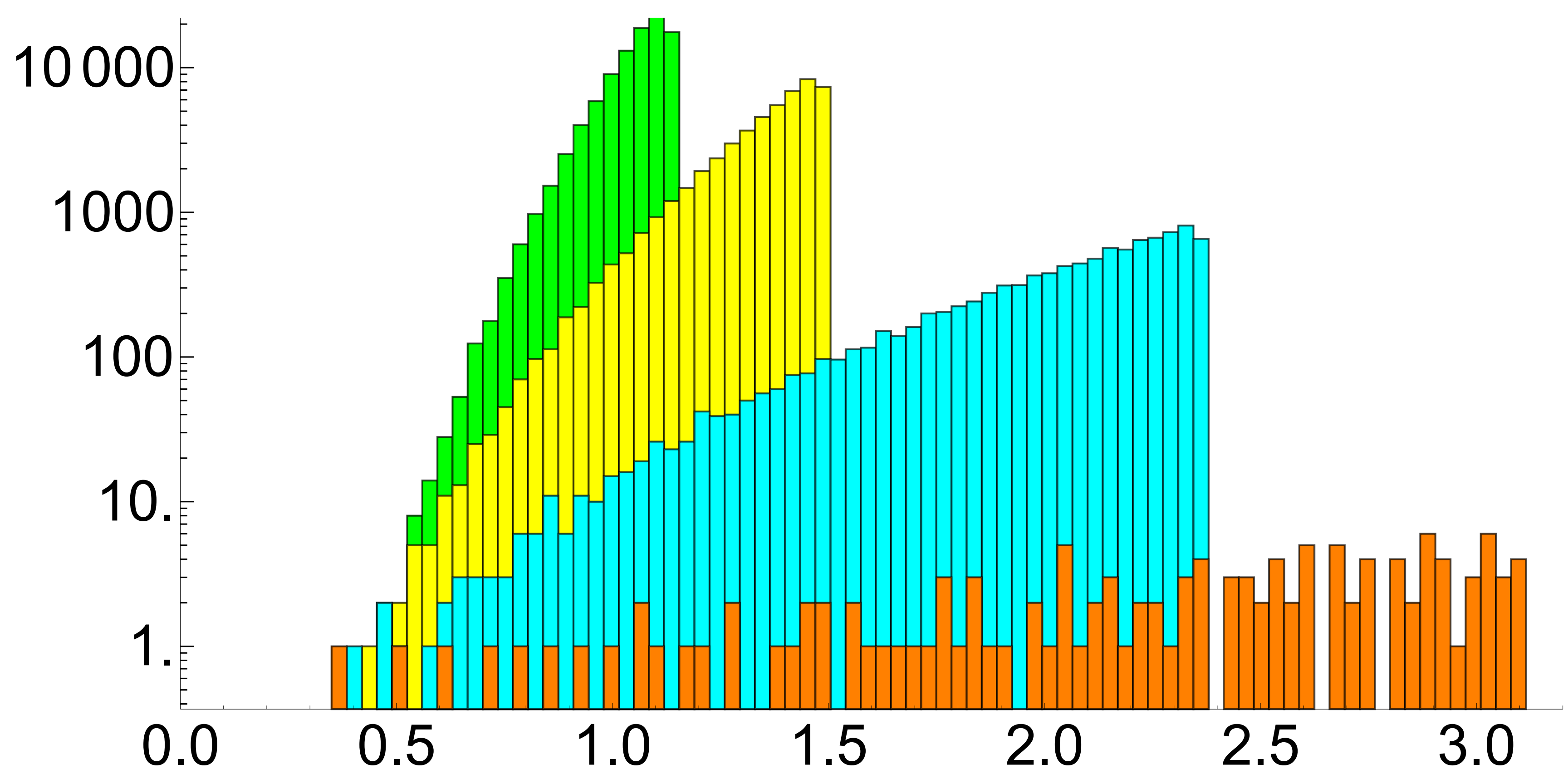
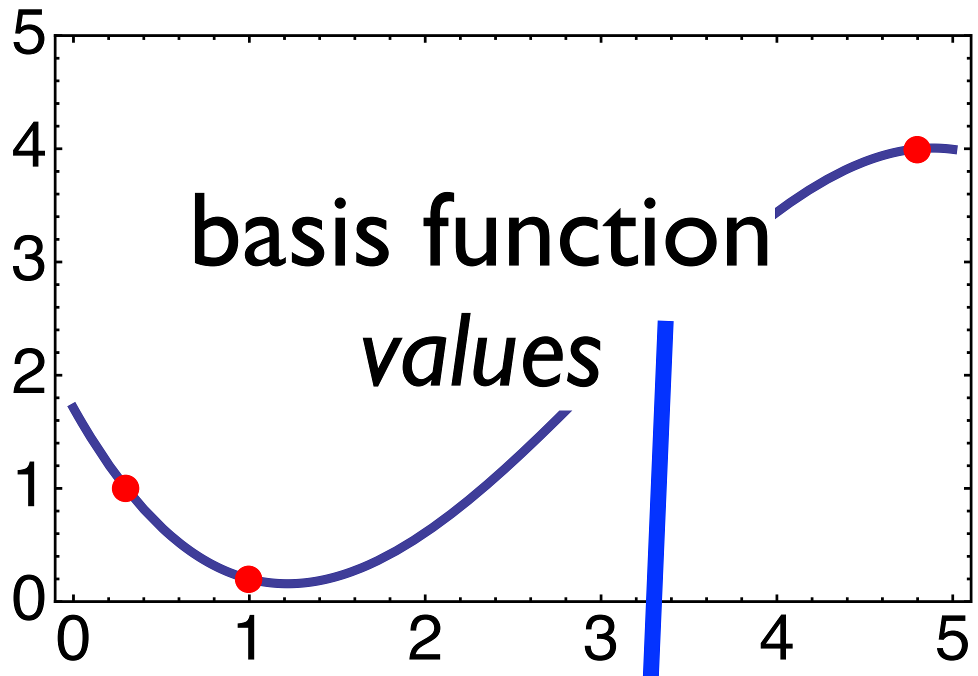



$+ \quad \vdots \quad + \cdots$



# Expanding in a power series




Data

basis function *values*

coefficients of the model

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

# Compressive sensing: It's like magic

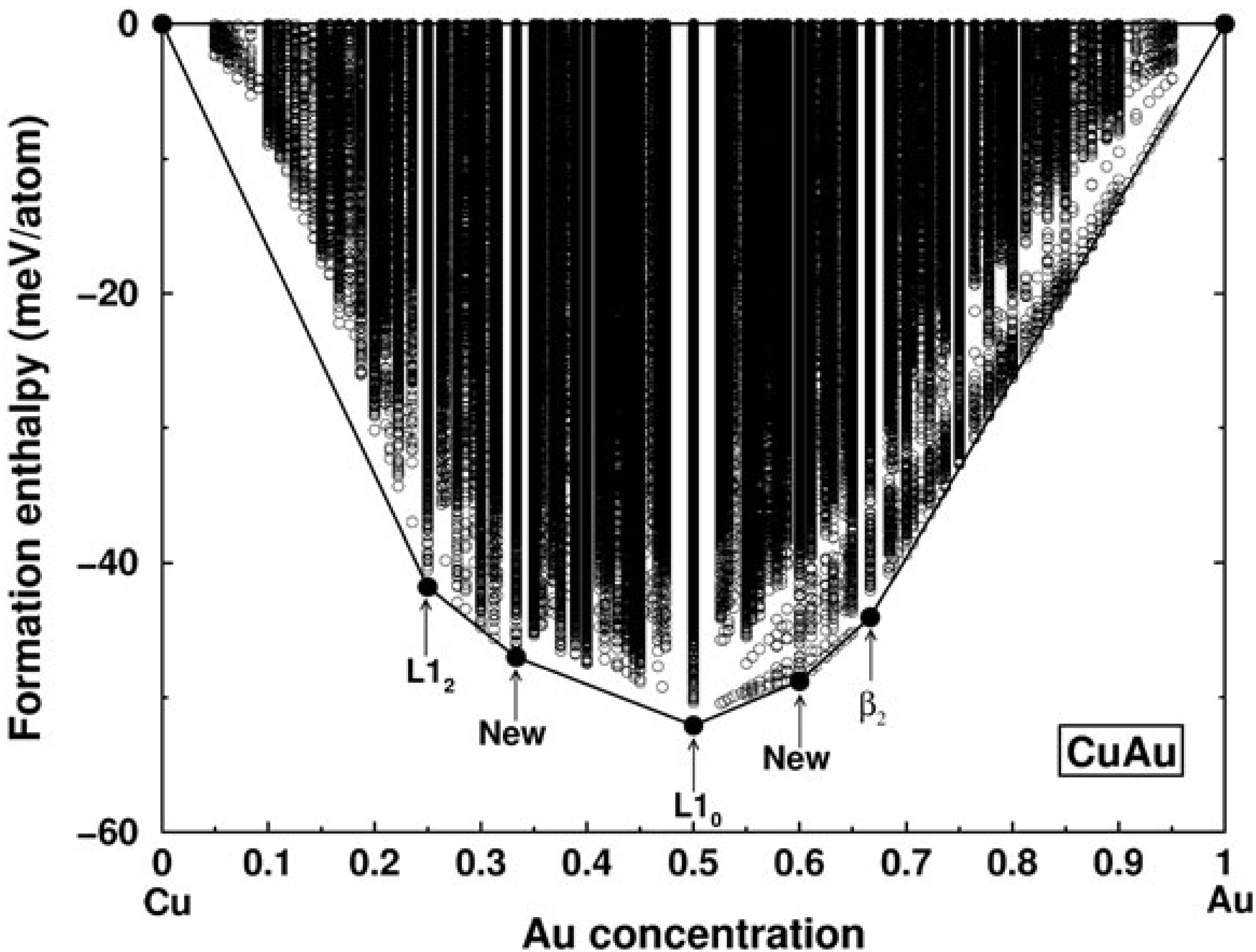
More info at the end of the talk

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

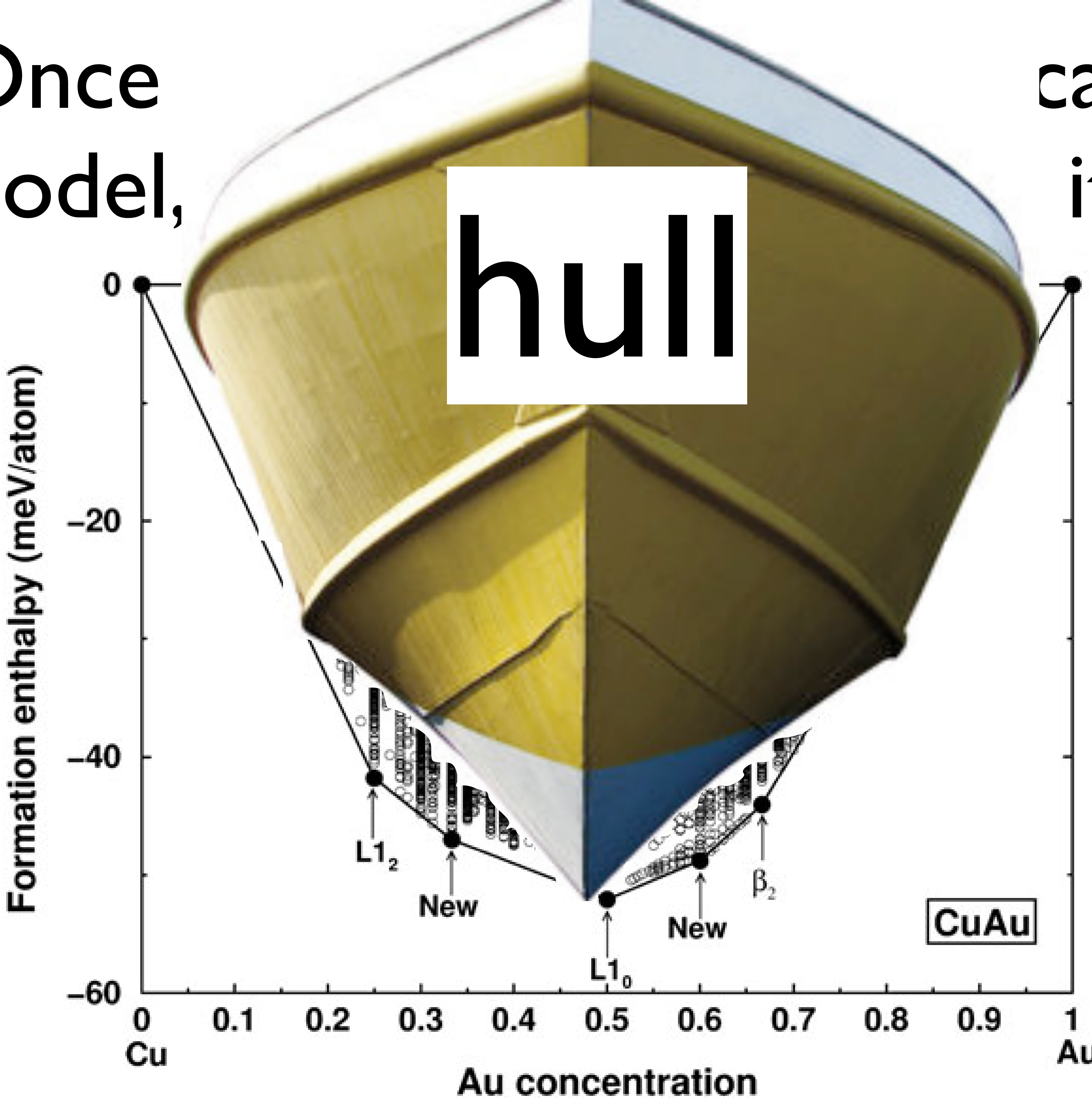
# Once you have a good physical model, what can you do with it?

Calculate the energy of
millions of configurations

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



Once cal
model, it?



