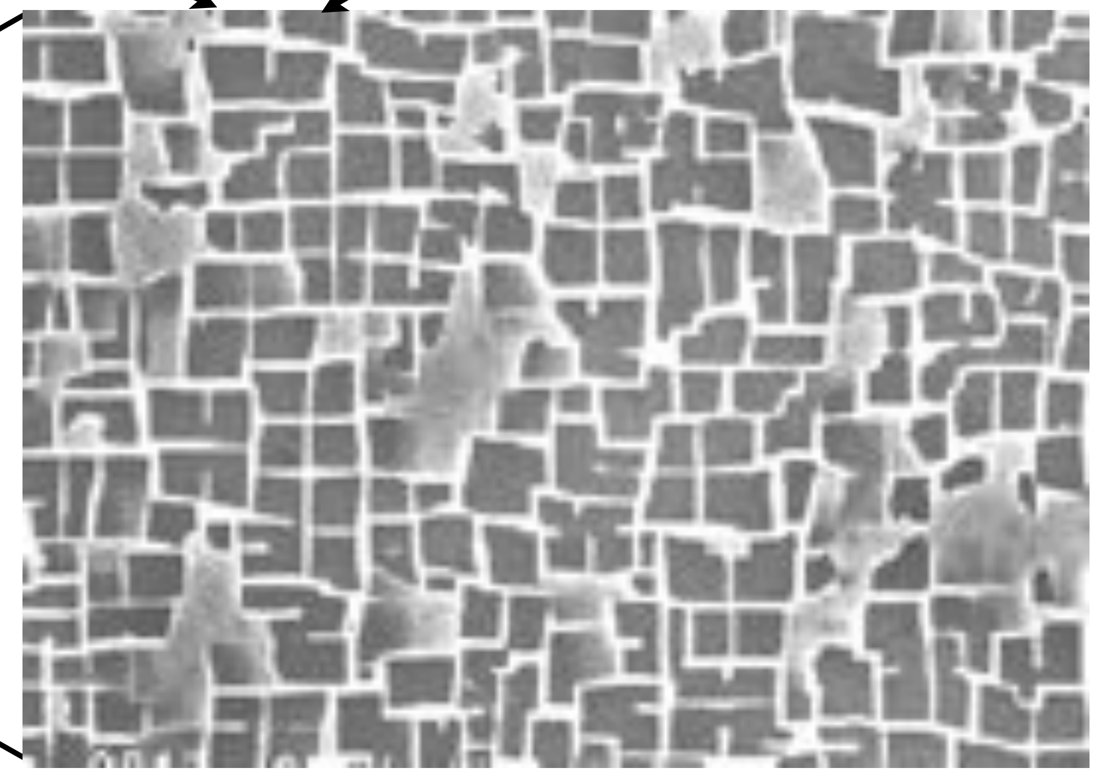
Alloy example (configurational problem)

disordered fcc Ni+(Co,Cr,Mo,W,...)

ordered $Ni_3(Al,Ti)$

Nickel superalloy jet engine turbine blade

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

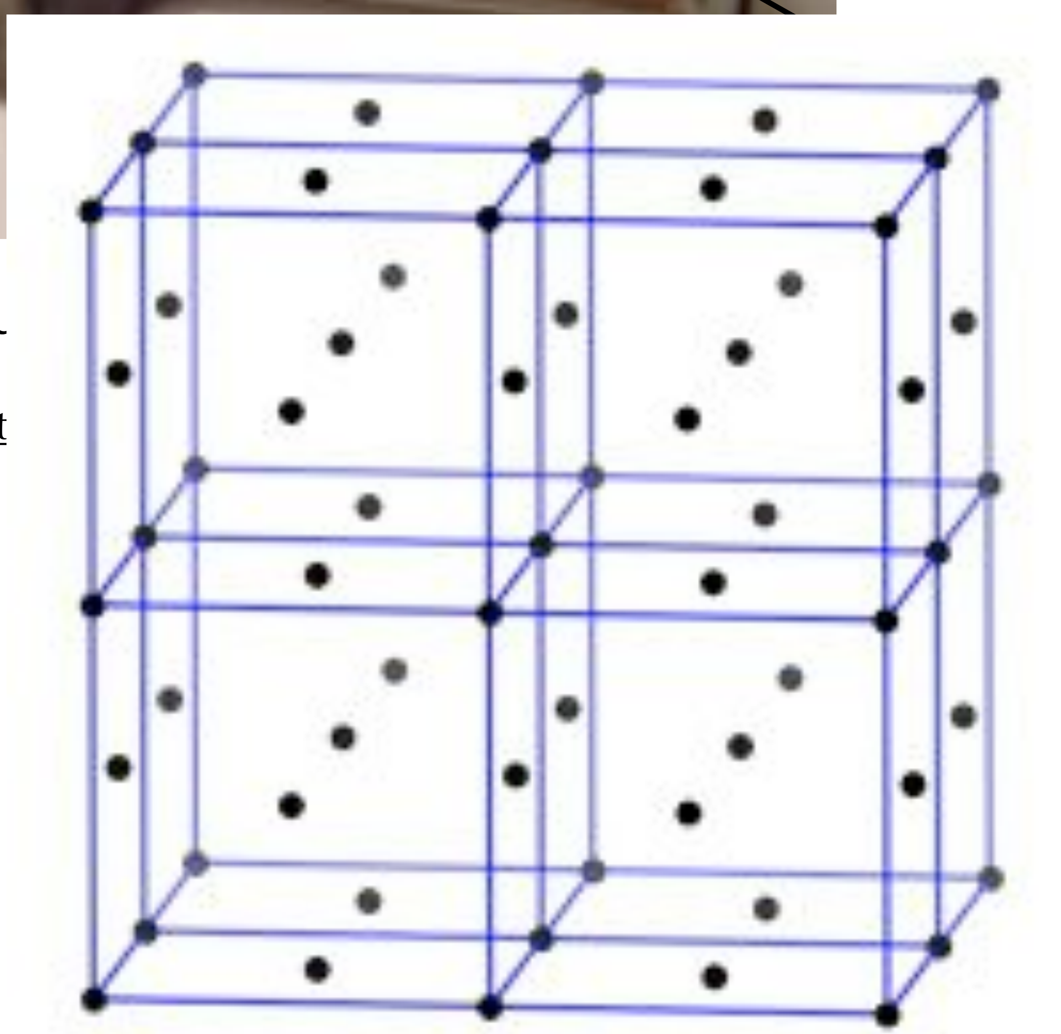


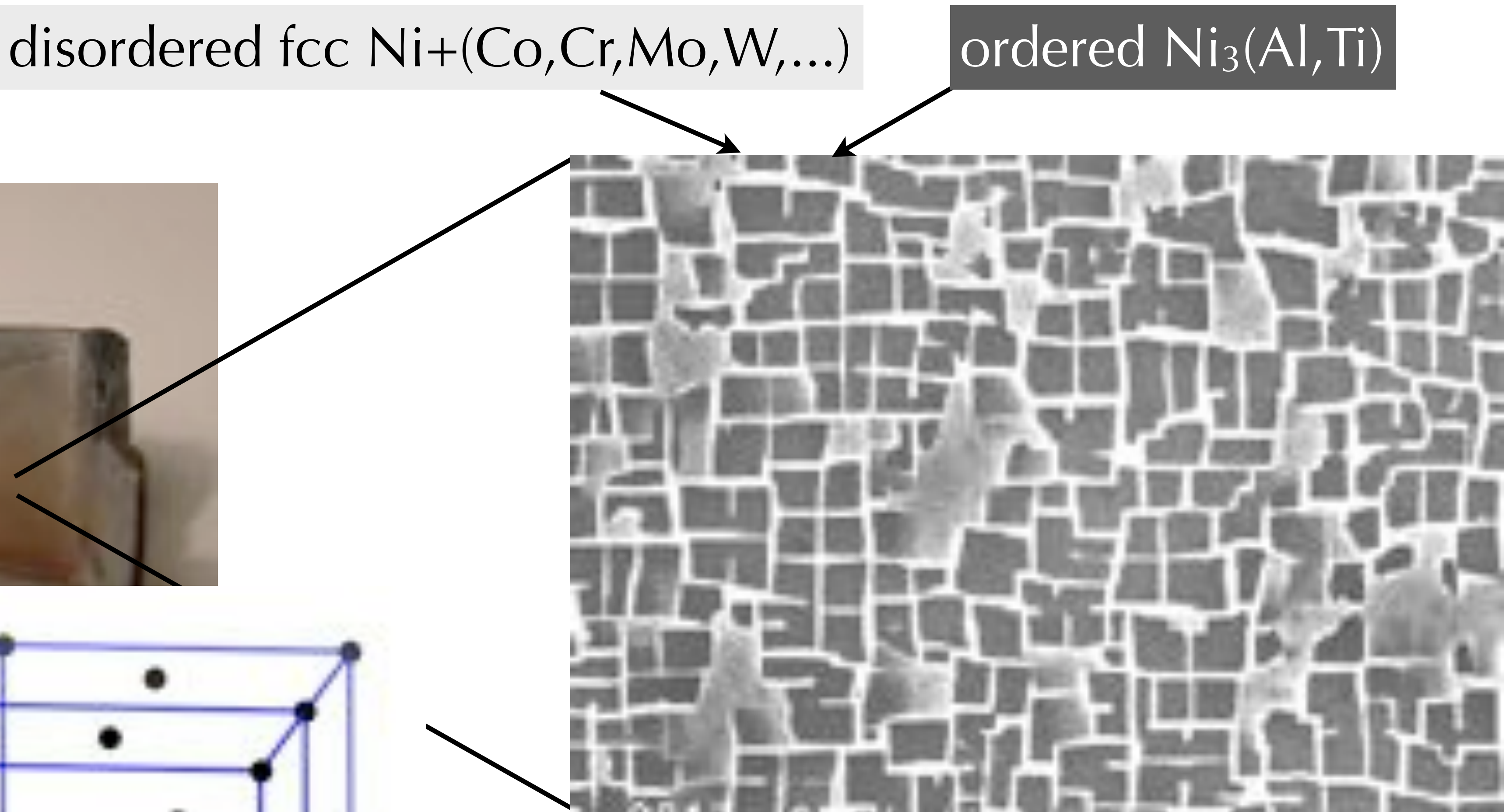
http://www.tms.org/meetings/specialty/superalloys2000/superalloyshistory.html