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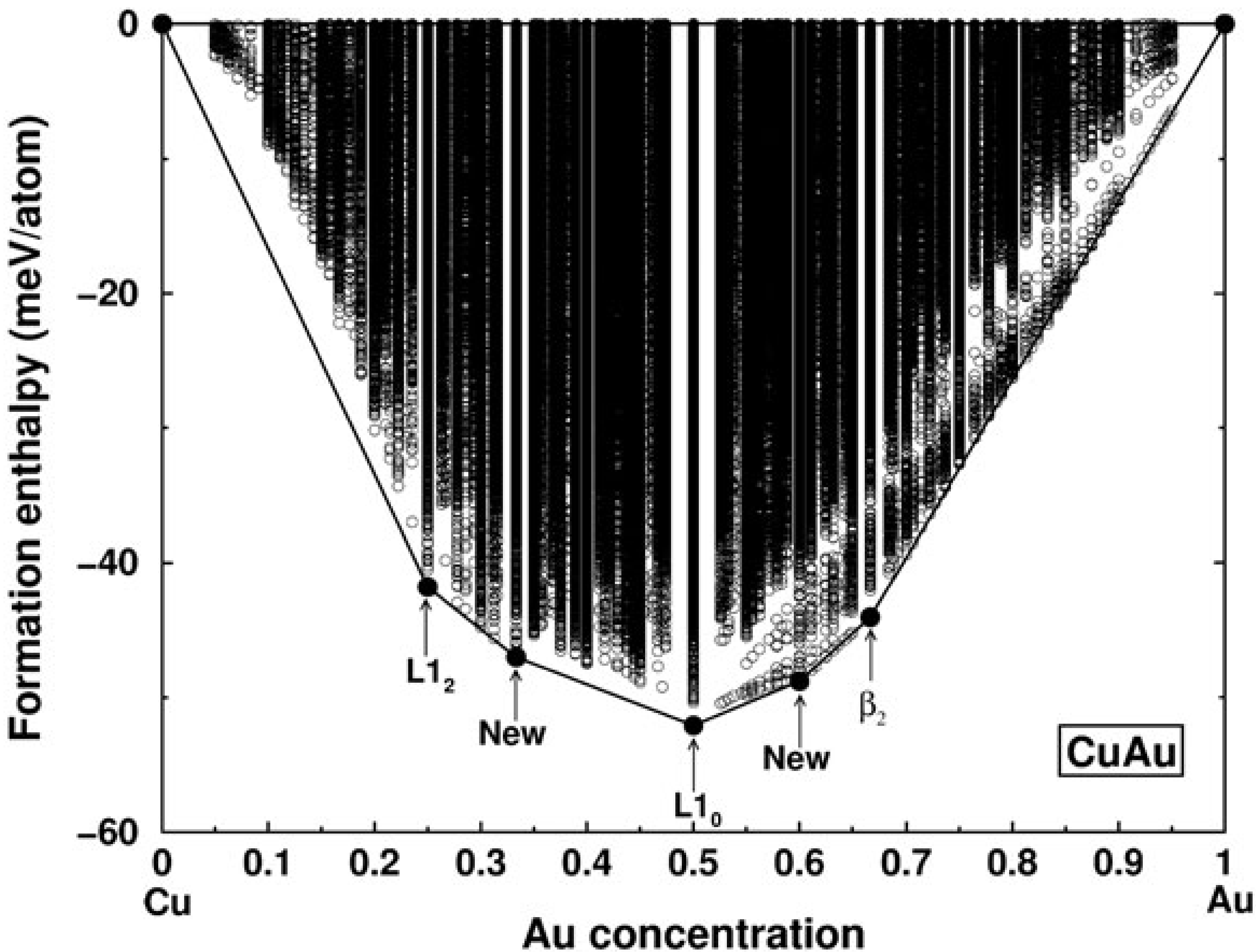
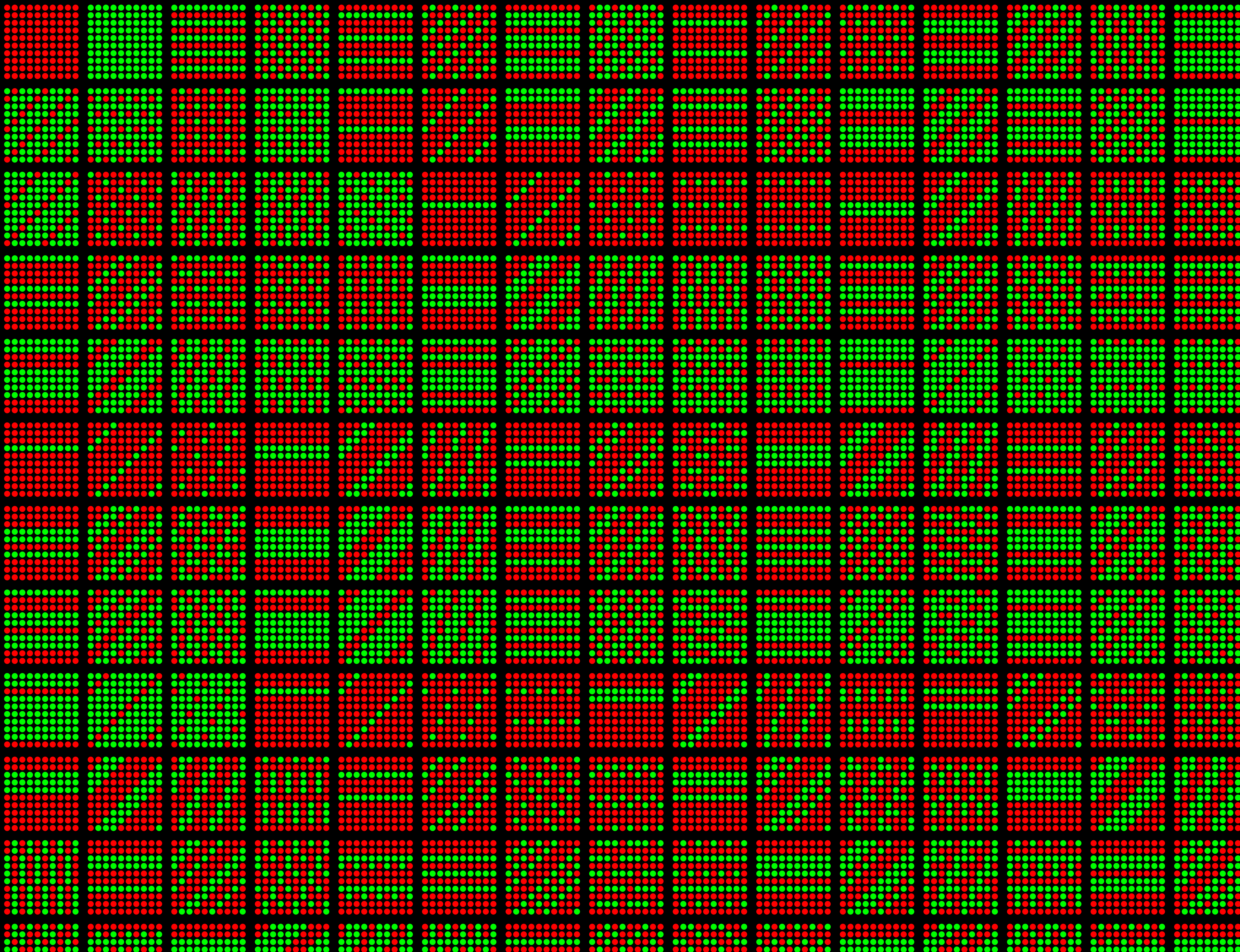
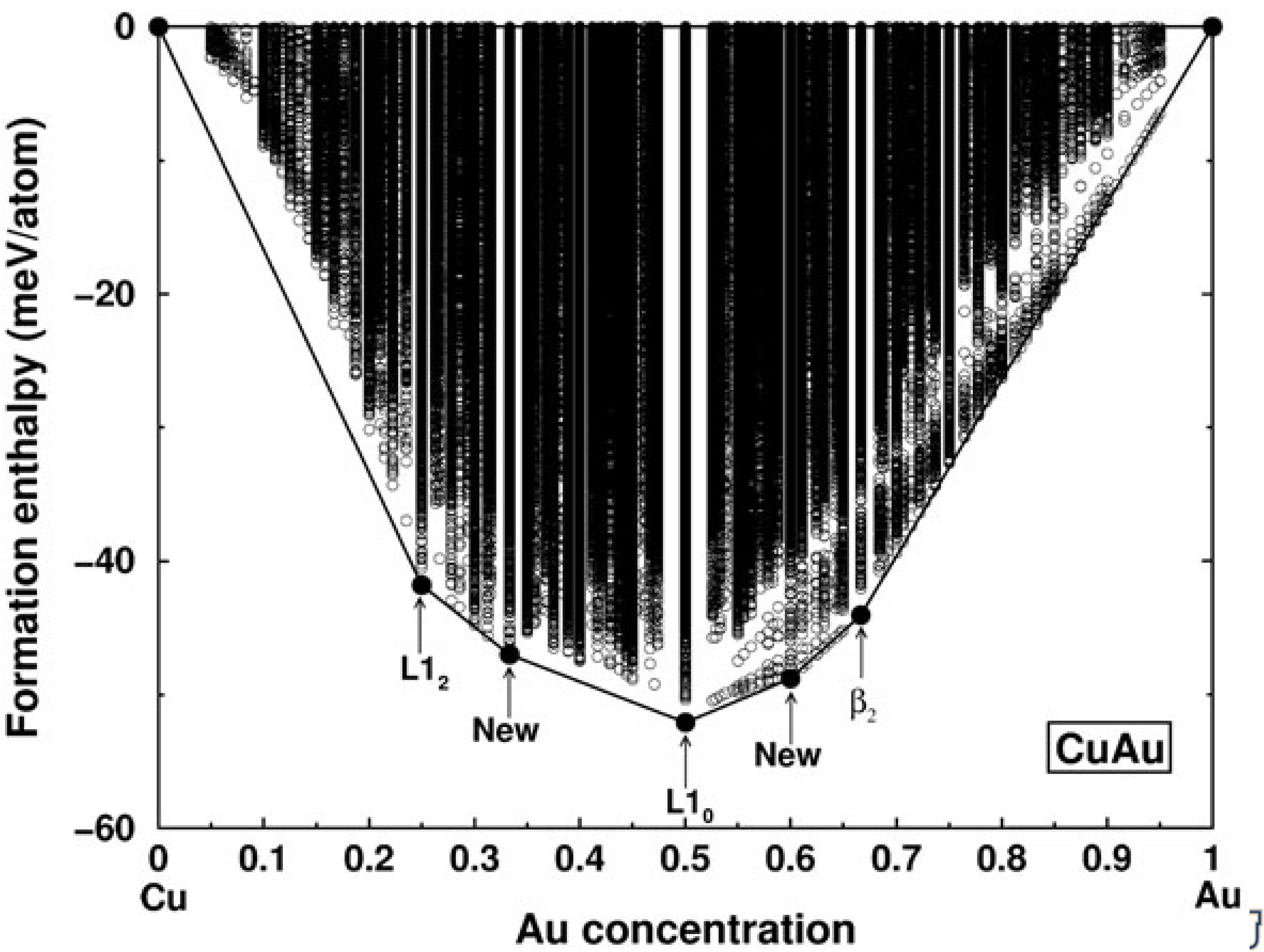
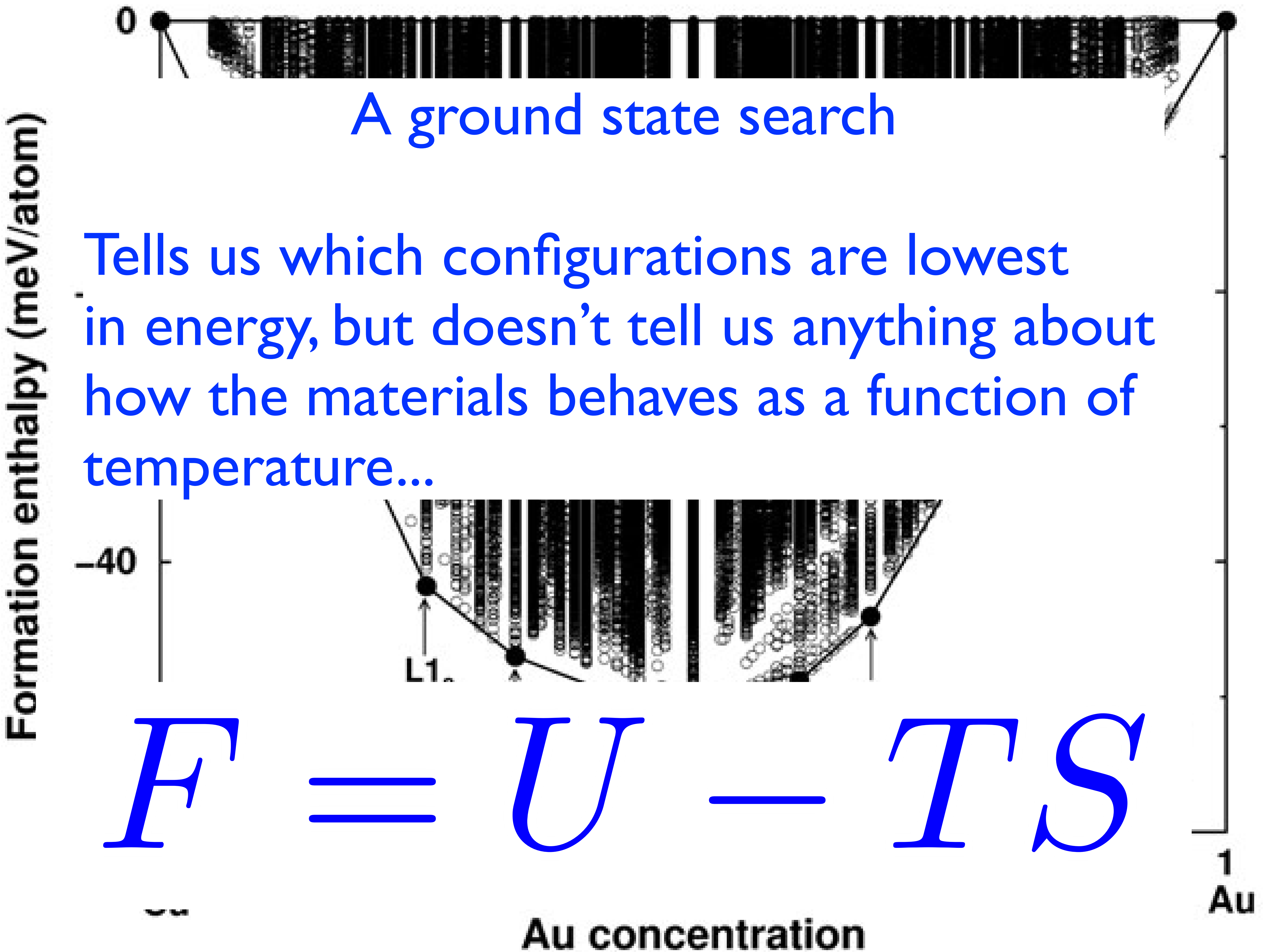






Formation enthalpy (meV/atom)
0
−20
−40
−60
L1$_2$
New
L1$_0$
New
β$_2$
CuAu
0
Cu
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Au
Au concentration

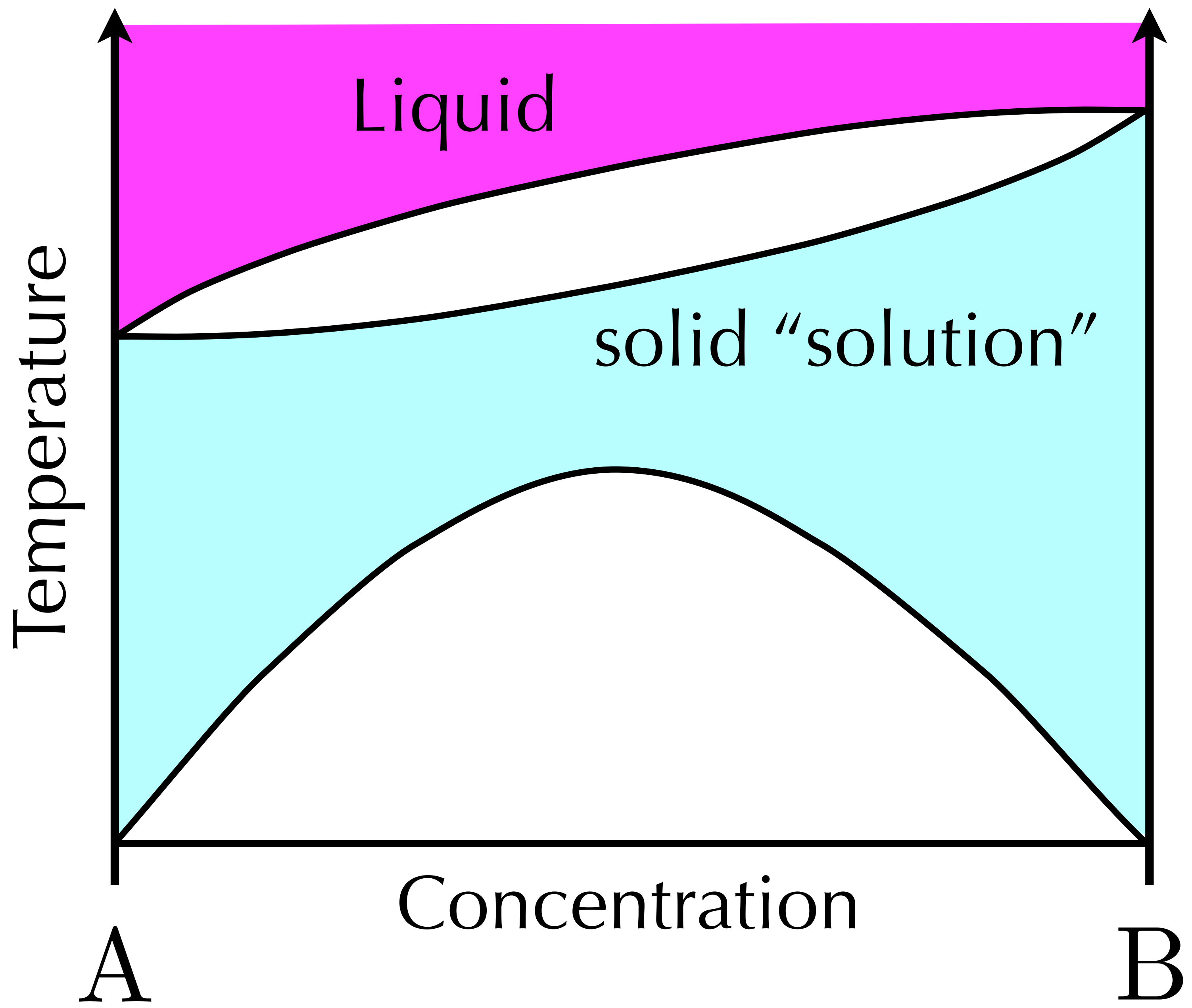



A ground state search

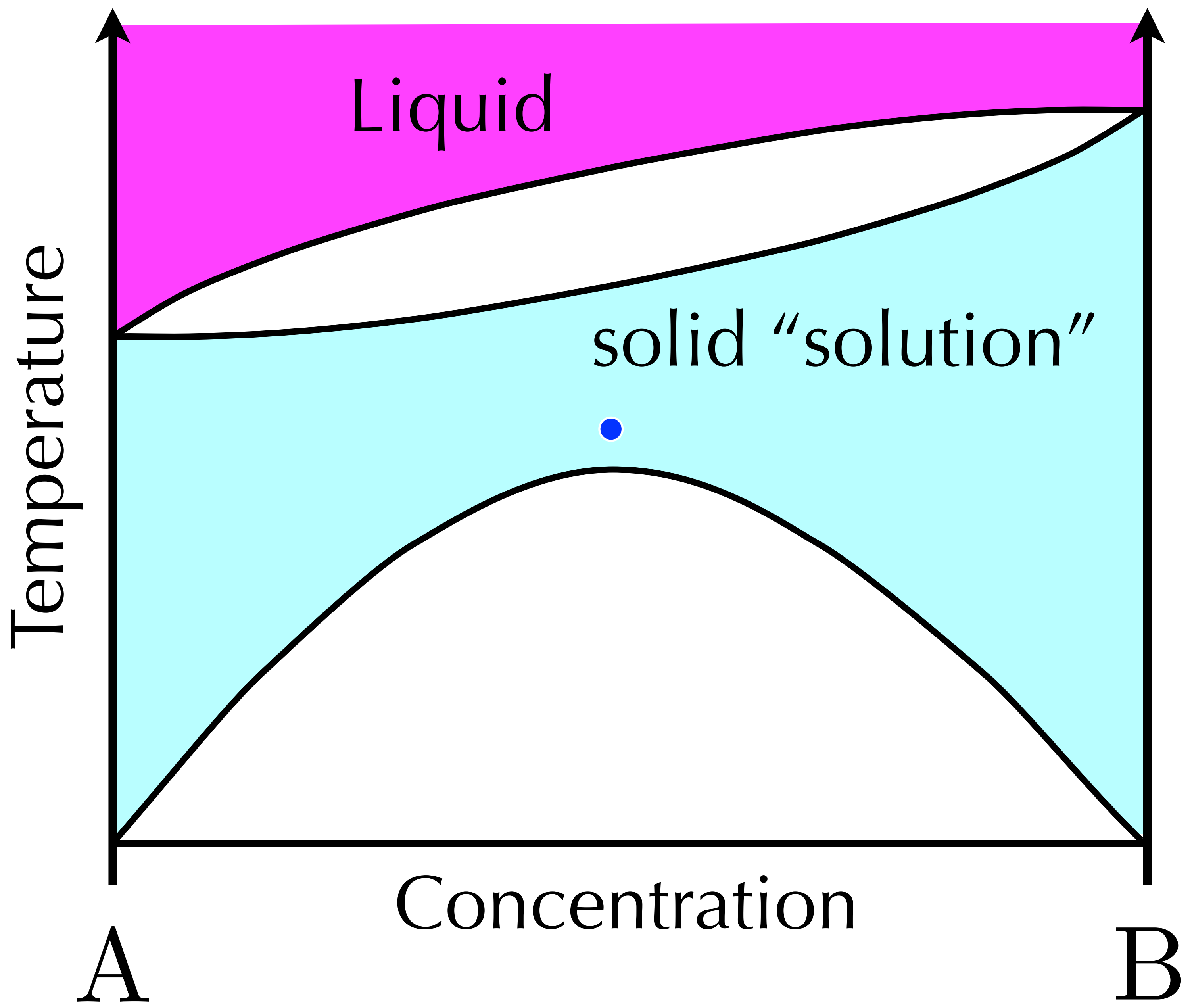
Tells us which configurations are lowest in energy, but doesn't tell us anything about how the materials behaves as a function of temperature...