Alloy example (configurational problem)

Nickel su

ht



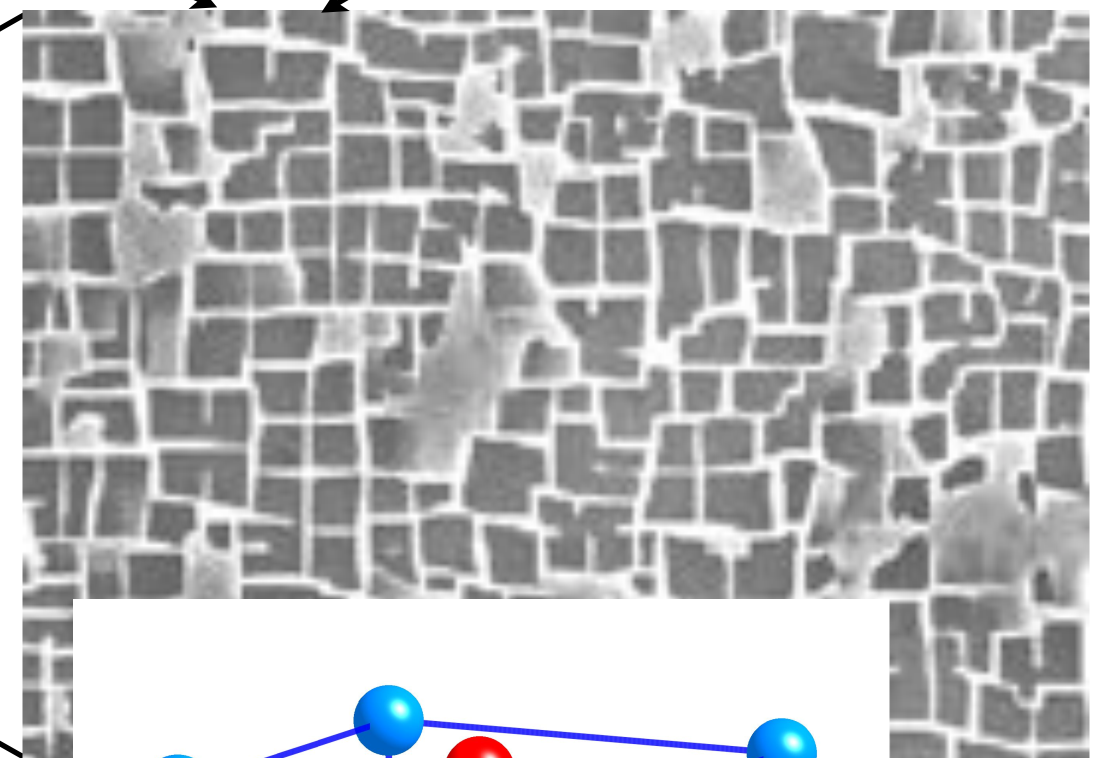


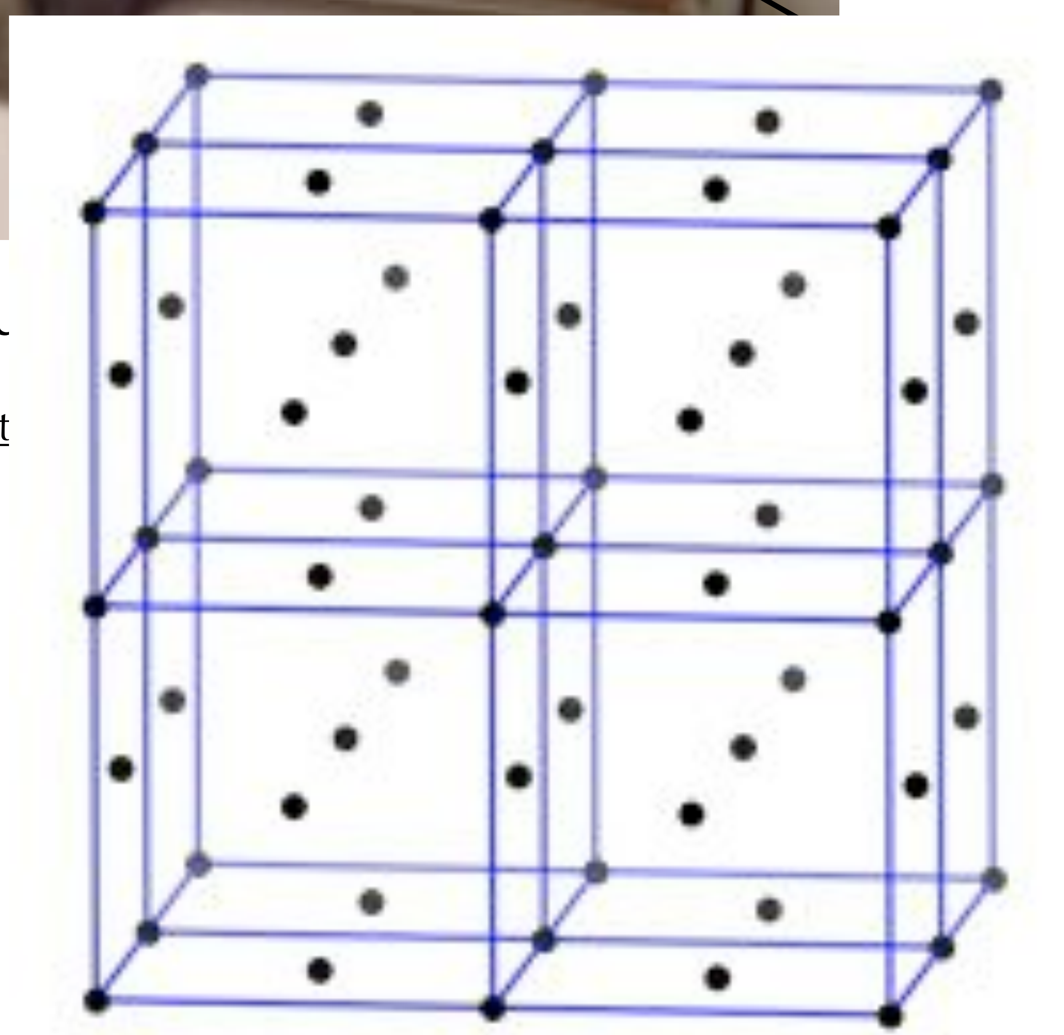
http://www.tms.org/meetings/specialty/superalloys2000/superalloyshistory.html

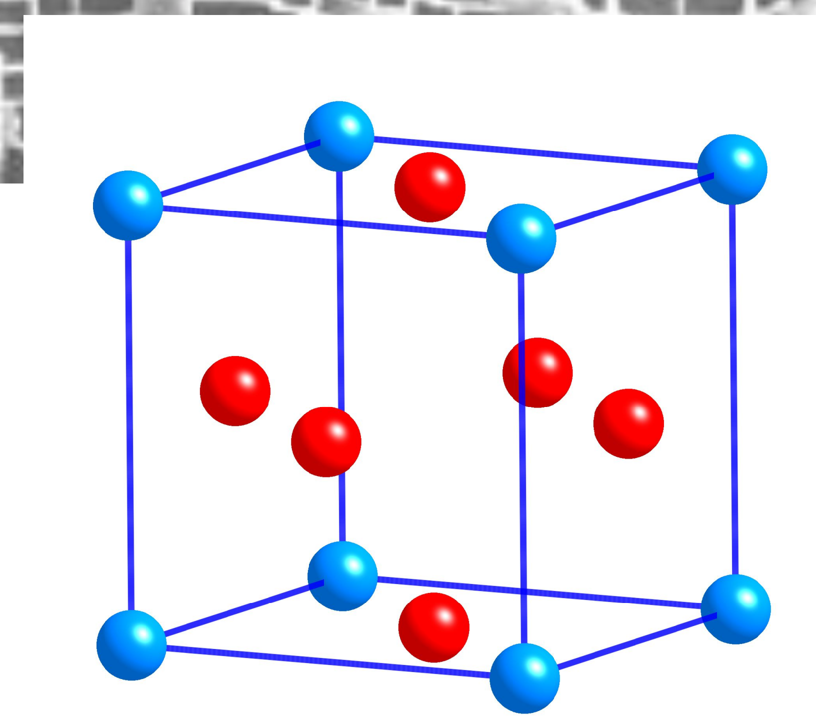
Alloy example (configurational problem)