$$F = U - TS$$

# Alloy phase diagrams



# What happens as it cools?



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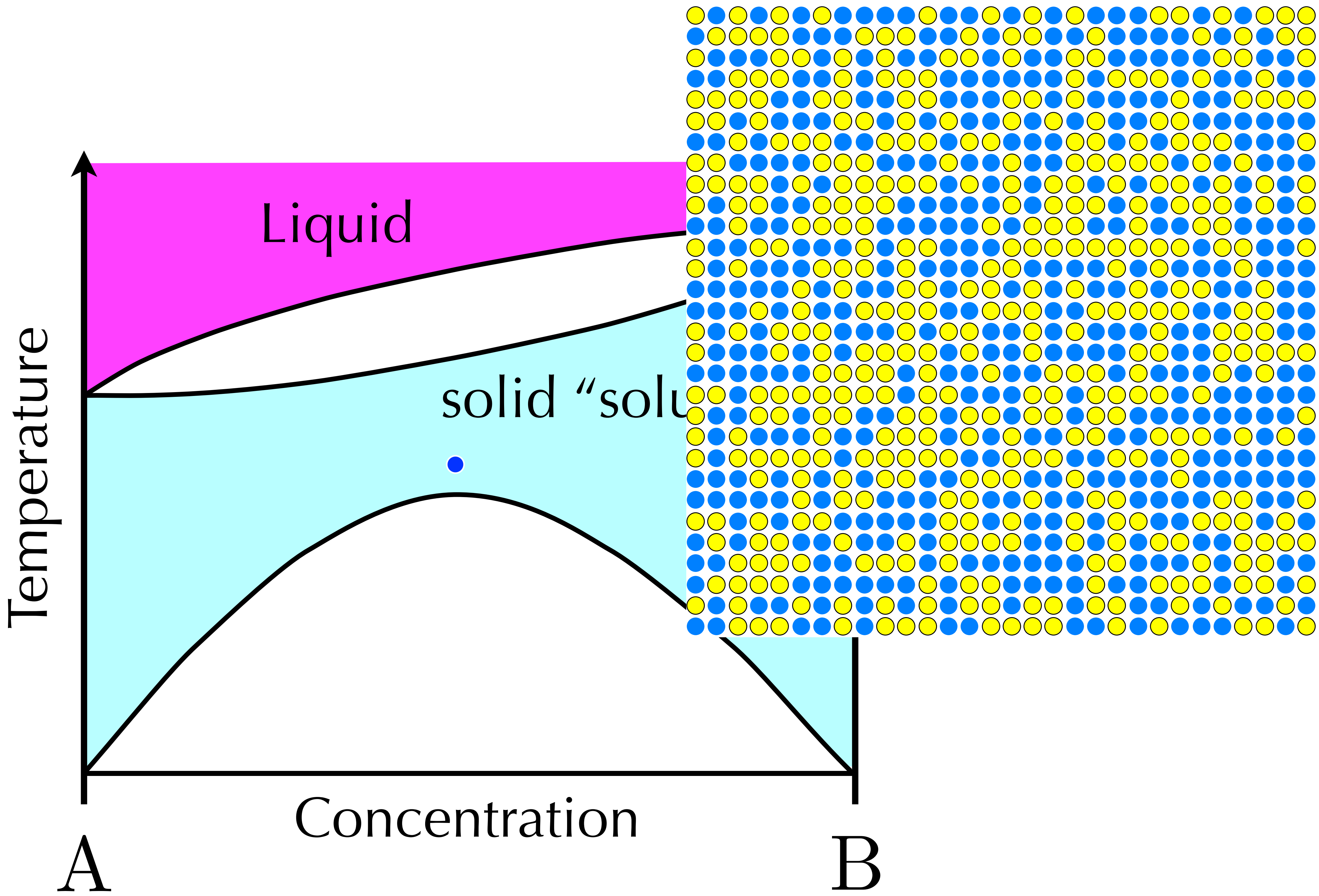

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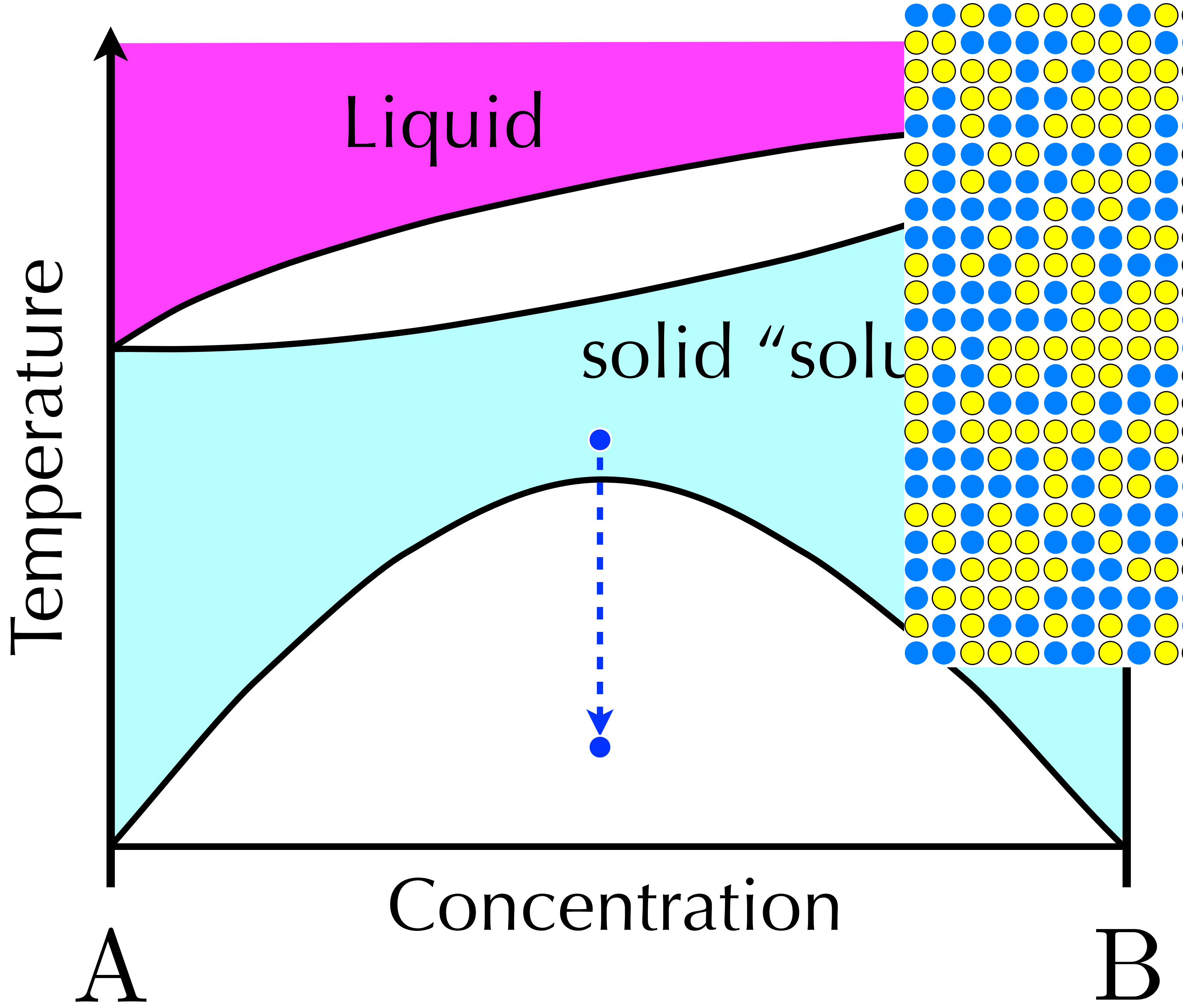


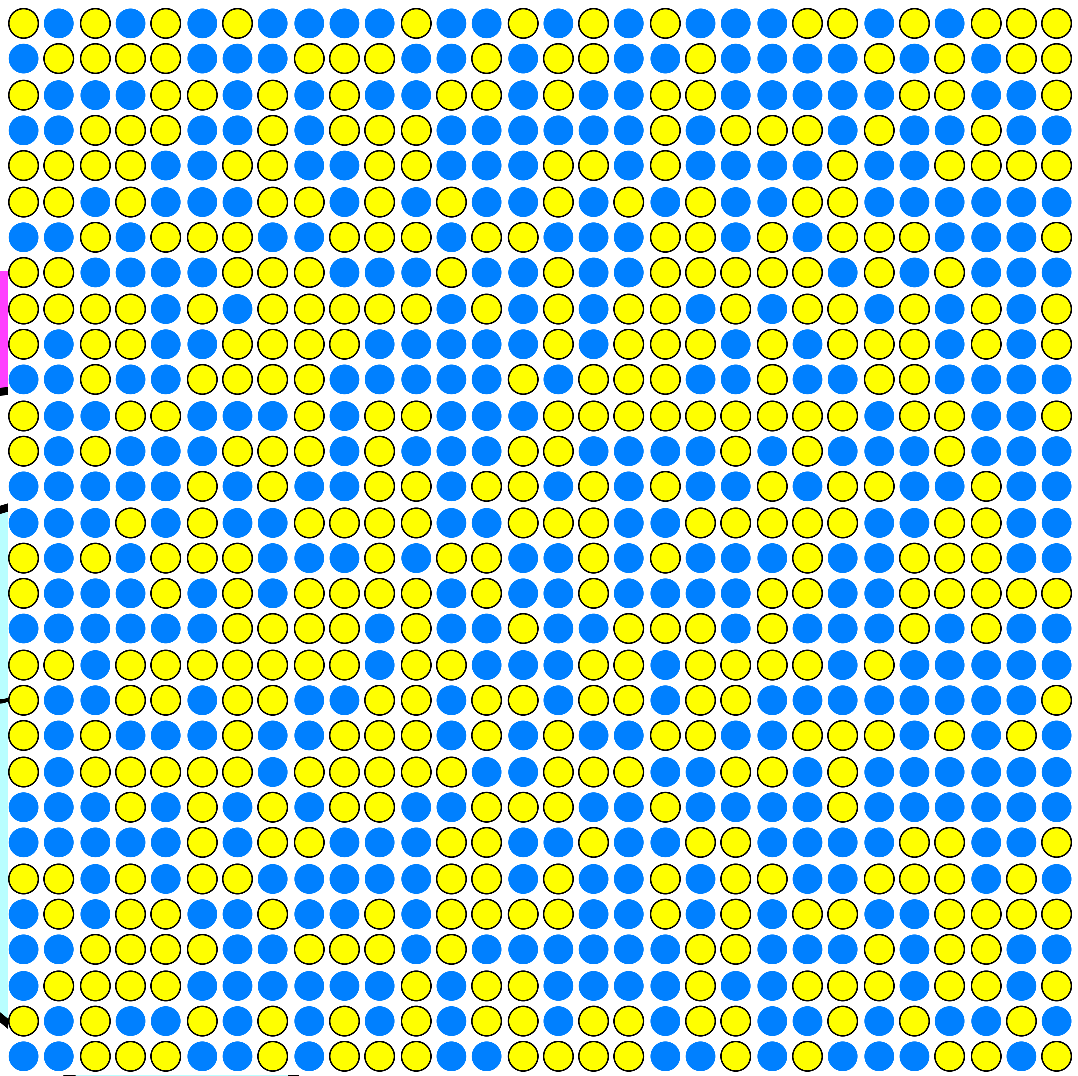

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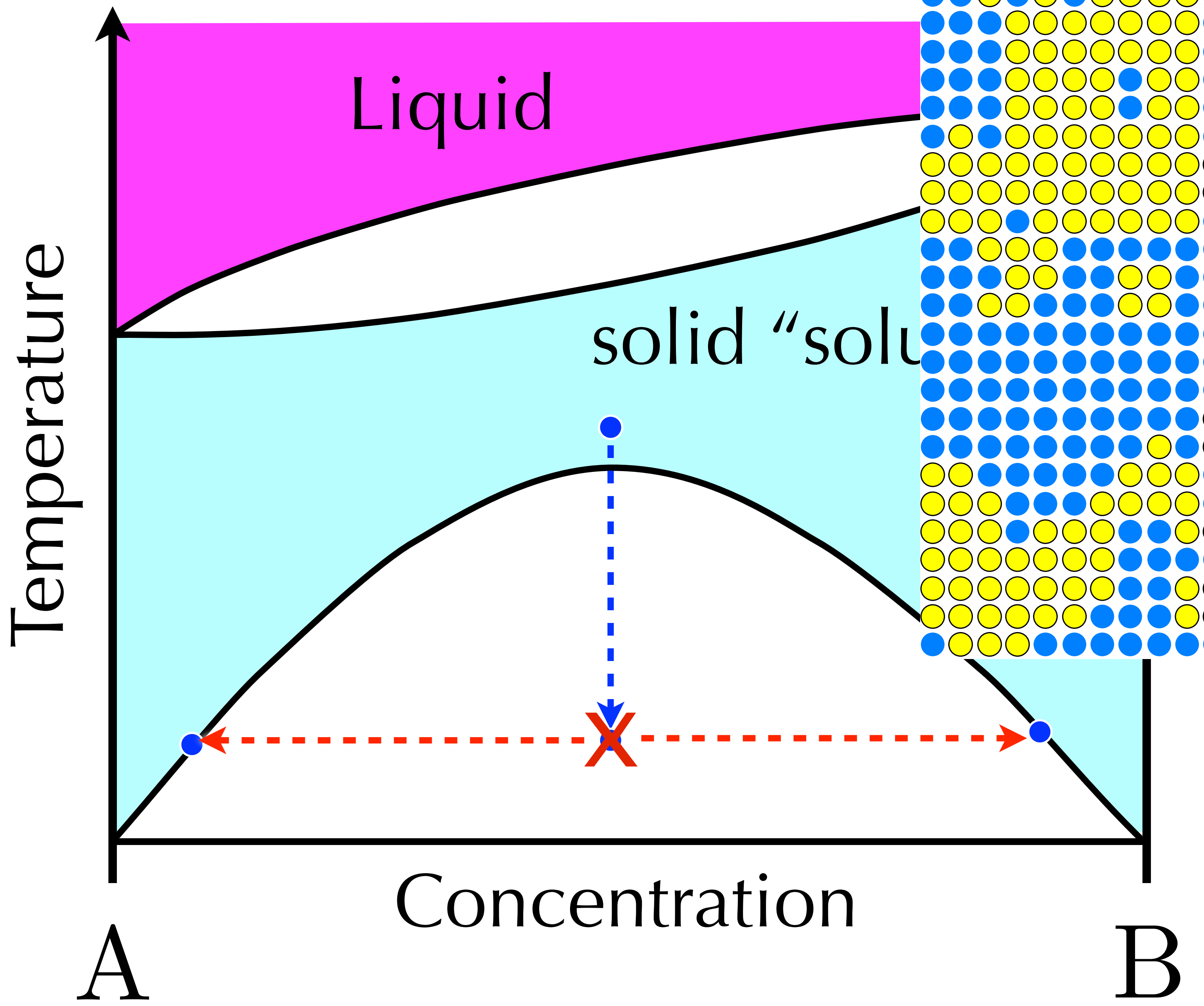
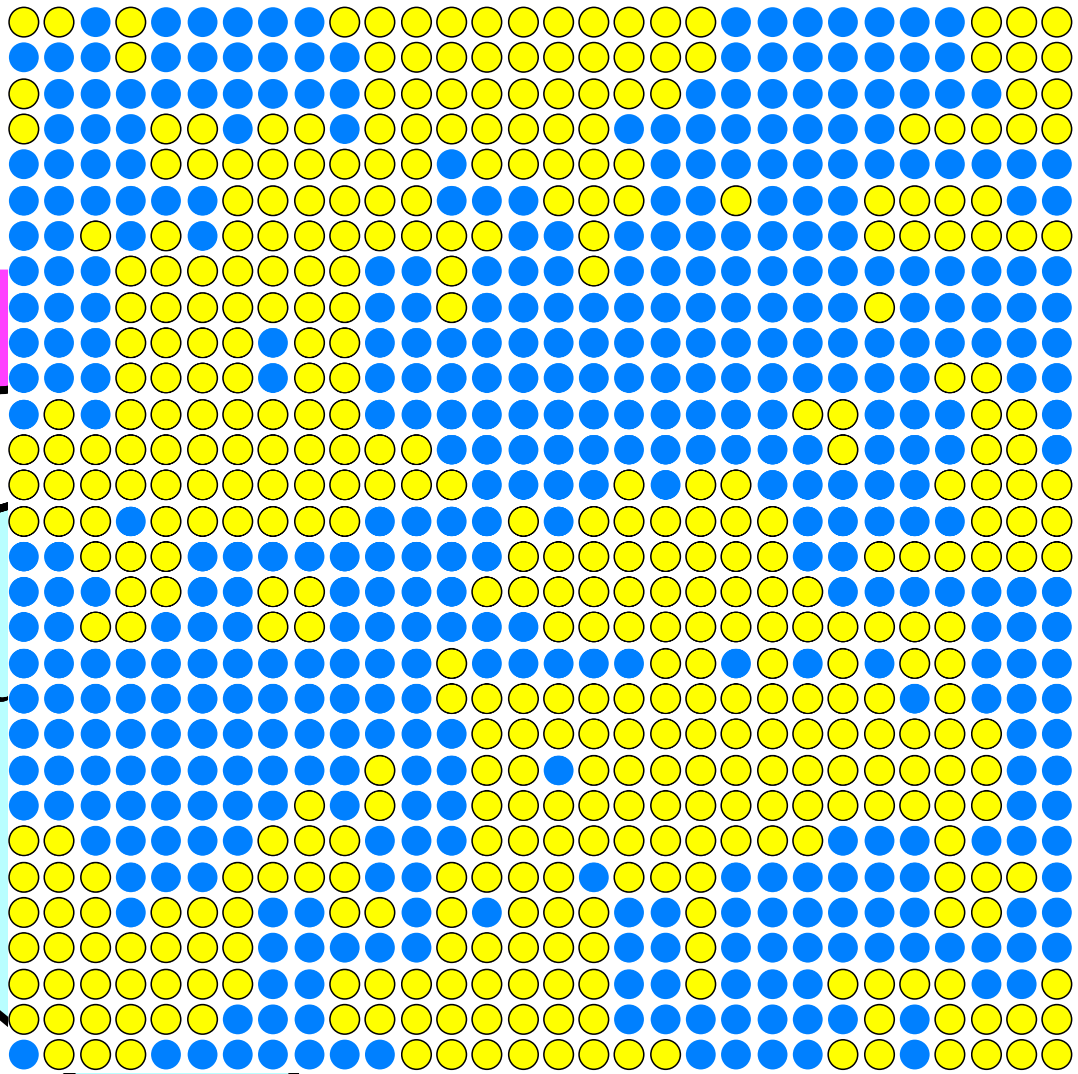
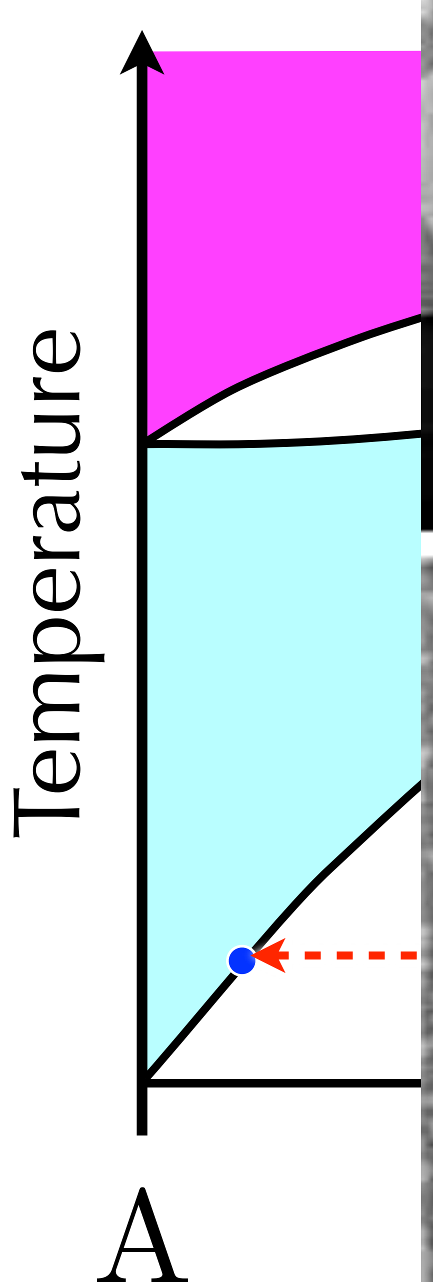
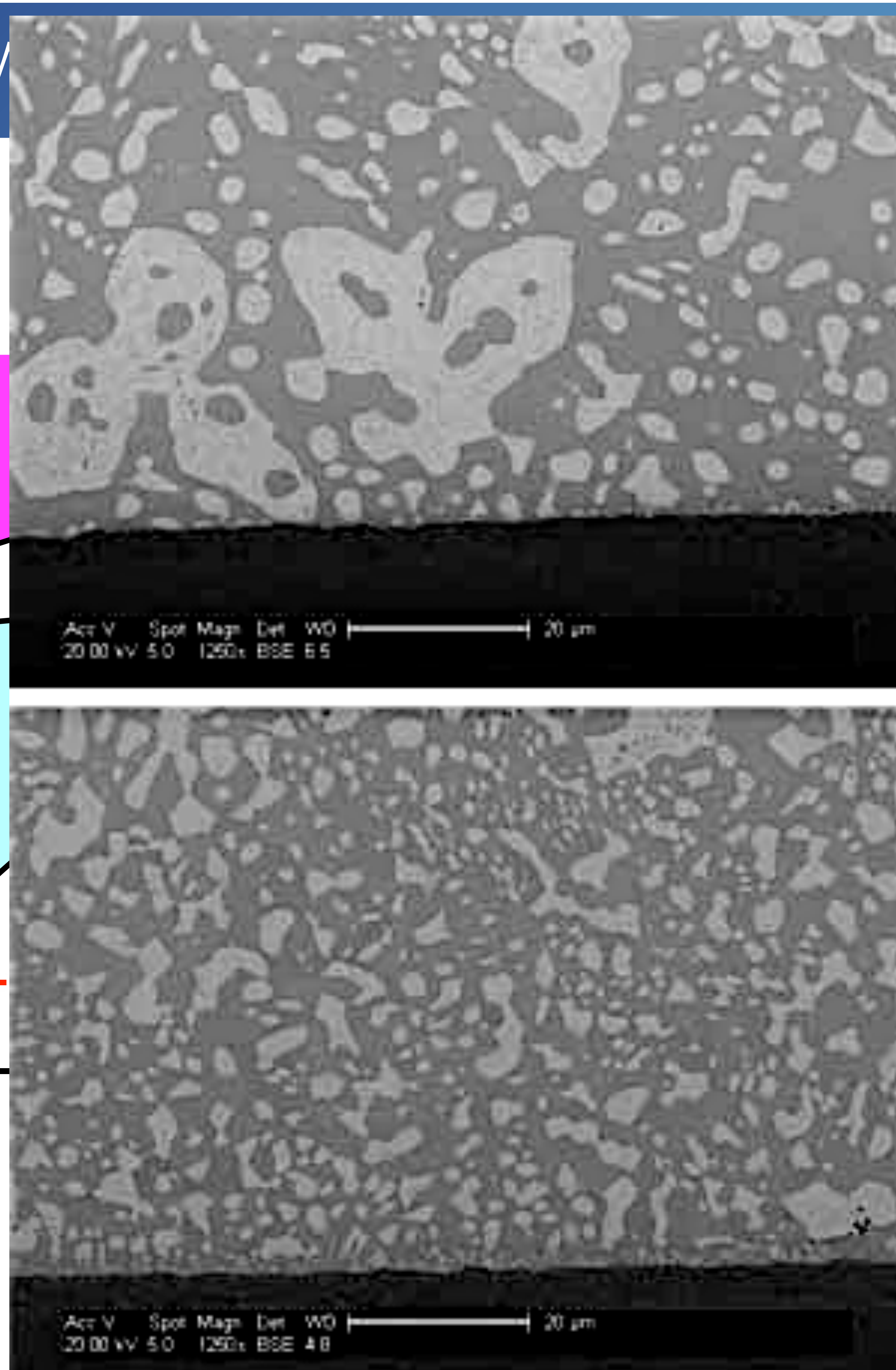