Nickel su

ht

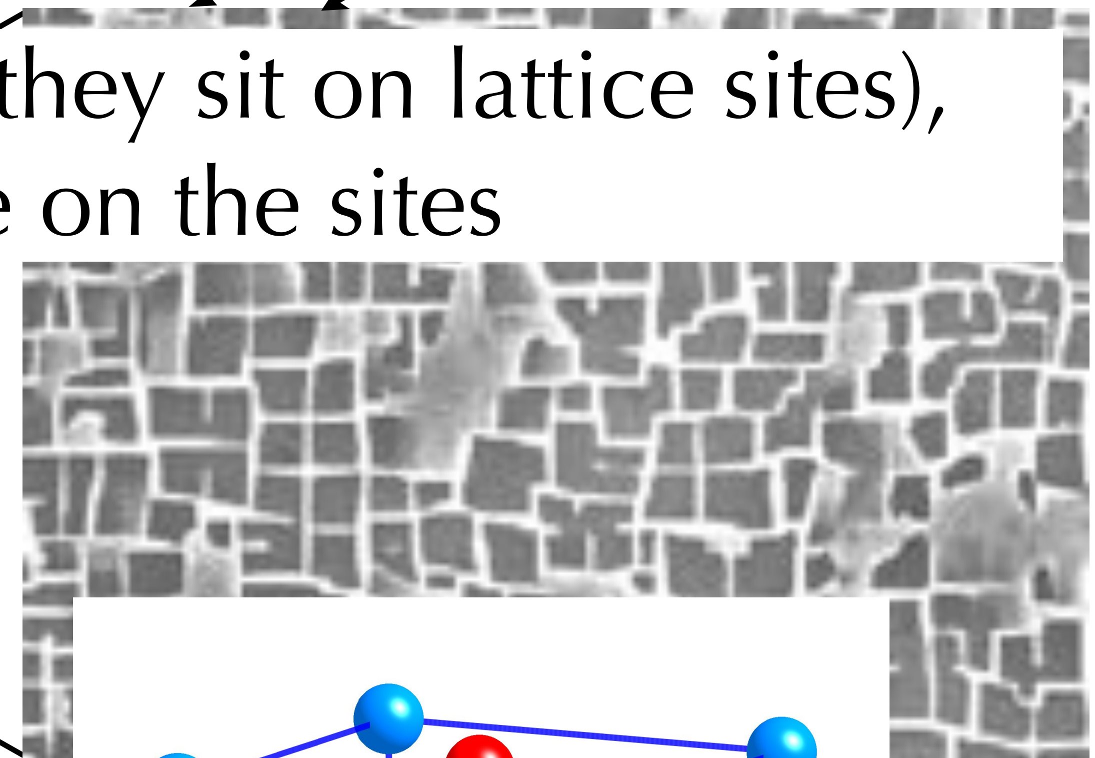




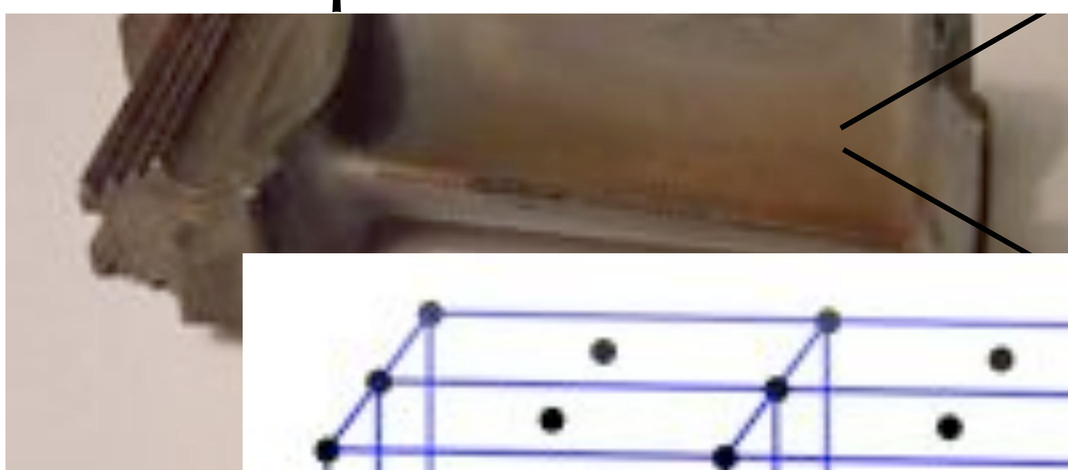


$L1_2$ (Cu_3Au)

Alloy example (configurational problem)

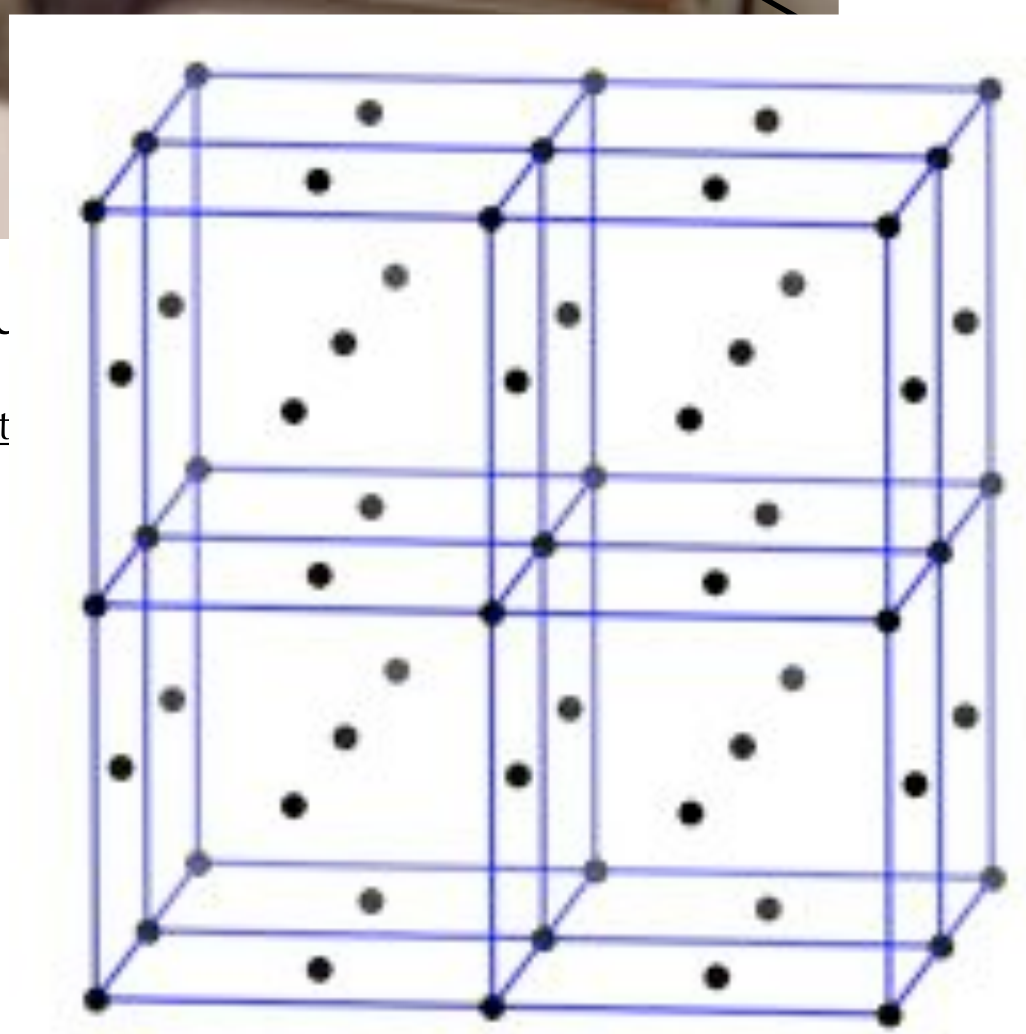


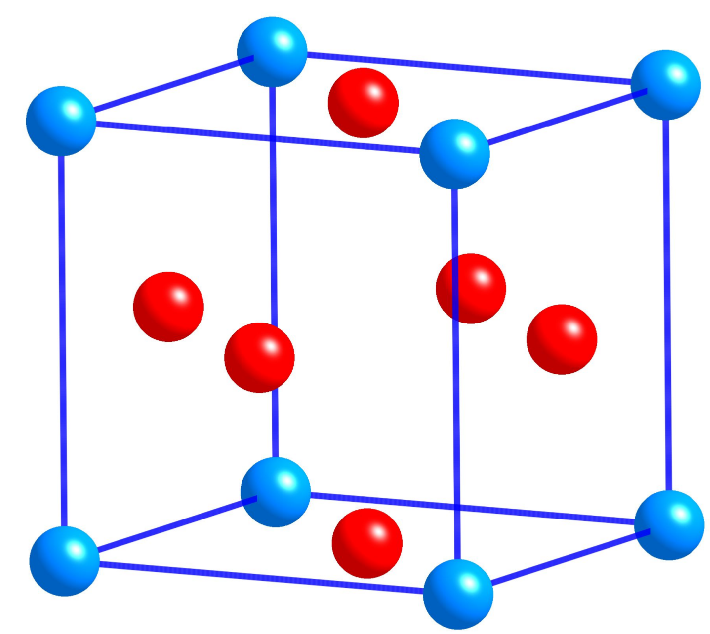
It's not about *where* the atoms are (they sit on lattice sites), but it's question of *which* atoms site on the sites



Nickel su

ht



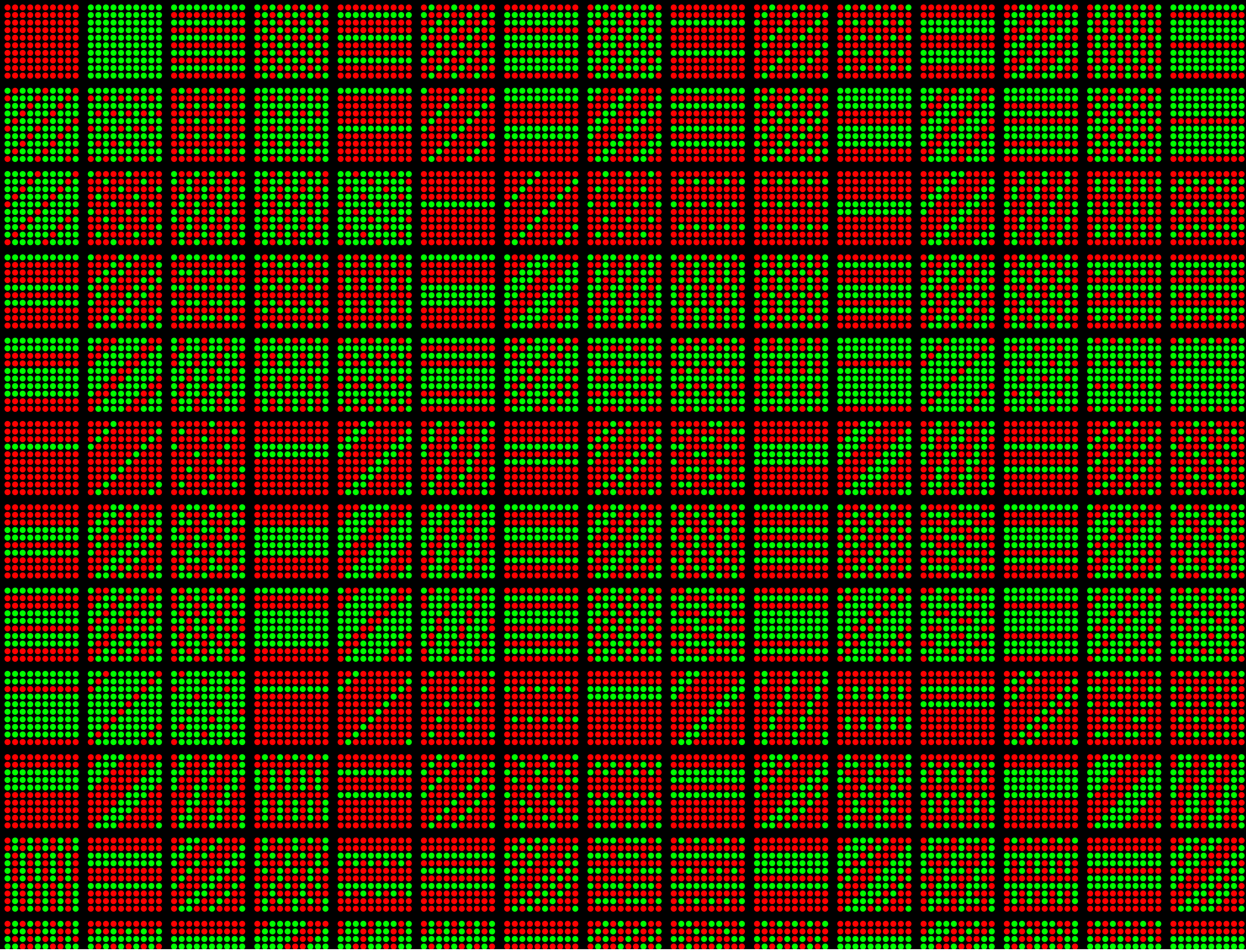


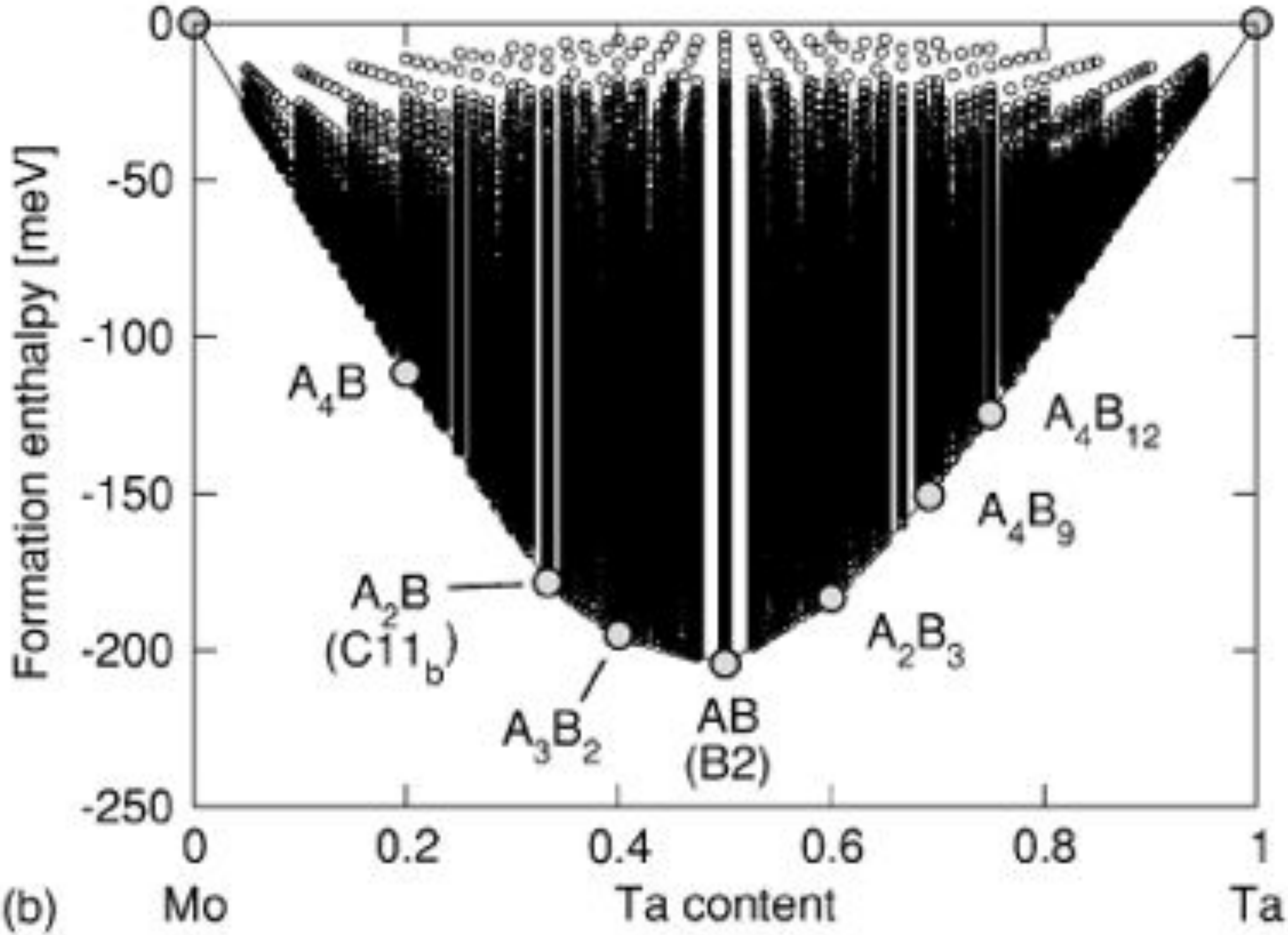
$L1_2$ (Cu_3Au)