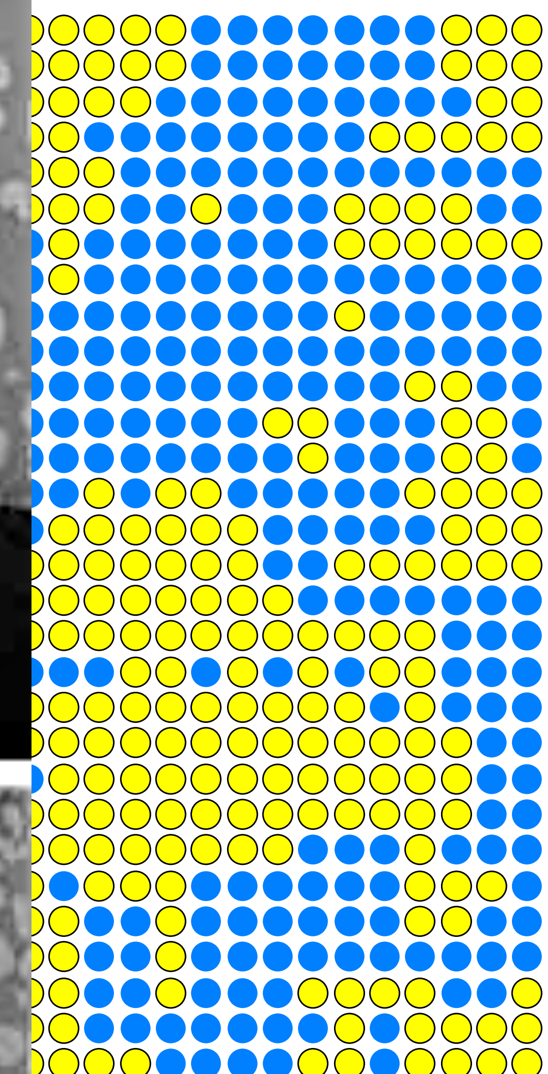
# V



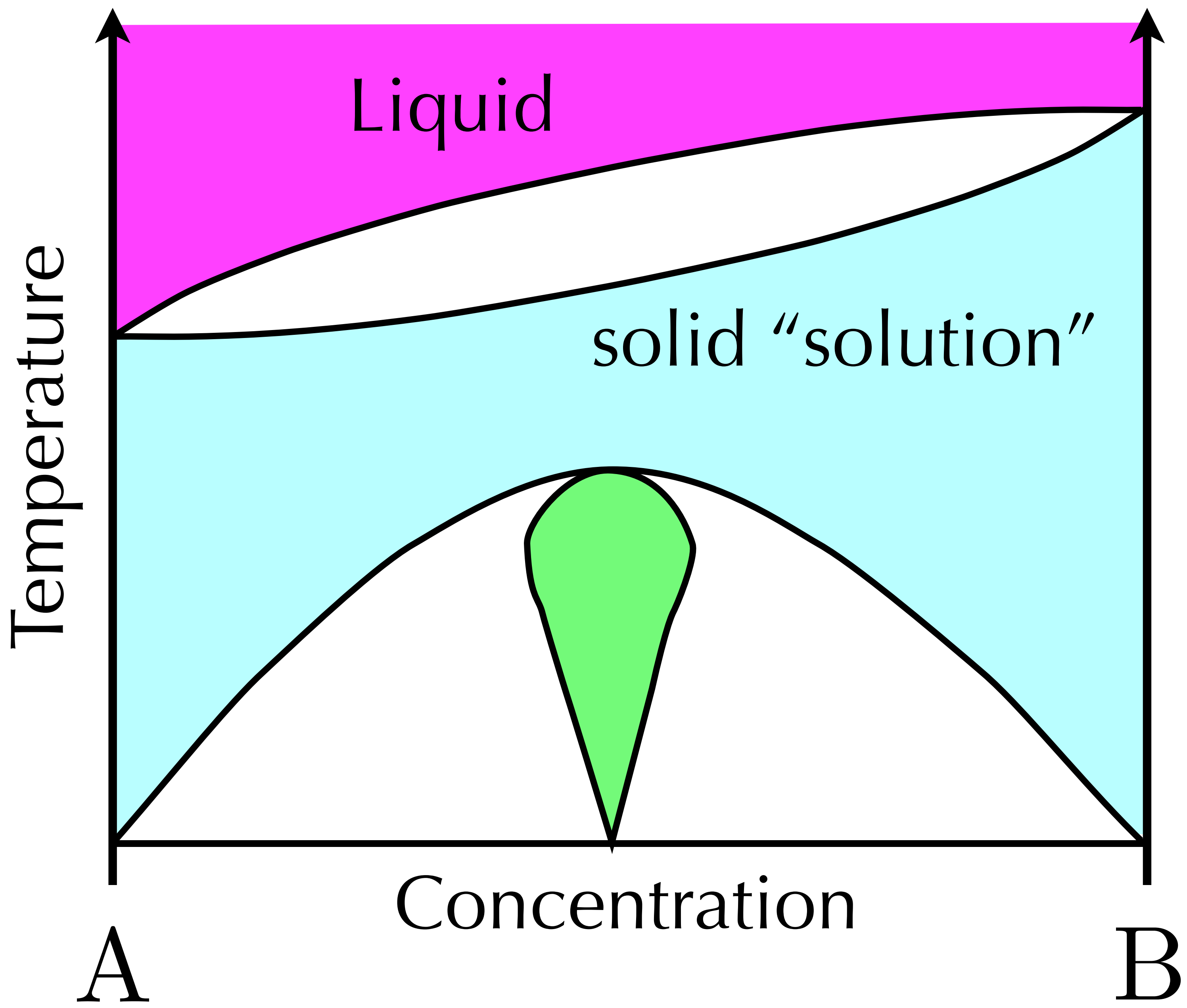
Temperature
A

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



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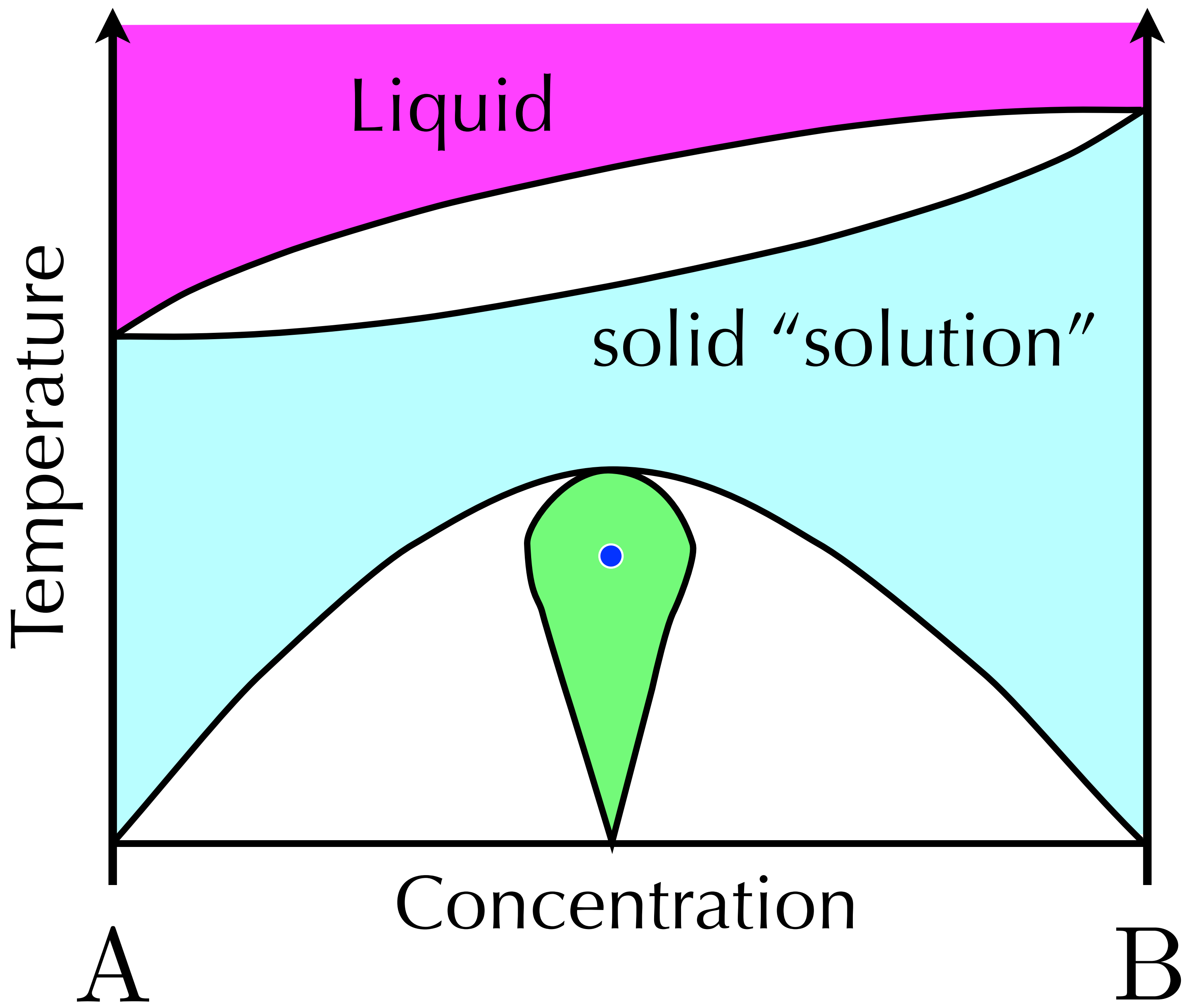

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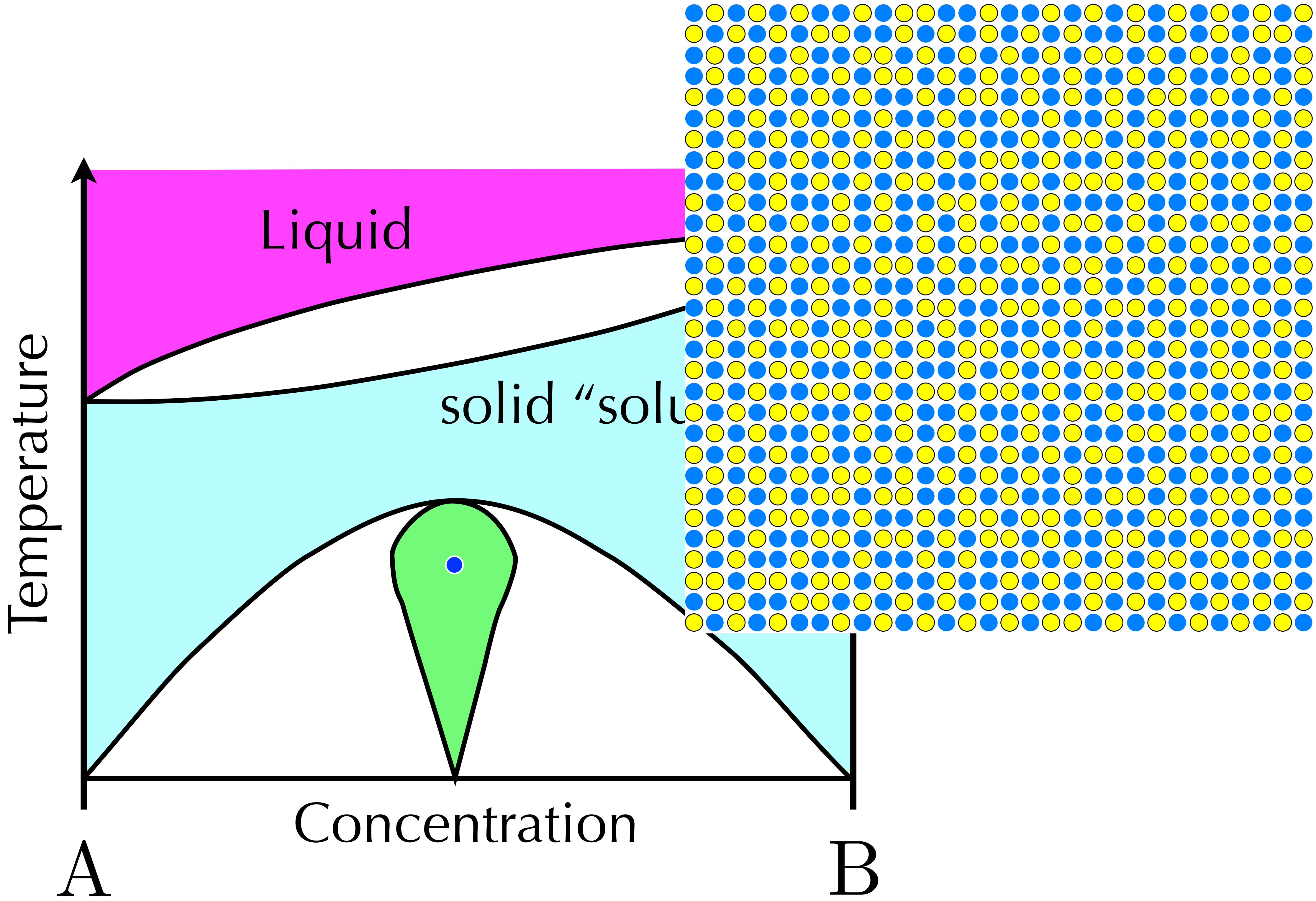