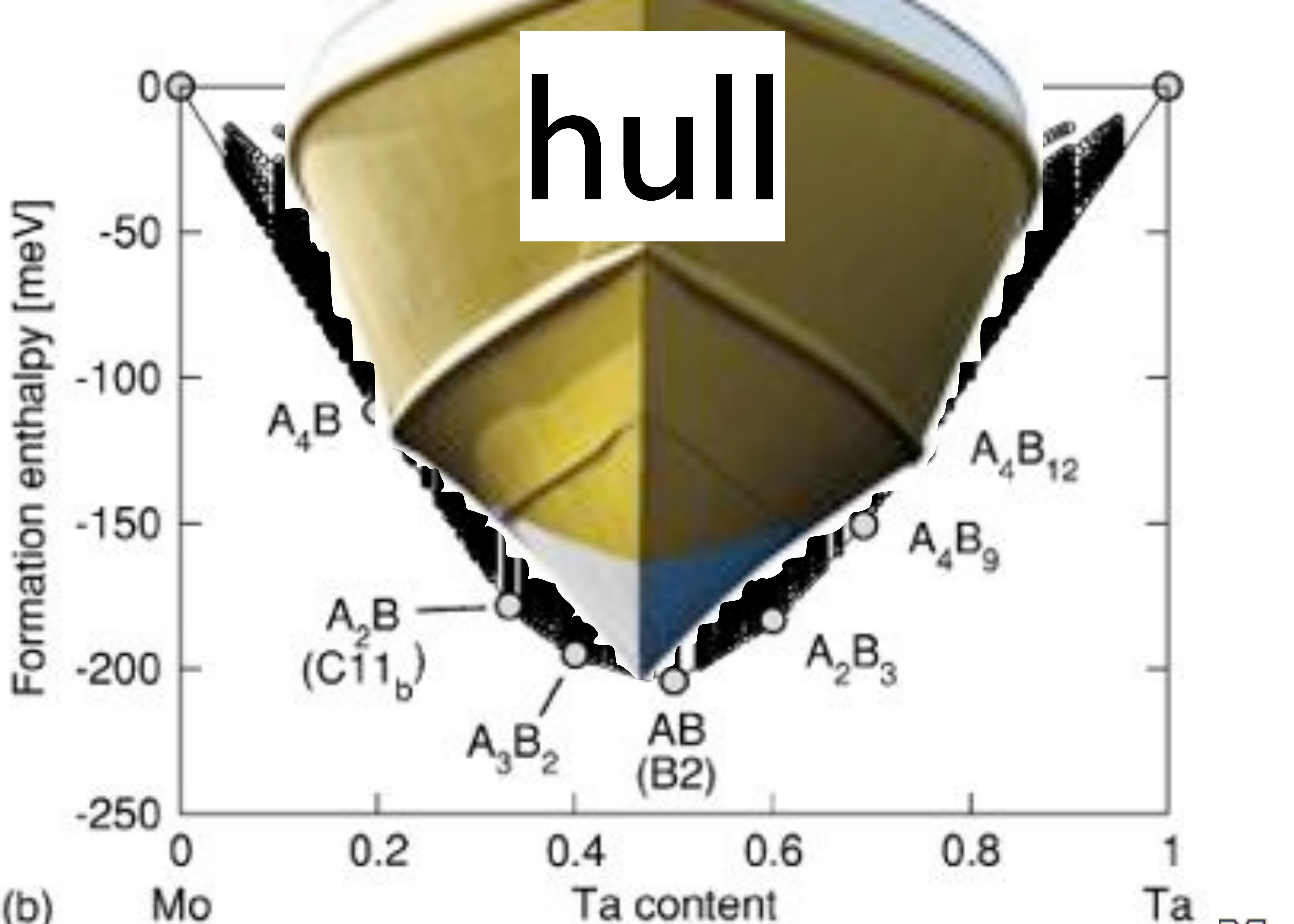
If we had a fast lattice Hamiltonian...

If we had a fast lattice Hamiltonian...

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



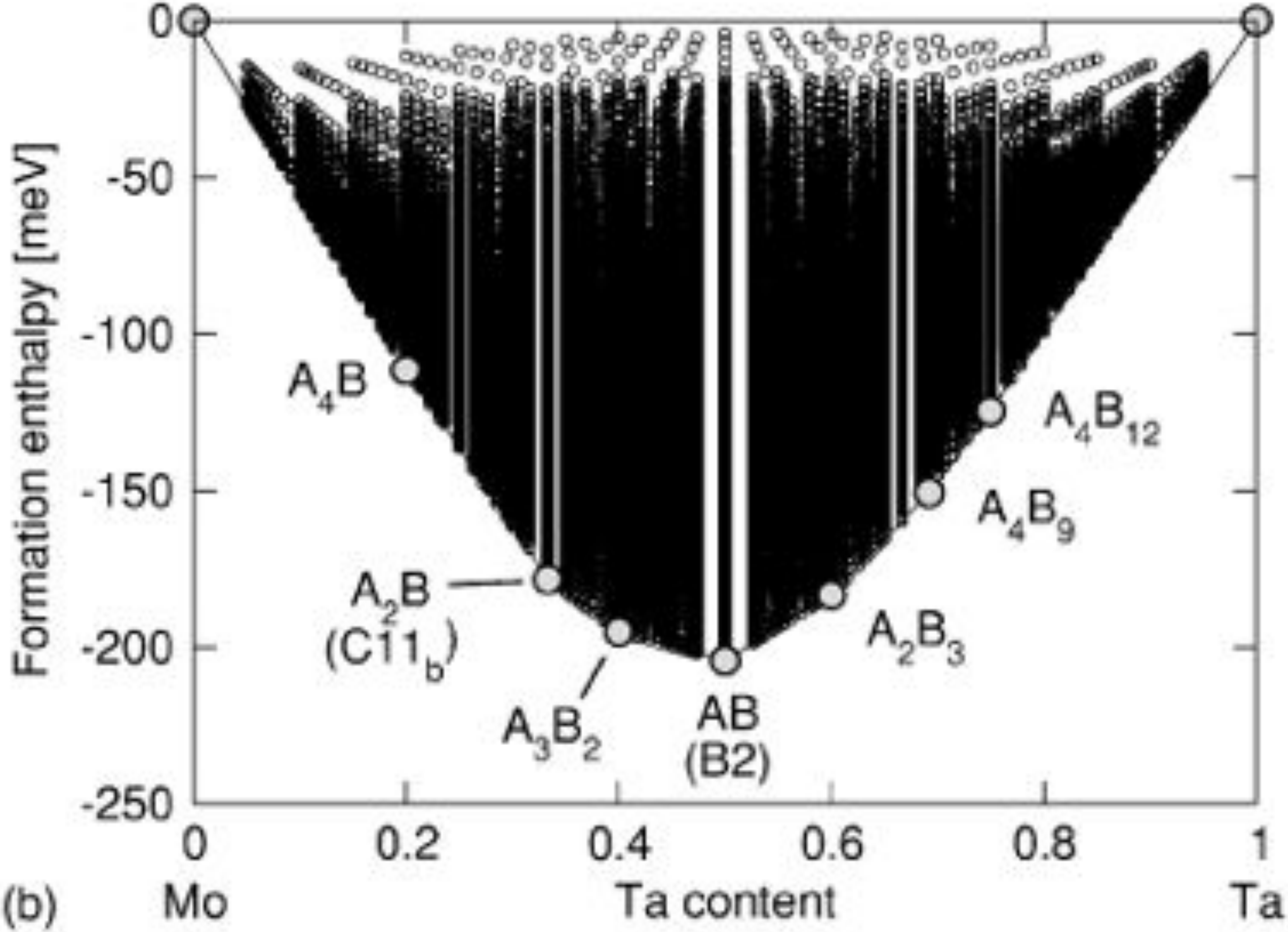

0
-50
-100
-150
-200
-250
Formation enthalpy [meV]
A$_4$B
A$_2$B
(C11$_b$)
A$_3$B$_2$
AB
(B2)
A$_2$B$_3$
A$_4$B$_9$
A$_4$B$_{12}$
0
0.2
0.4
0.6
0.8
1
(b)
Mo
Ta content
Ta


hull
Formation enthalpy [meV]
0
-50
-100
-150
-200
-250
A4B
A4B12
A4B9
A2B
(C11b)
A3B2
AB
(B2)
A2B3
0
0.2
0.4
0.6
0.8
1
(b)
Mo
Ta content
Ta

If we had a fast lattice Hamiltonian...