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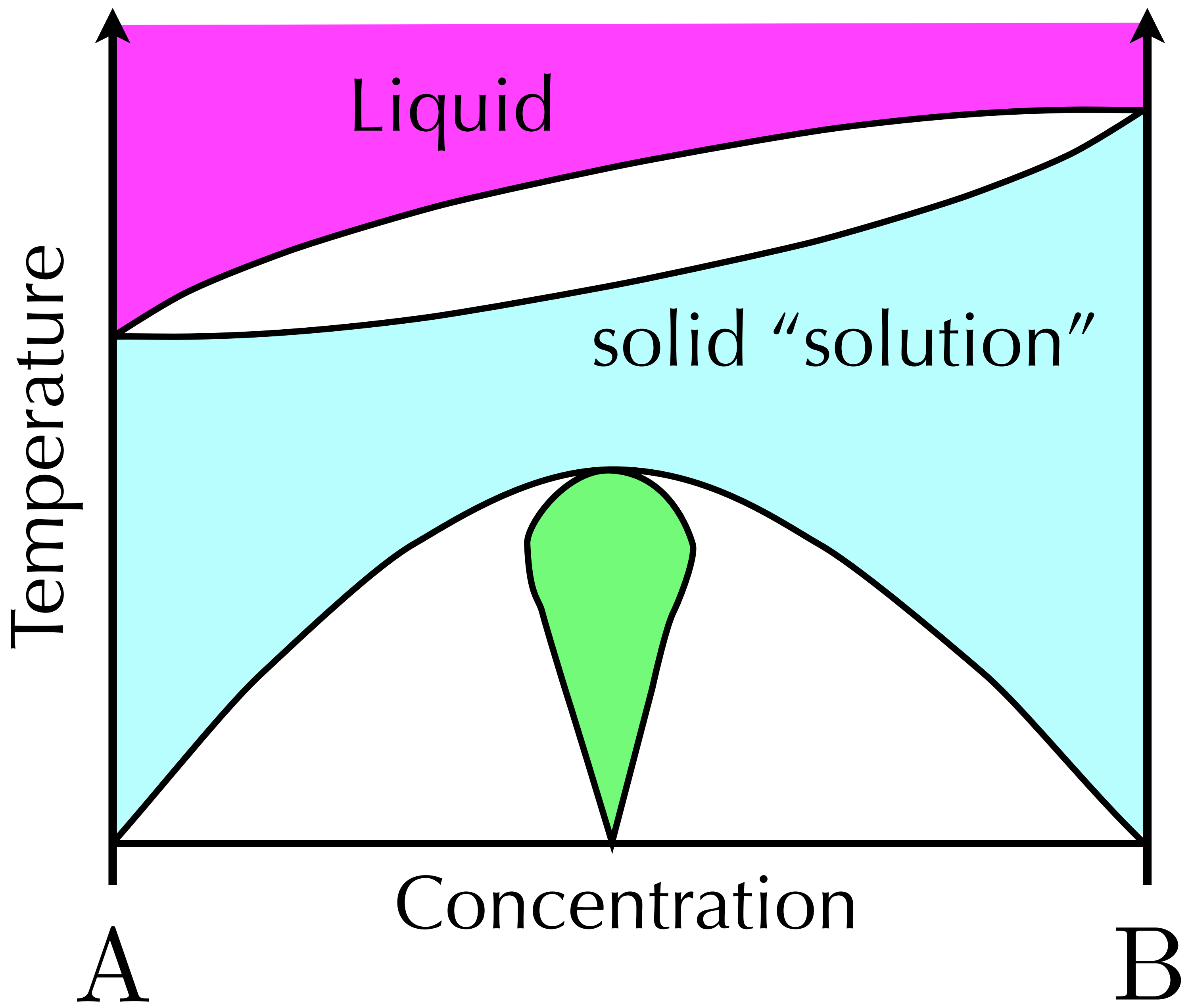

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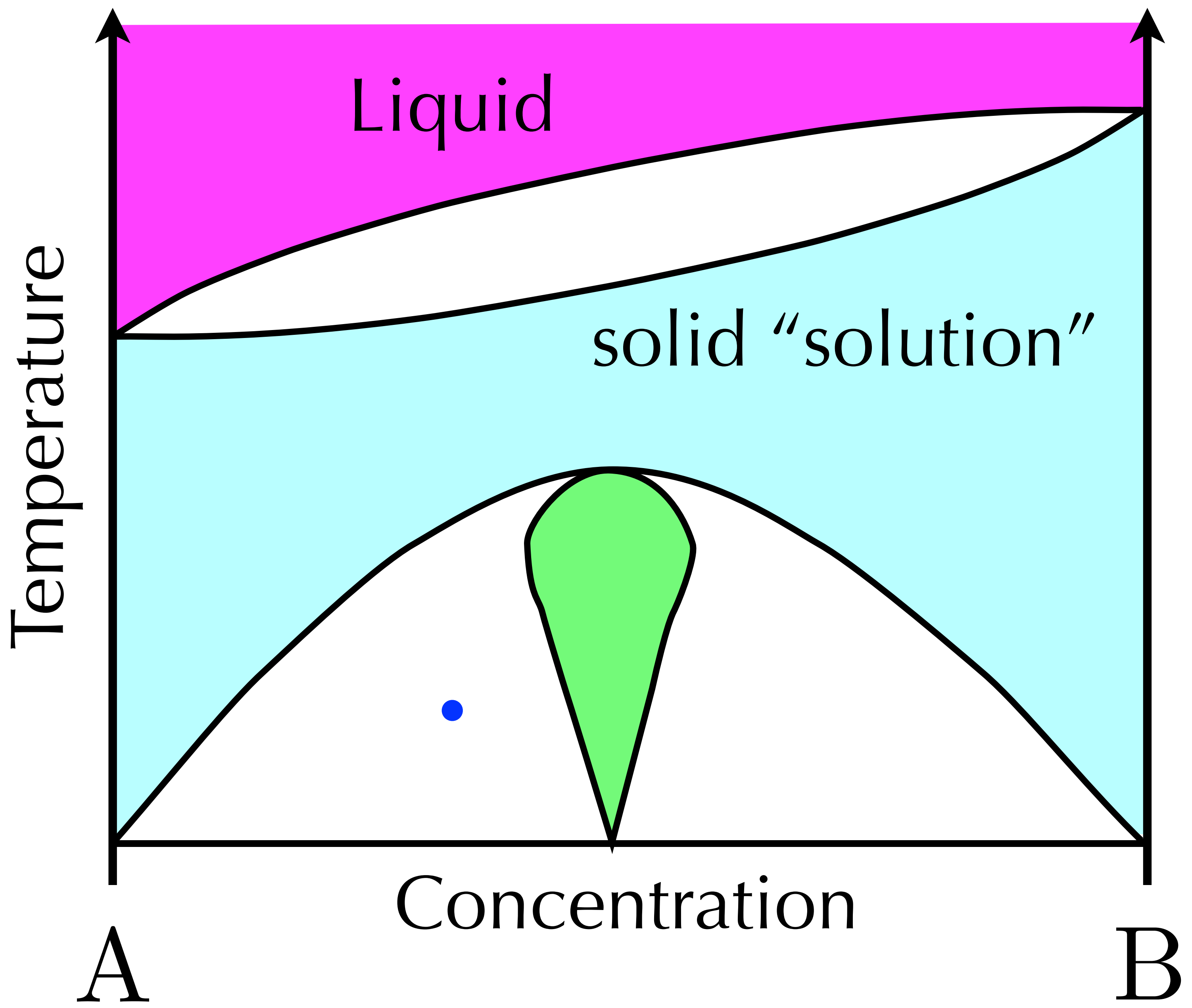

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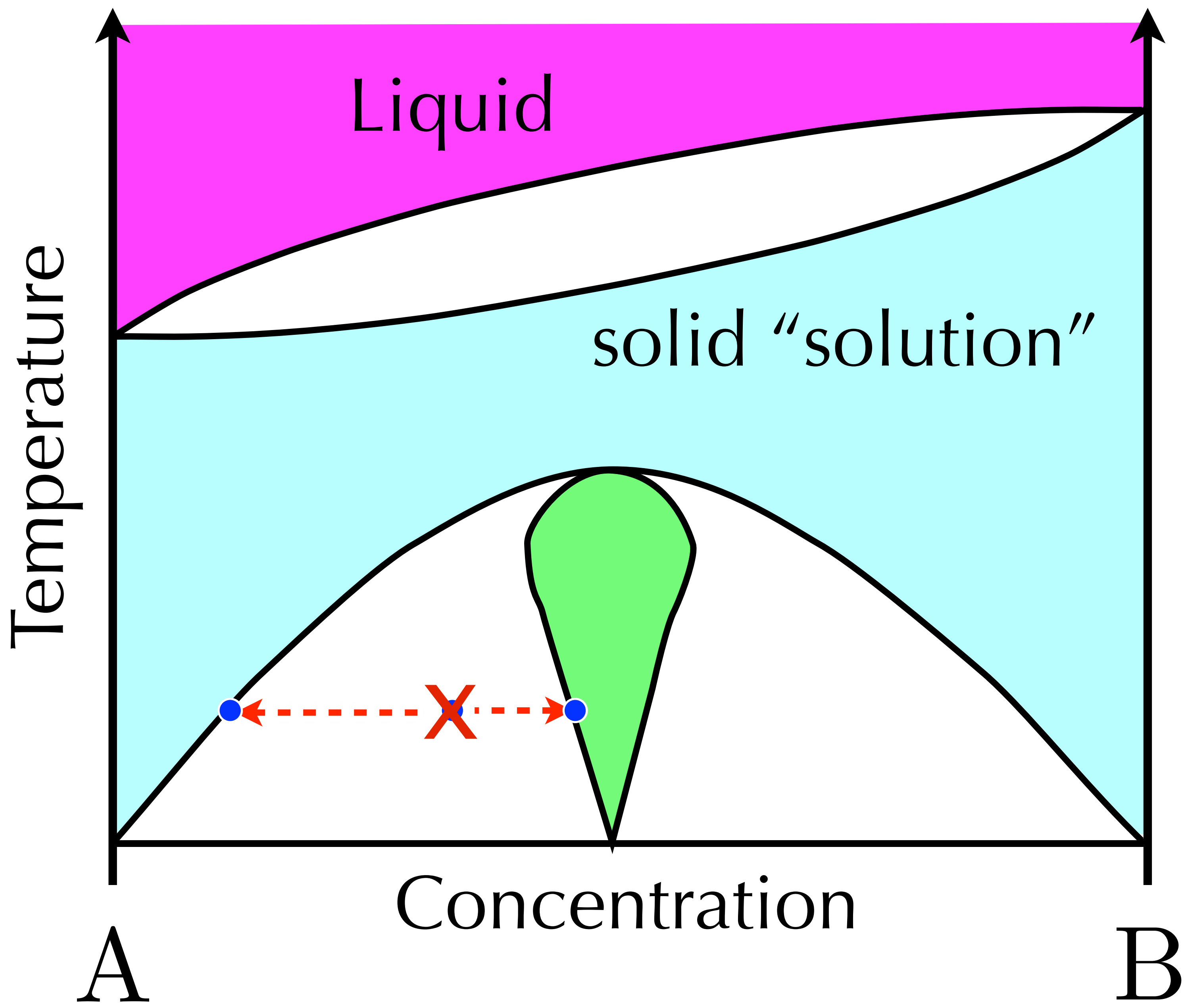

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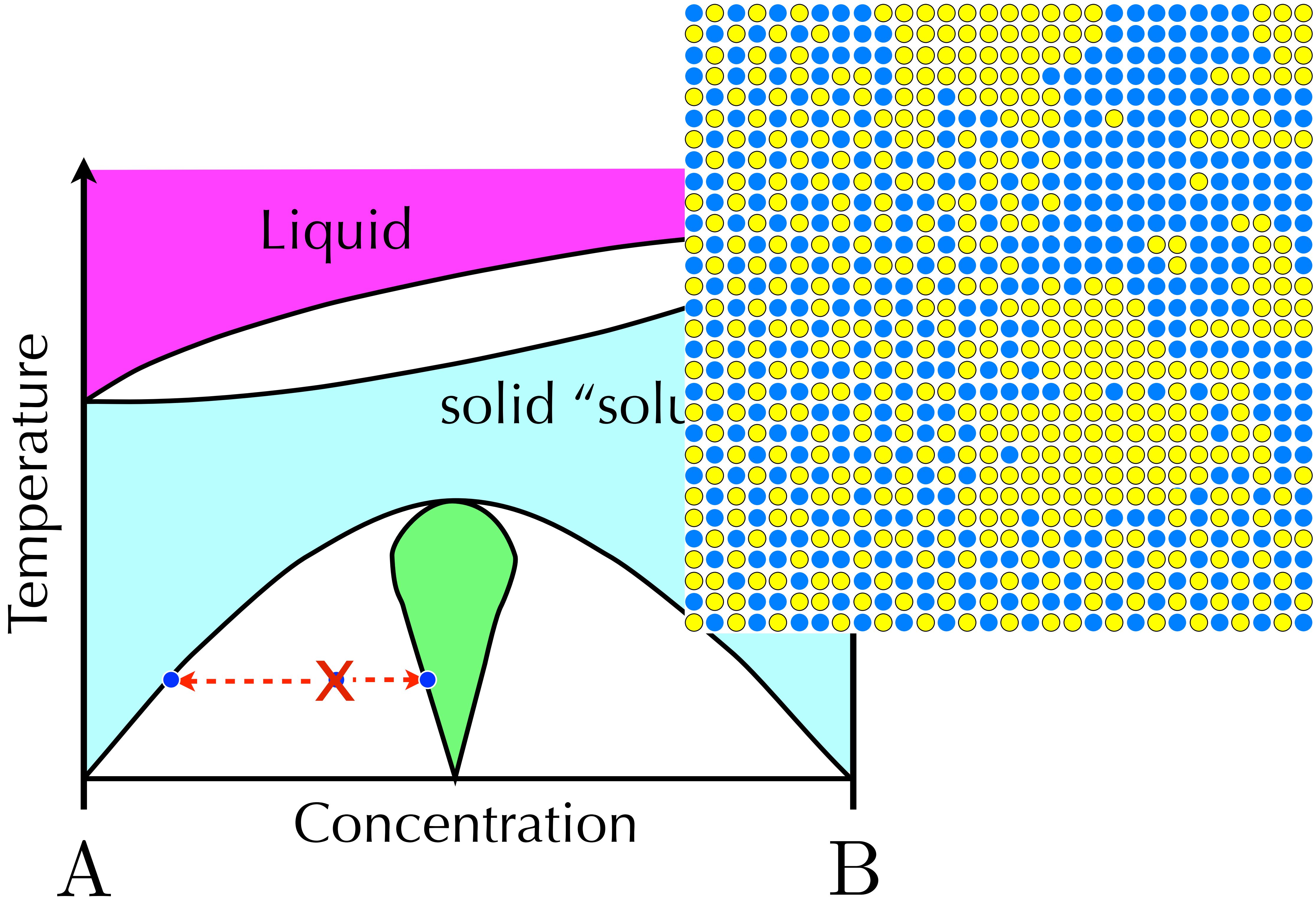

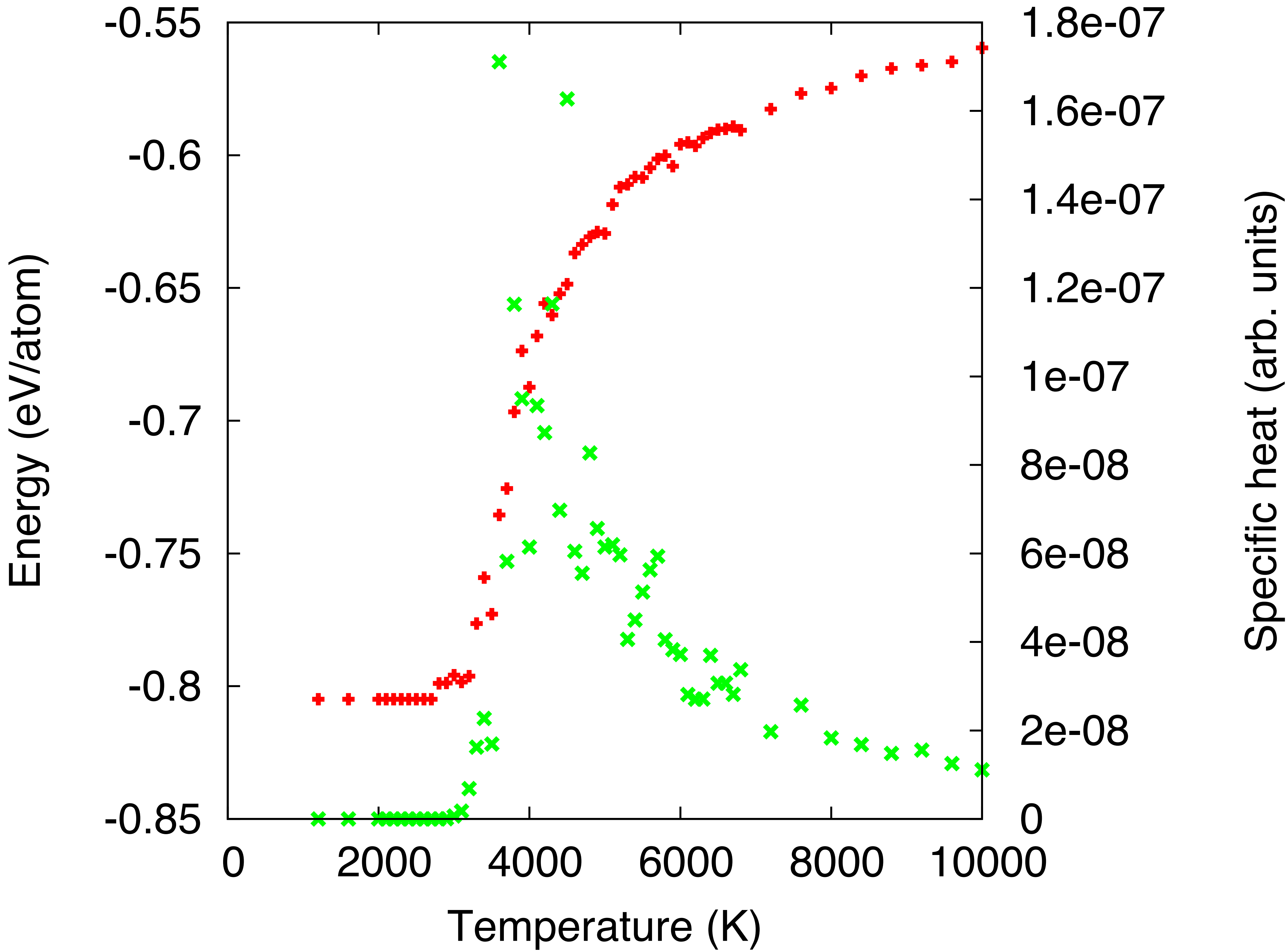

Energy (eV/atom)
Specific heat (arb. units)
Temperature (K)
-0.55
-0.6
-0.65
-0.7
-0.75
-0.8
-0.85
1.8e-07
1.6e-07
1.4e-07
1.2e-07
1e-07
8e-08
6e-08
4e-08
2e-08
0
0
2000
4000
6000
8000
10000

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

In a nutshell: **Better models, faster**

**Basic idea:**

Instead of adding complexity (terms) to a model until it fits the data and predicts well…(normal approach)…

…start with an infinite set of models (containing all possible terms). Discard all models except the simplest one (Compressive Sensing approach). Surprisingly perhaps, this is really efficient.

# Going beyond a linear model fit (adding terms)

$$f(x,y) = \boxed{a_0 + a_1 x + a_2 y + a_3 xy + a_4 x^2 + a_5 y^2} + \cdots$$

$$\begin{pmatrix} 1 & x_1 & y_1 & x_1 y_1 & x_1^2 & y_1^2 \\ 1 & x_2 & y_2 & x_2 y_2 & x_2^2 & y_2^2 \\ 1 & x_3 & y_3 & x_3 y_3 & x_3^2 & y_3^2 \\ 1 & x_4 & y_4 & x_4 y_4 & x_4^2 & y_4^2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}$$

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$$\ell_2 \equiv \left( \sum_i |u_i|^2 \right)^{\frac{1}{2}} \qquad \ell_1 \equiv \left( \sum_i |u_i|^1 \right)^{\frac{1}{1}}$$

# Basic ideas of Compressive Sensing

- Solution must be “sparse” in some basis
- Numerical application of ell-1 norm is fast
- Choose a big basis so that you’ve captured all the relevant components
- Like a Fourier Transform...except that you can sample way below the Nyquist frequency
- Sample points must be “uncorrelated”—selected at random from the domain.