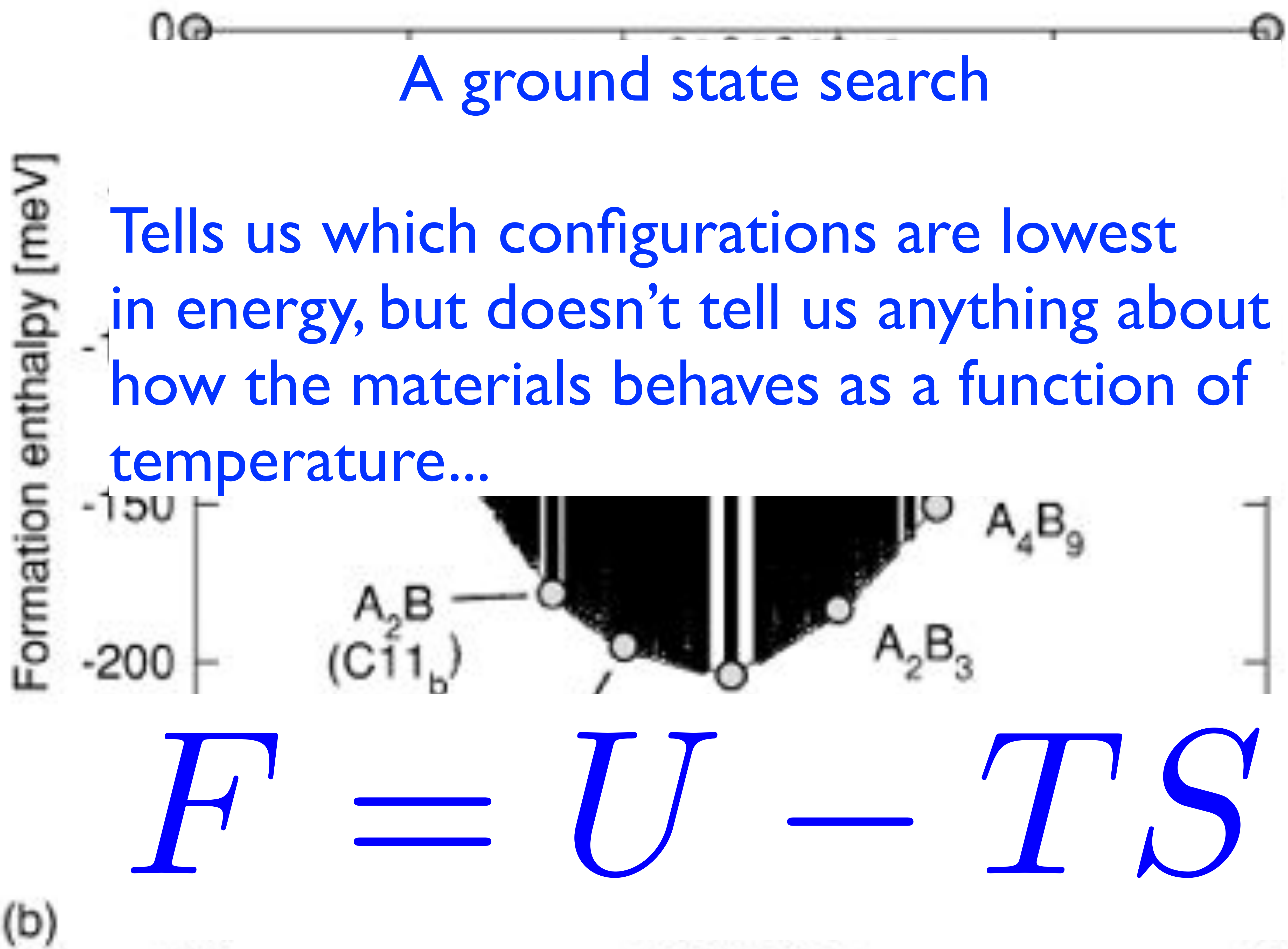
1. Search for new phases (step through millions of candidate configurations)
Ground State Search

2. Apply thermodynamic modeling (to identify phase transitions)

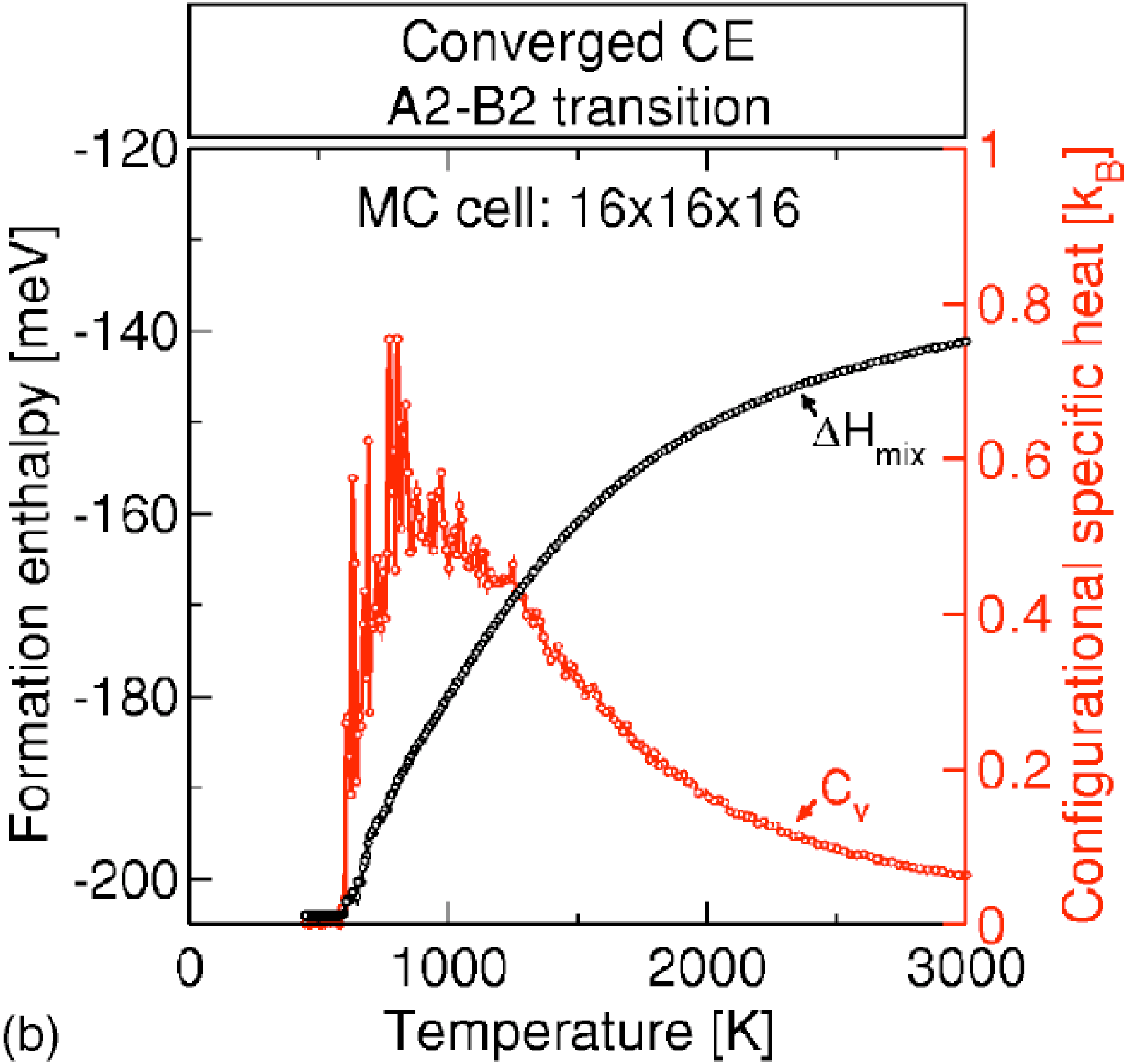

0
-50
-100
-150
-200
-250
Formation enthalpy [meV]
A4B
A2B
(C11b)
A3B2
AB
(B2)
A2B3
A4B9
A4B12
0
0.2
0.4
0.6
0.8
1
(b)
Mo
Ta content
Ta

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...