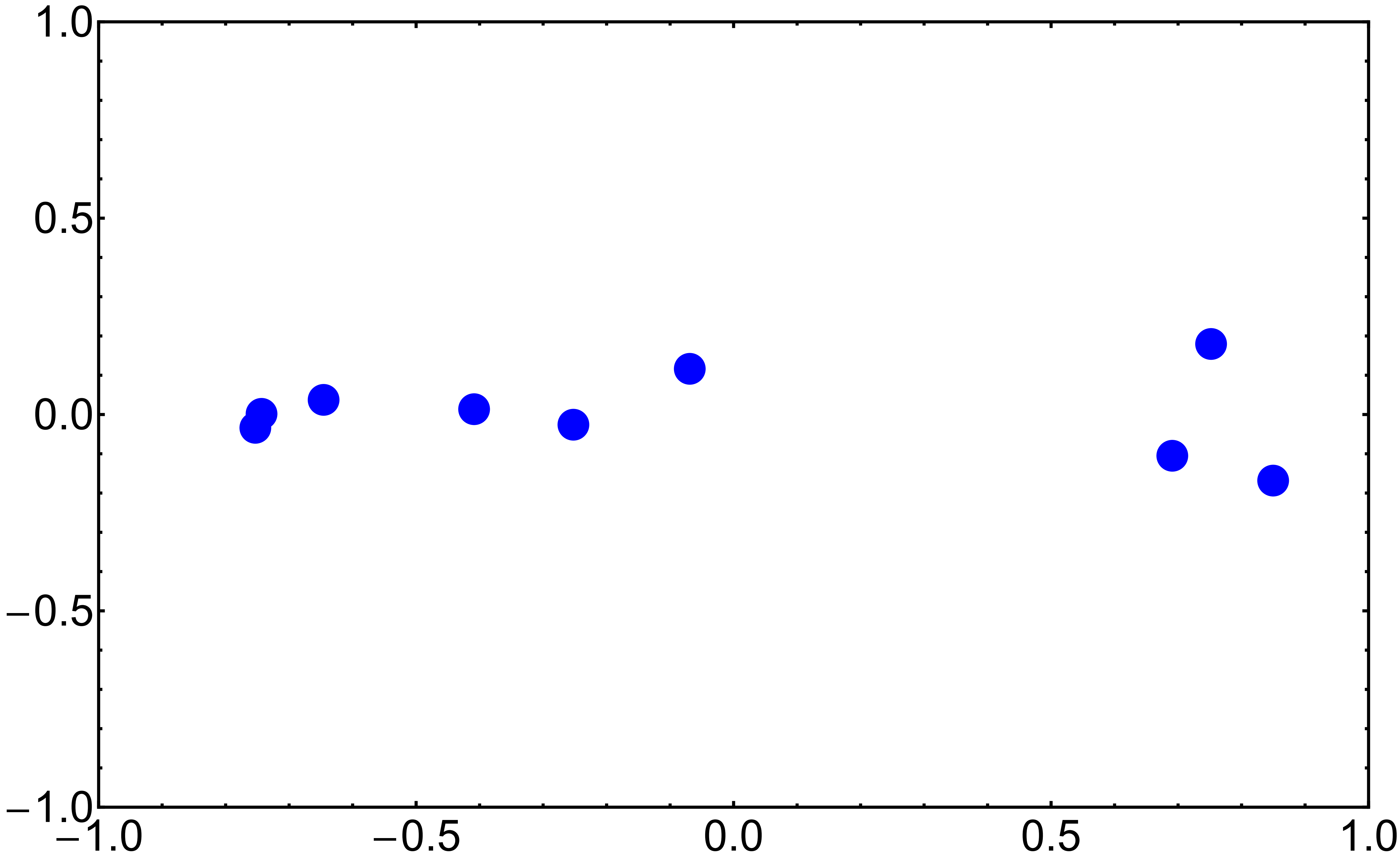

# An Introduction To Compressive Sampling

[A sensing/sampling paradigm that goes against the common knowledge in data acquisition]

[Emmanuel J. Candès and Michael B. Wakin]

Conventional approaches to sampling signals or images follow Shannon's celebrated theorem: the sampling rate must be at least twice the maximum frequency present in the signal (the so-called Nyquist rate). In fact, this principle underlies nearly all signal acquisition protocols used in consumer

# Under-determined problem: Example



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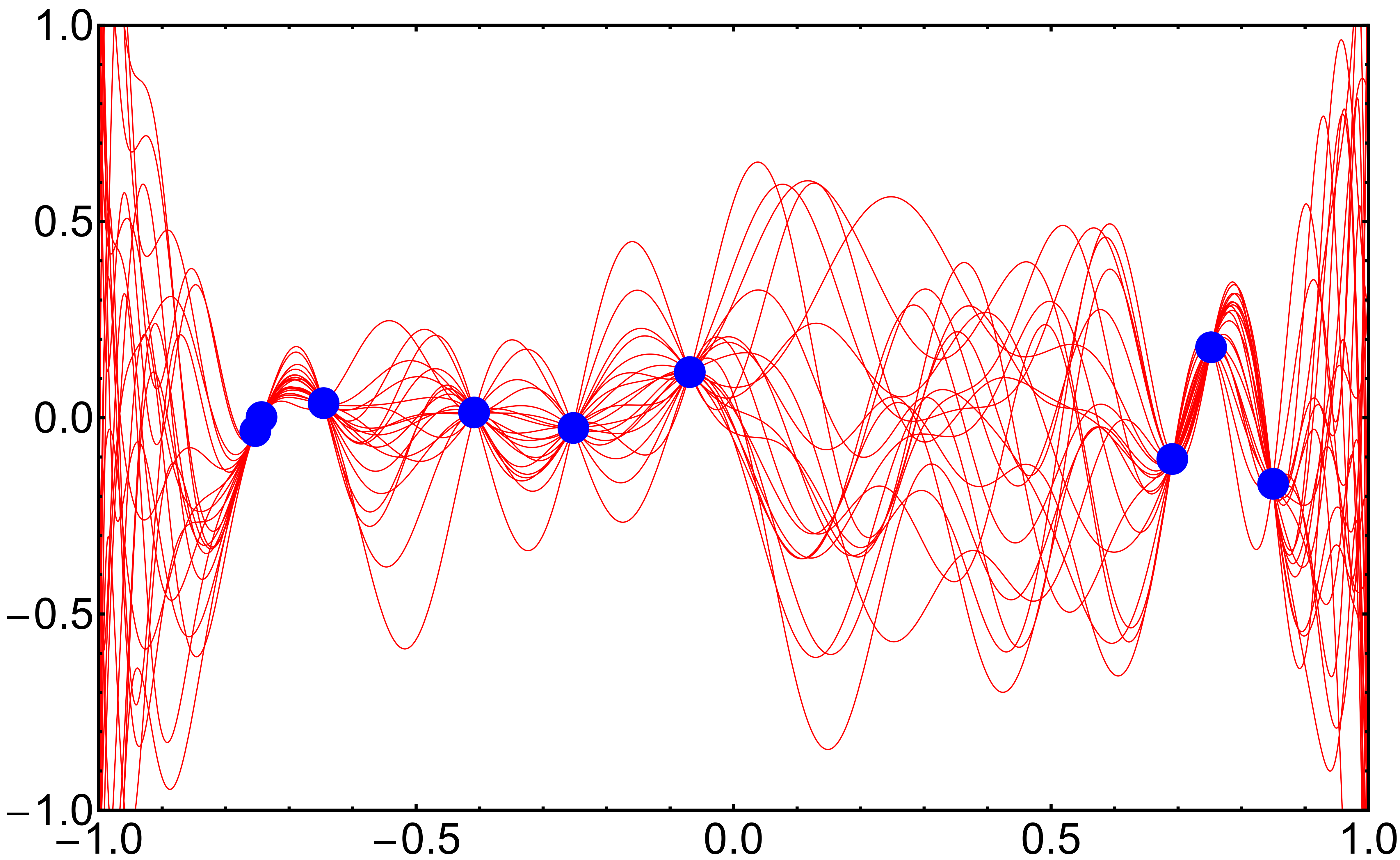

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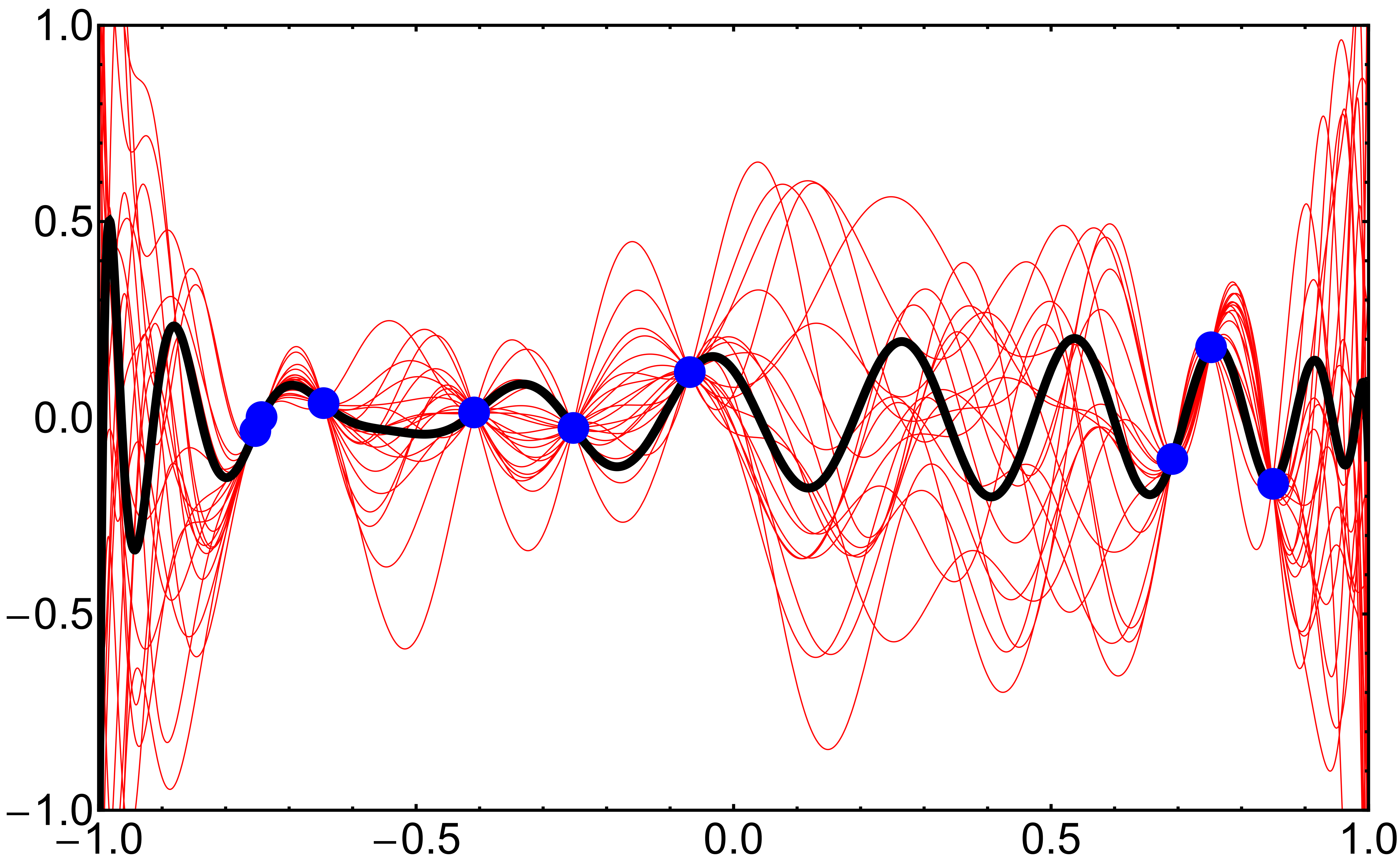
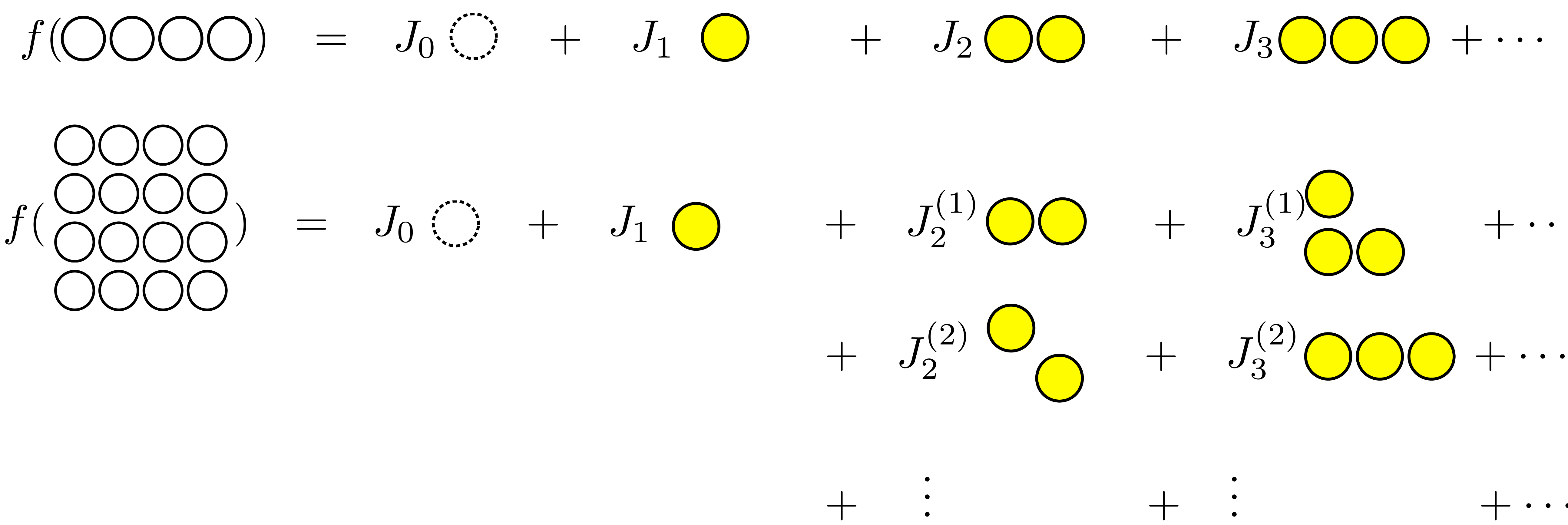