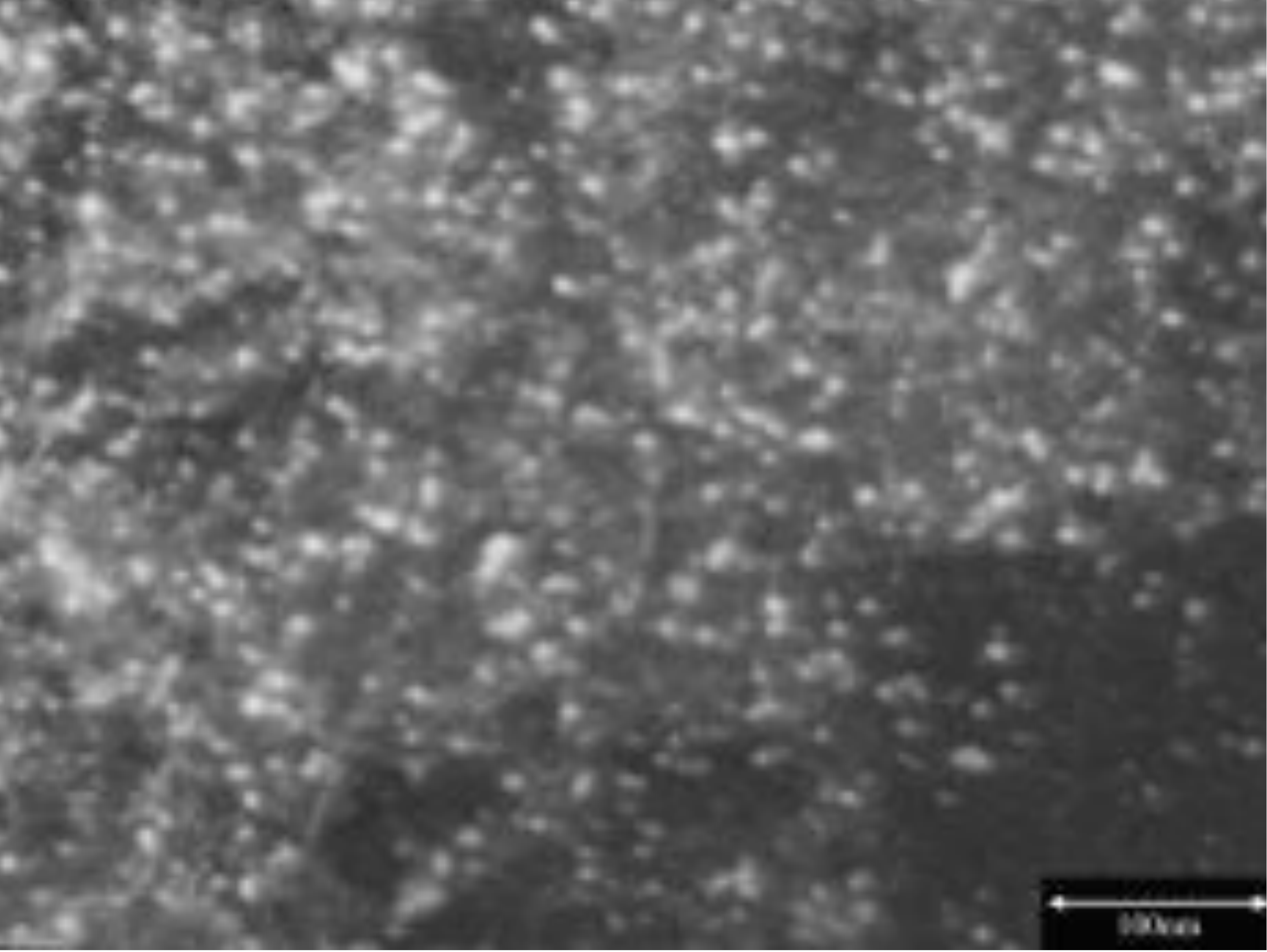


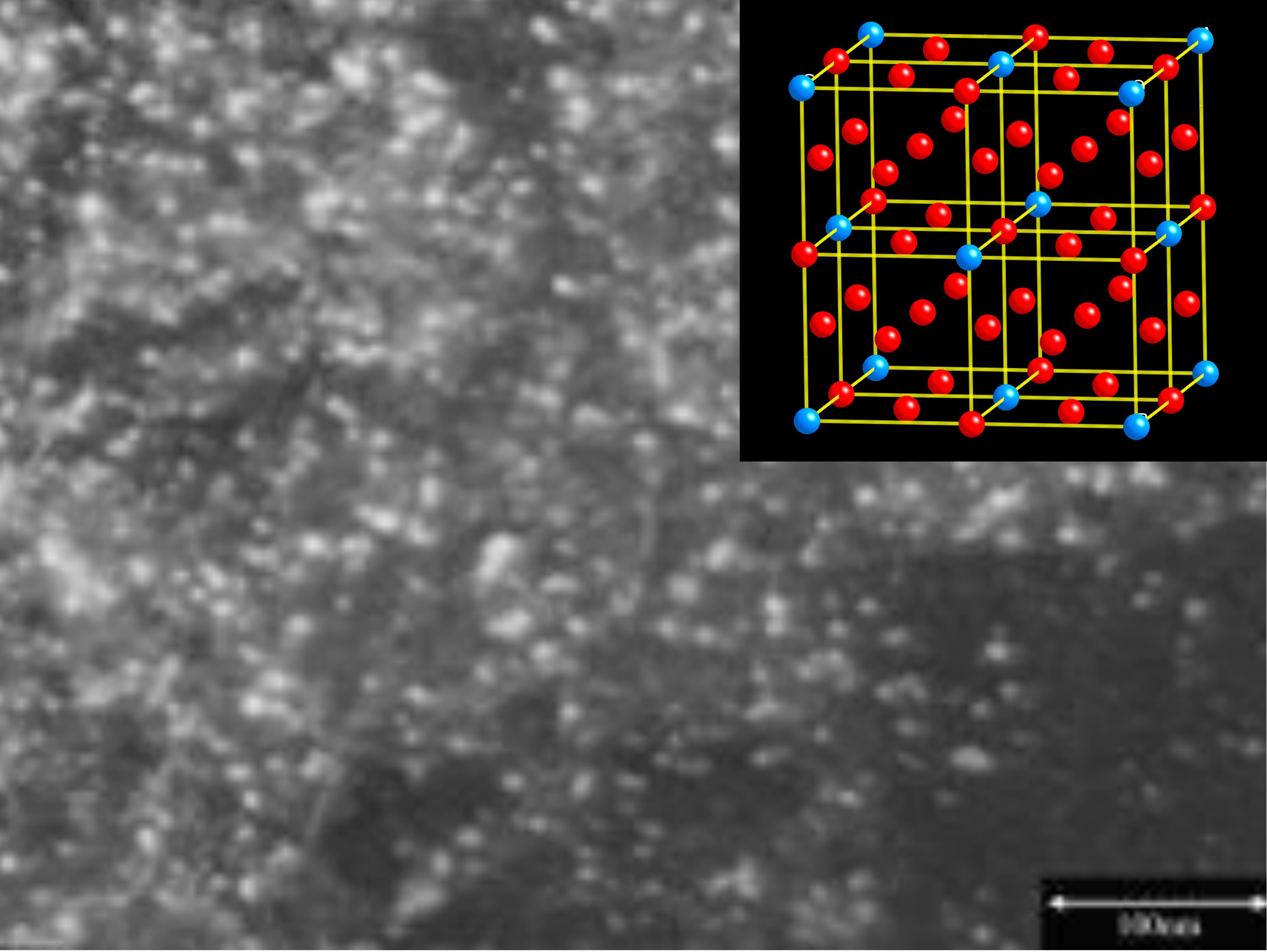
$$F = U - TS$$

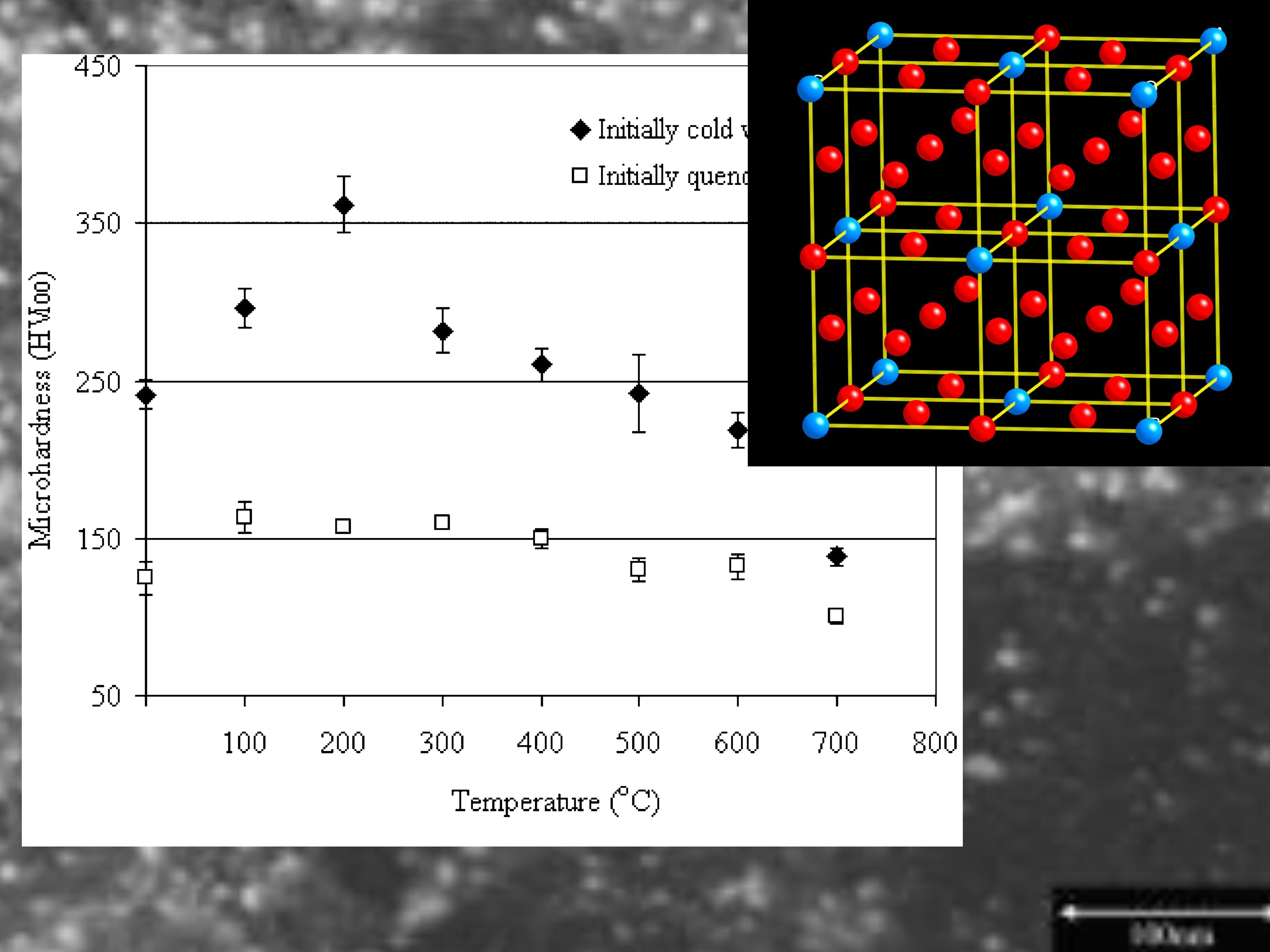


Converged CE
A2-B2 transition
MC cell: 16x16x16
-120
-140
-160
-180
-200
0
1000
2000
3000
1
0.8
0.6
0.4
0.2
0
ΔH$_{mix}$
C$_V$
Formation enthalpy [meV]
Configurational specific heat [k$_B$]
Temperature [K]