# In more than one dimension...



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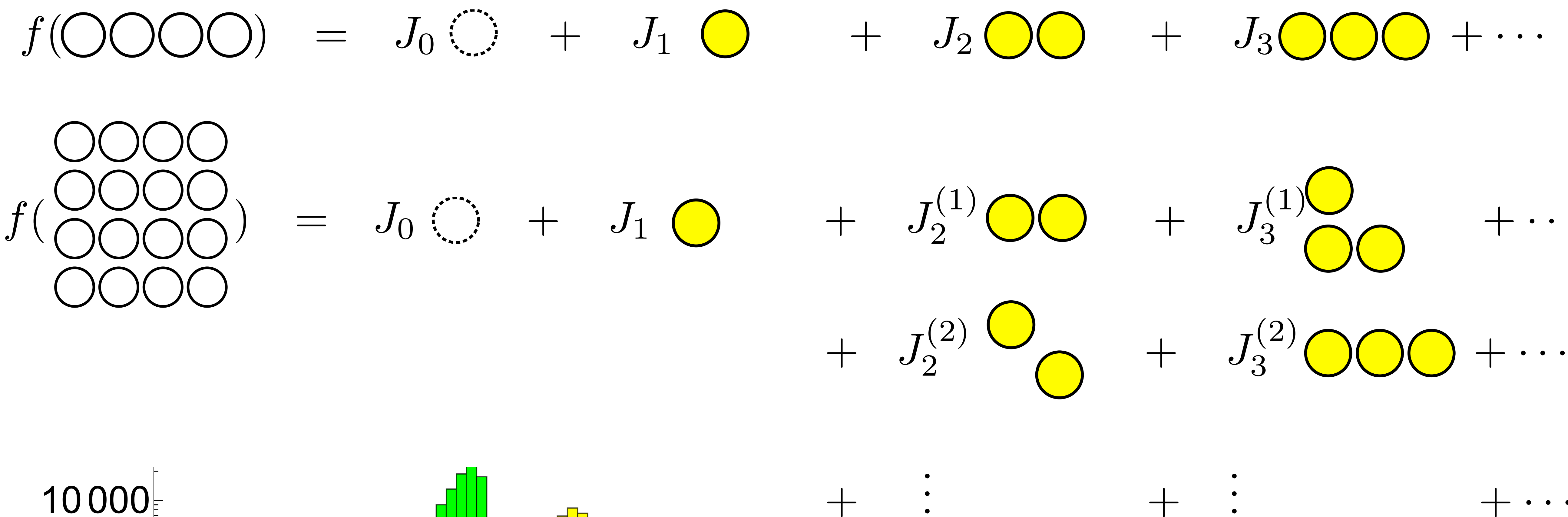
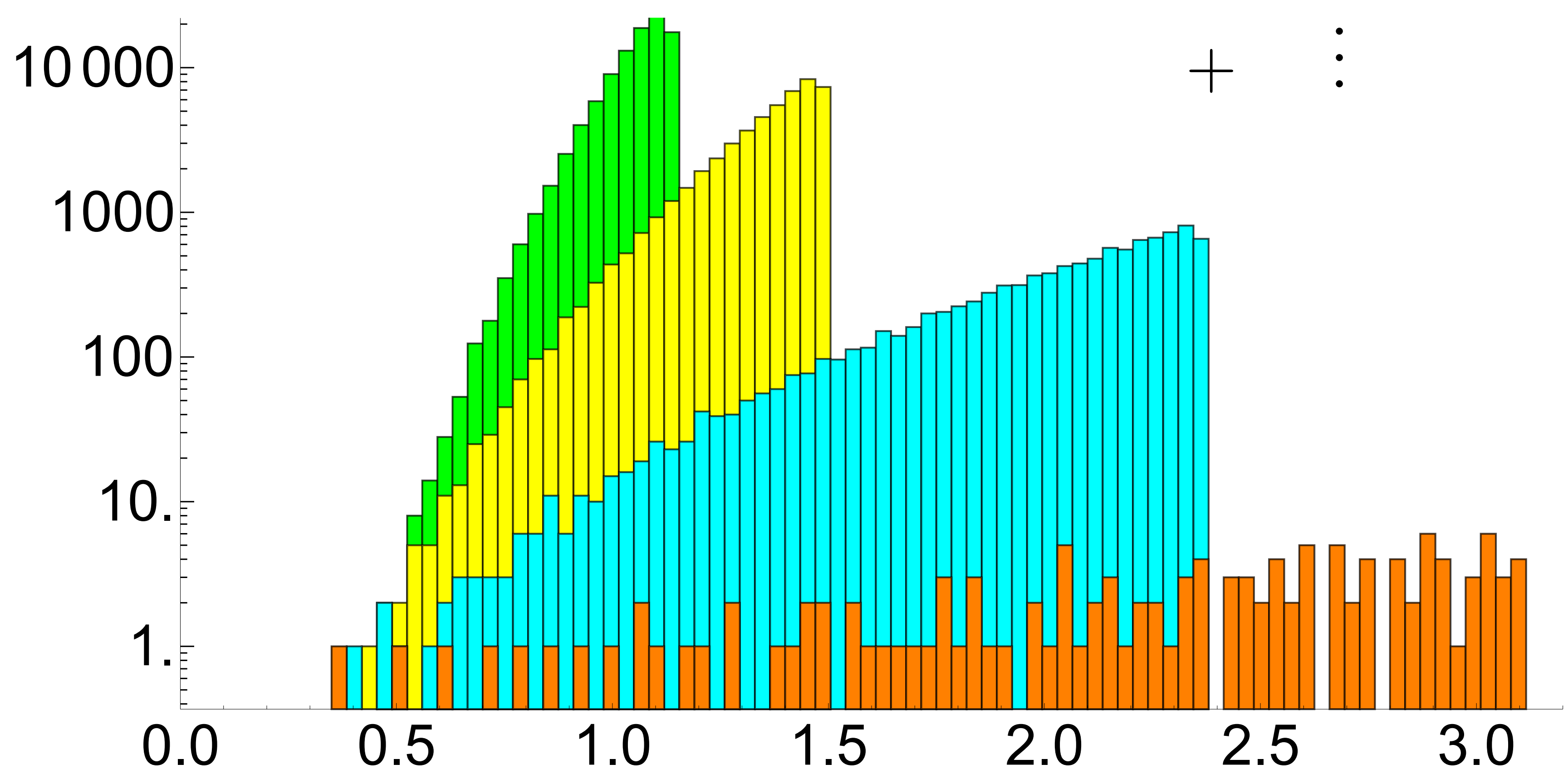
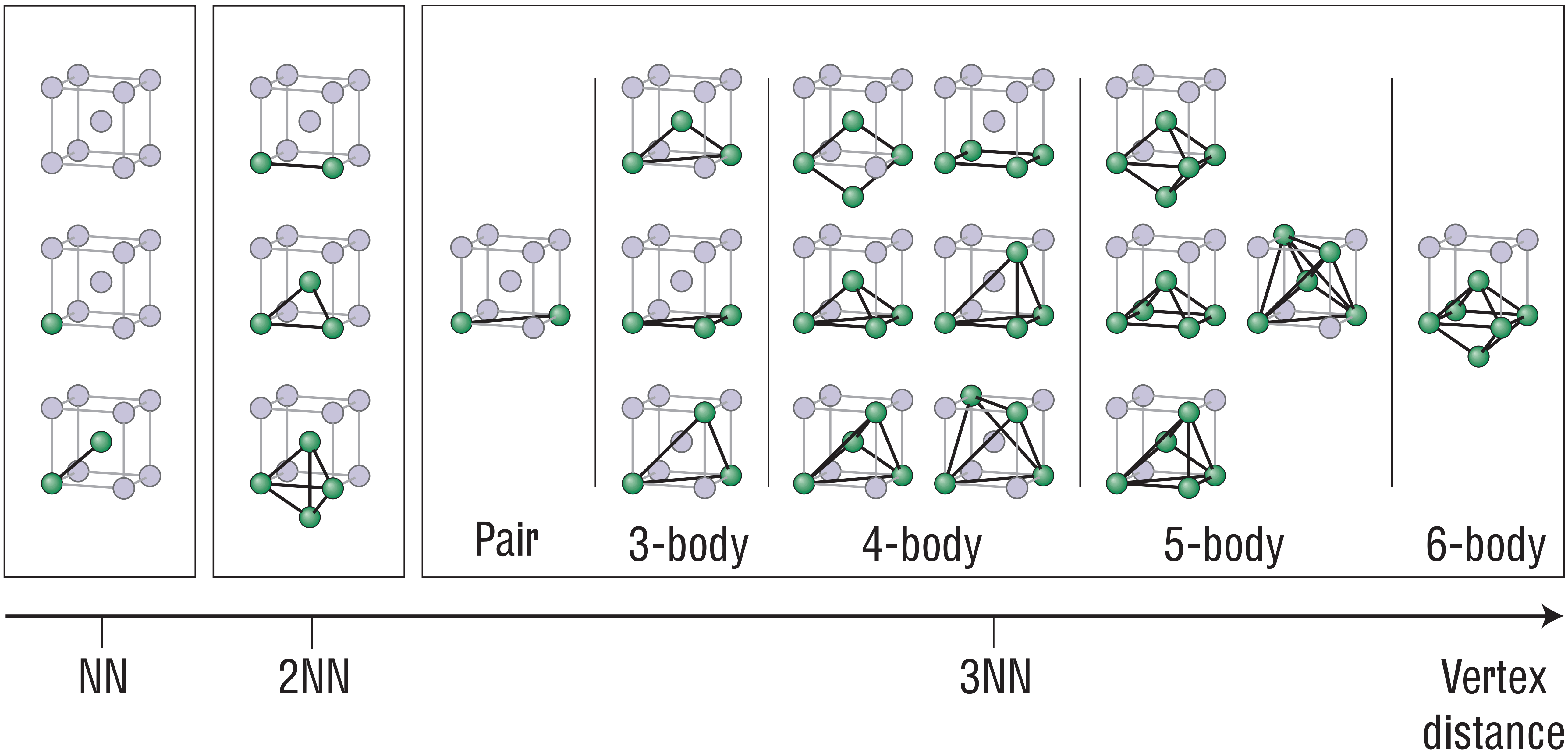
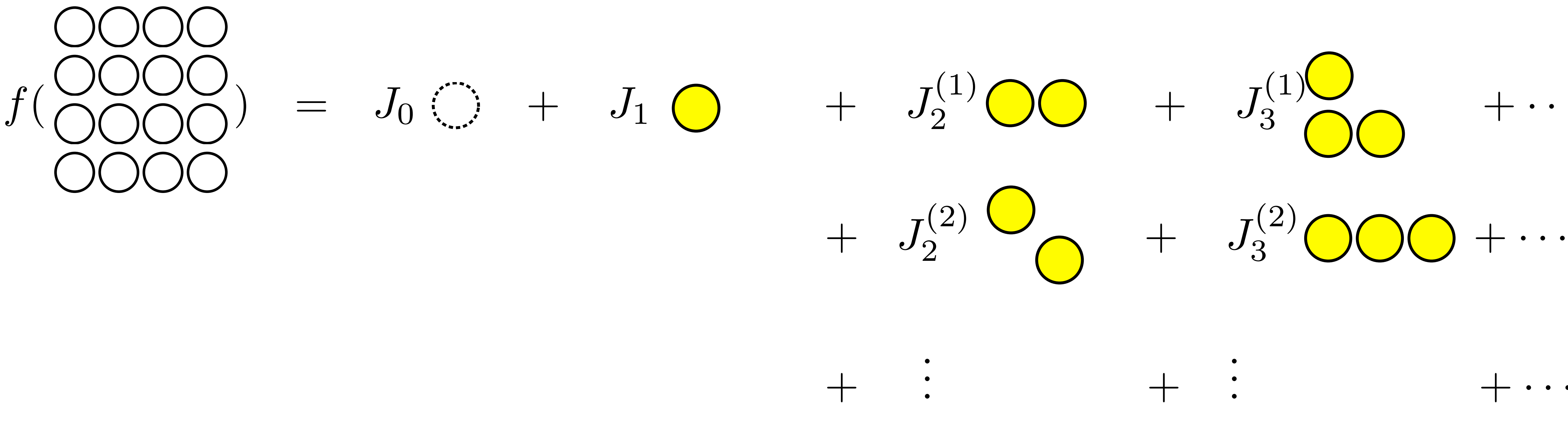


# In three dimensions...



# Models built via Compressive Sensing



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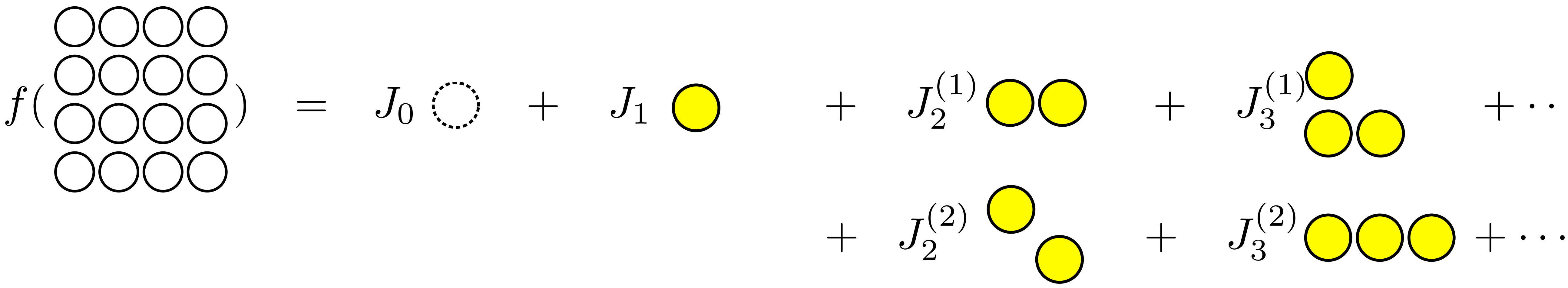
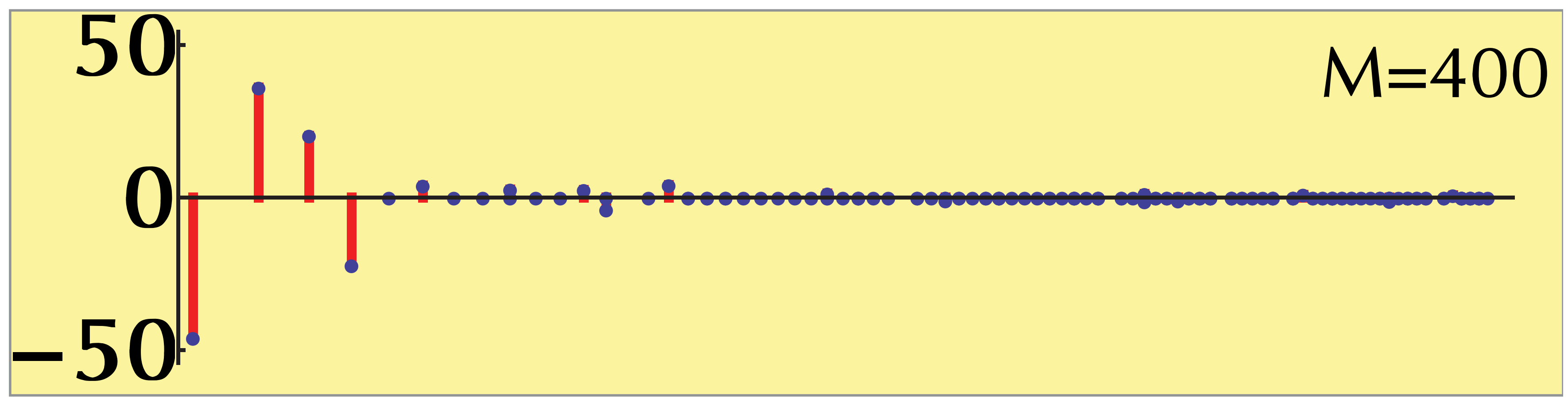



Pairs



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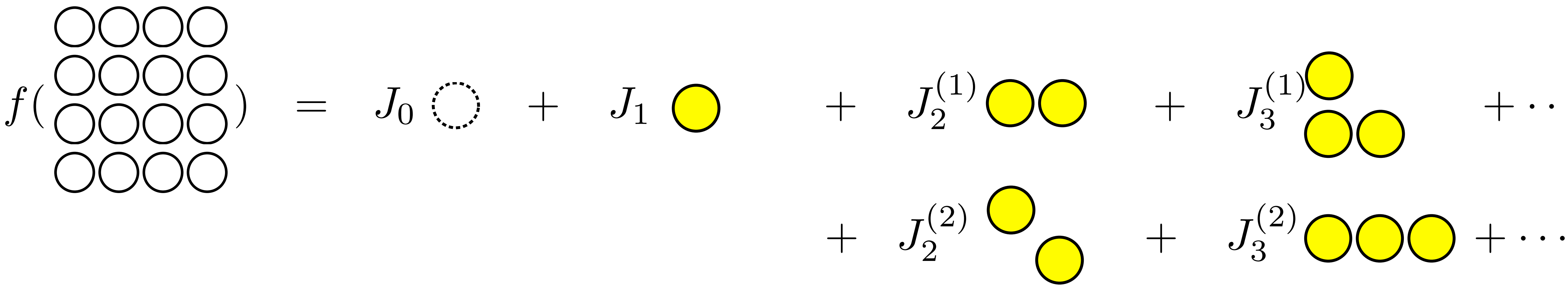


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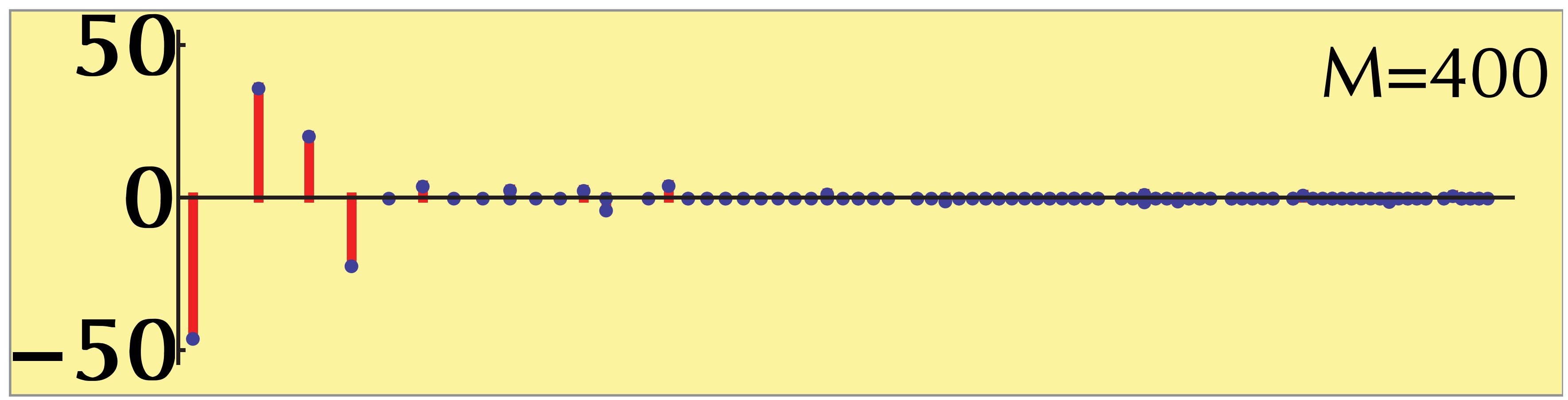
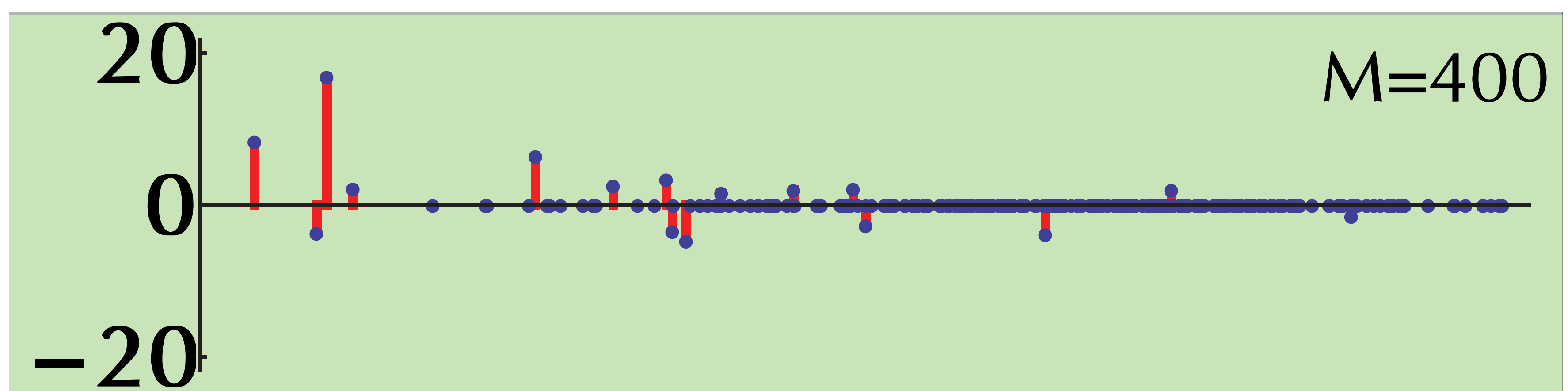



Triplets



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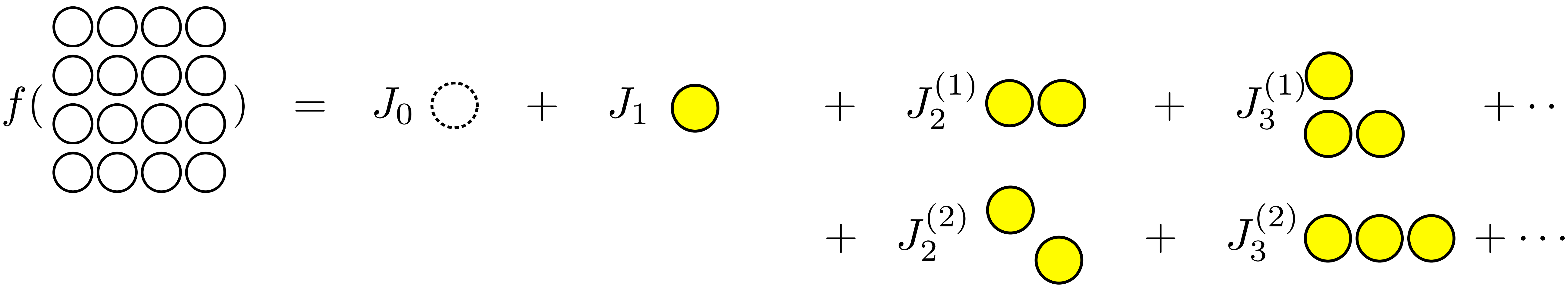
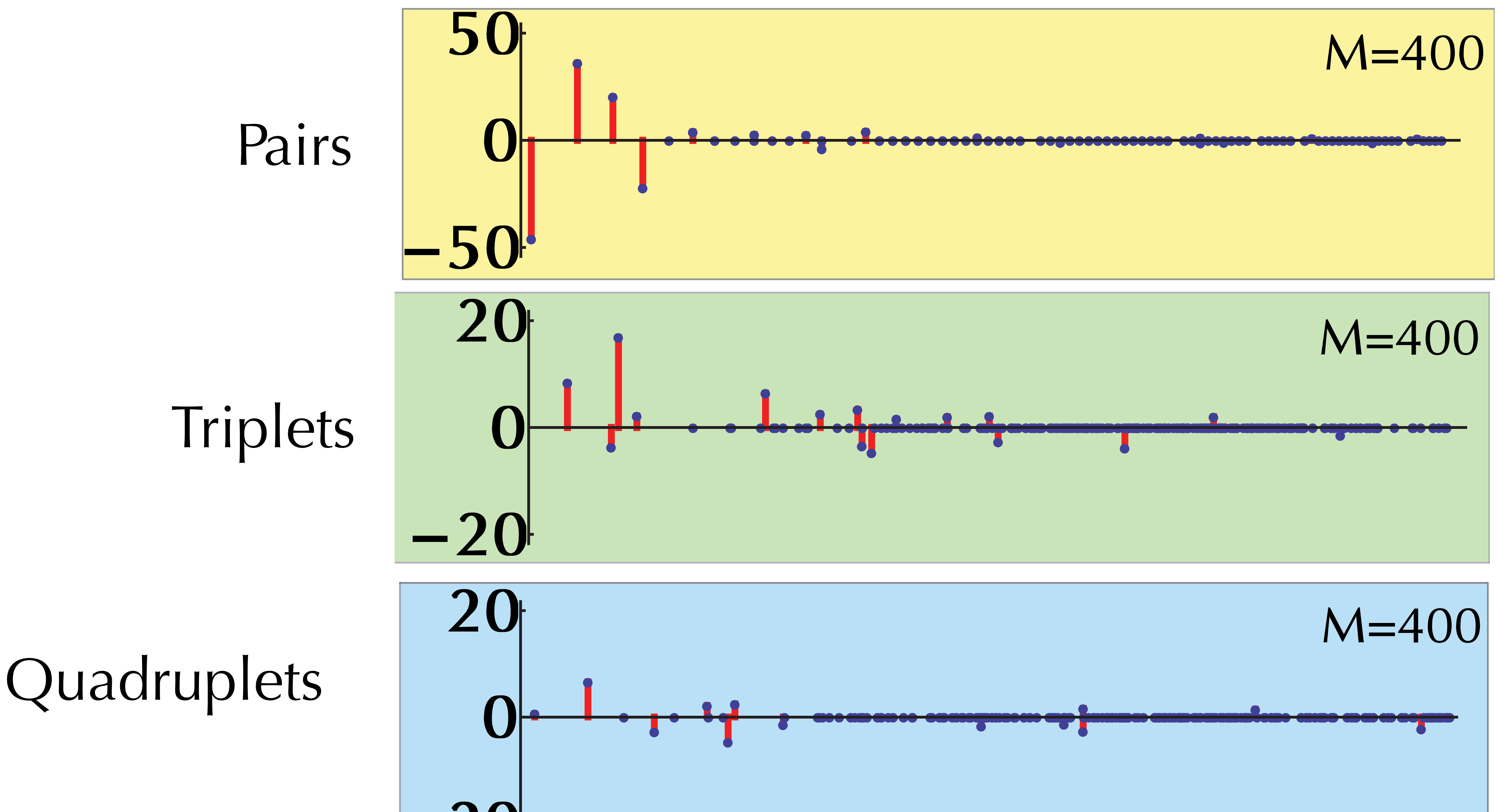
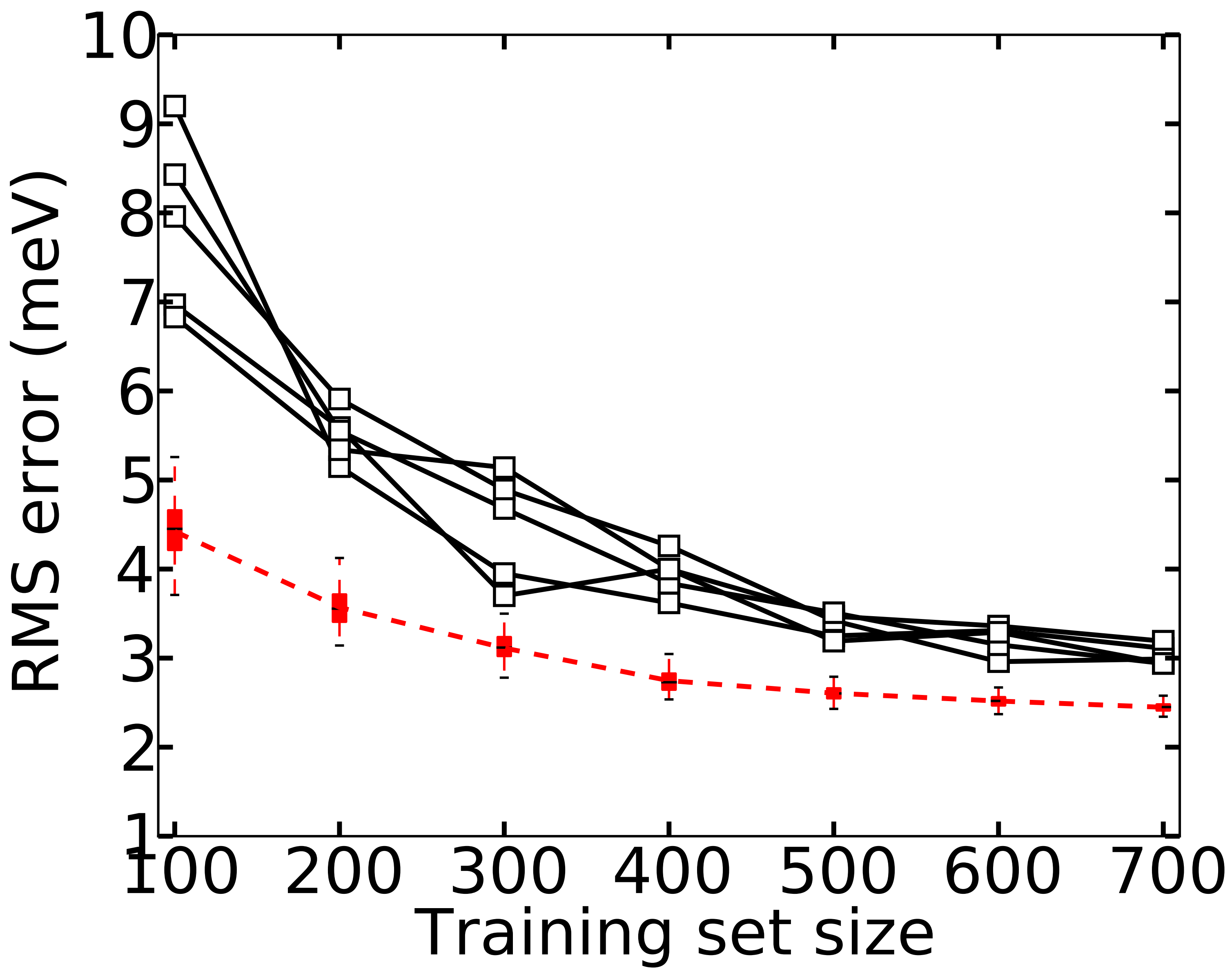


# Bayesian Compressive Sensing vs. GA



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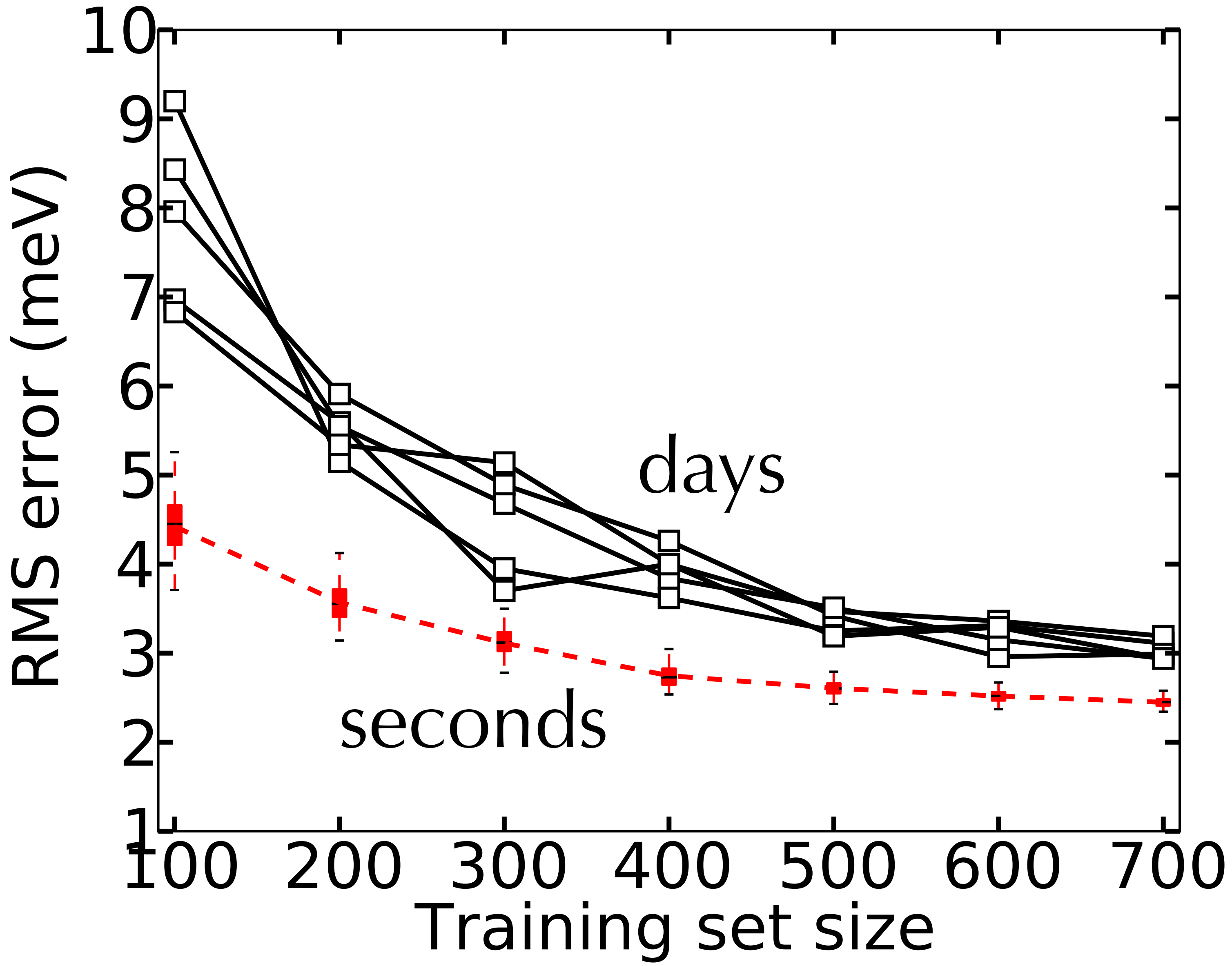

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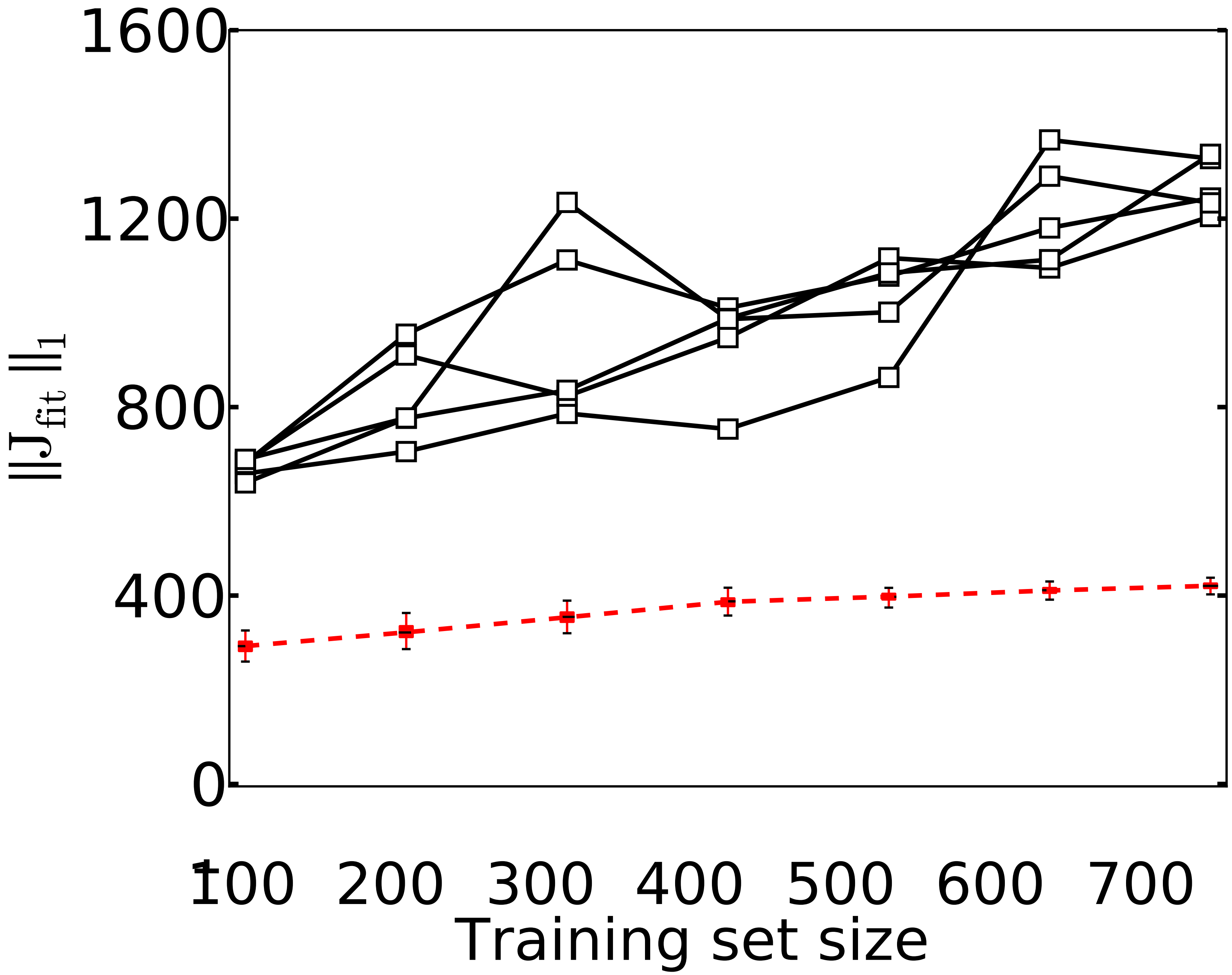

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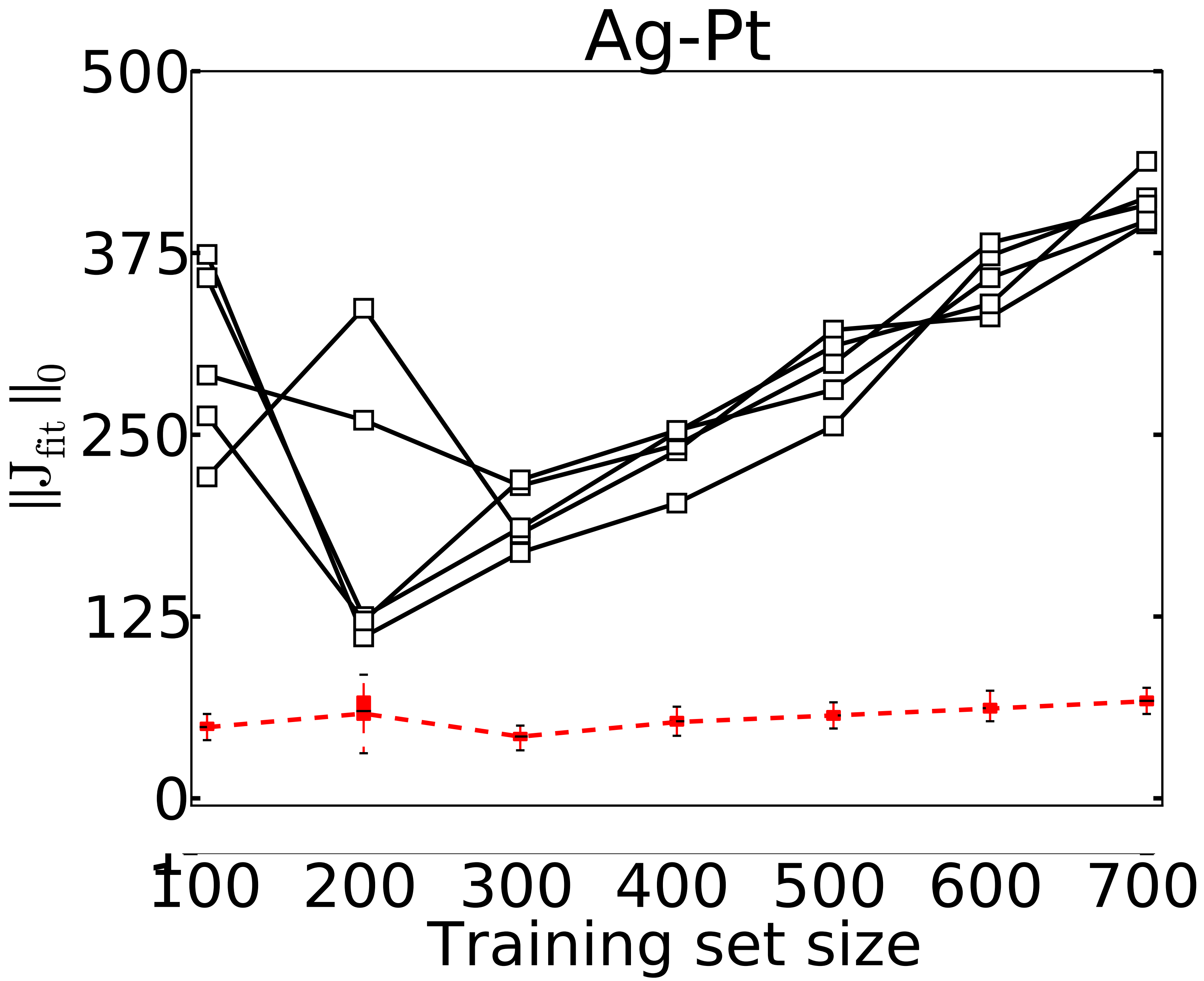

# Further reading


Lance J. Nelson, Gus L. W. Hart, Fei Zhou, and Vidvuds Ozolins, "*Cluster expansion made easy with Bayesian compressive sensing*," Phys. Rev. B **88** 155105 (Oct. 2013)

Lance J. Nelson, Gus L. W. Hart, Fei Zhou, and Vidvuds Ozolins, "*Compressive sensing as a paradigm for building physics models*," Phys. Rev. B **87** 035125 (2013).

E. J. Candès and M. B. Wakin, "*An introduction to compressive sampling*," Signal Processing Magazine, IEEE, **25** 21–30 (2008).

T. Strohmer, "*Measure What Should be Measured: Progress and Challenges in Compressive Sensing*," Signal Processing Letters **19** 887 (2012).

# Happy Birthday

Manuel from Rostock

Oliver from Graz