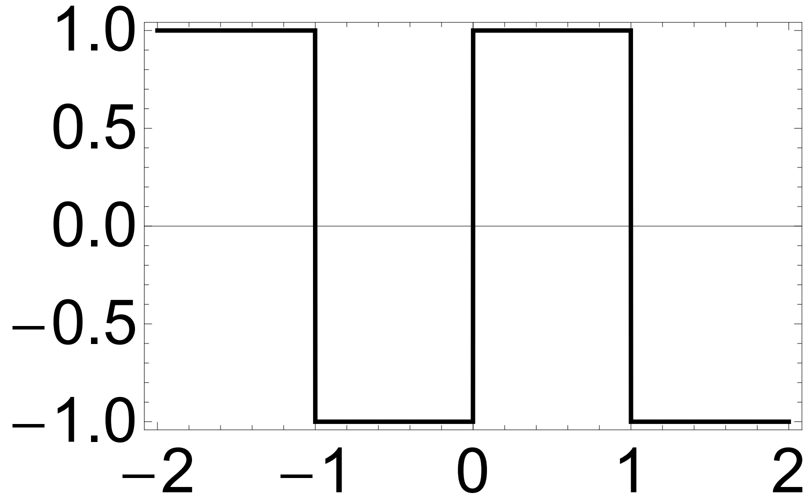
(b)

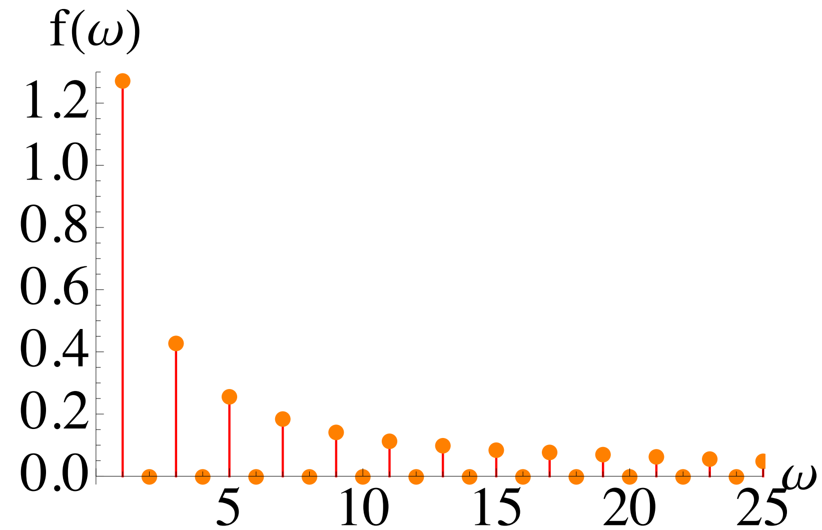


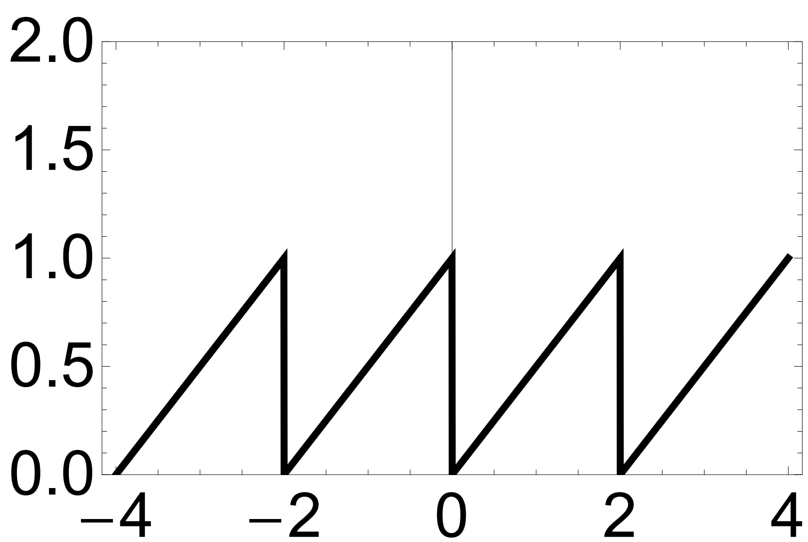


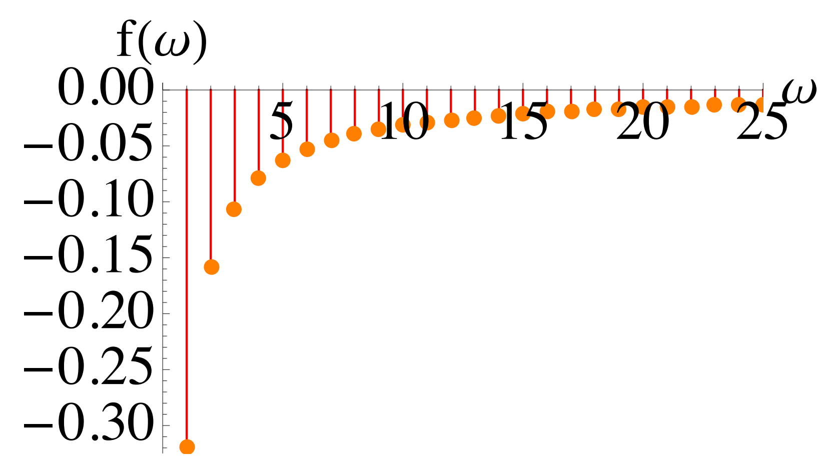

Microhardness (HVoo)
450
350
250
150
50
Initially cold
Initially quenc
100
200
300
400
500
600
700
800
Temperature (°C)

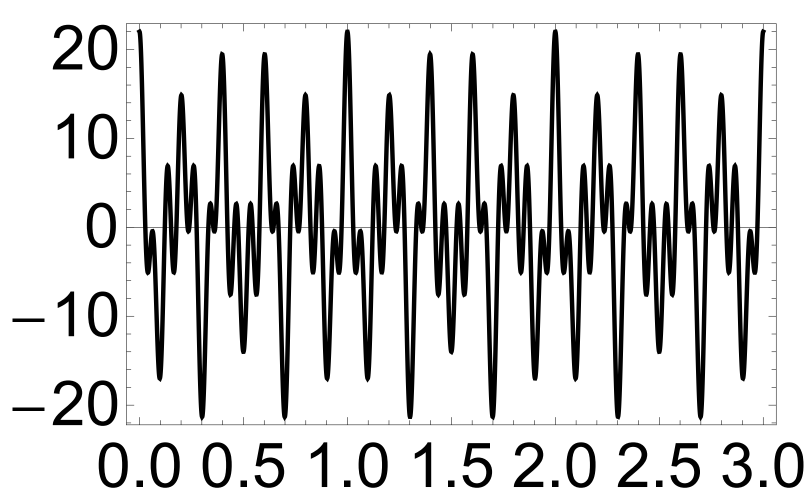
Periodic signals as Fourier series

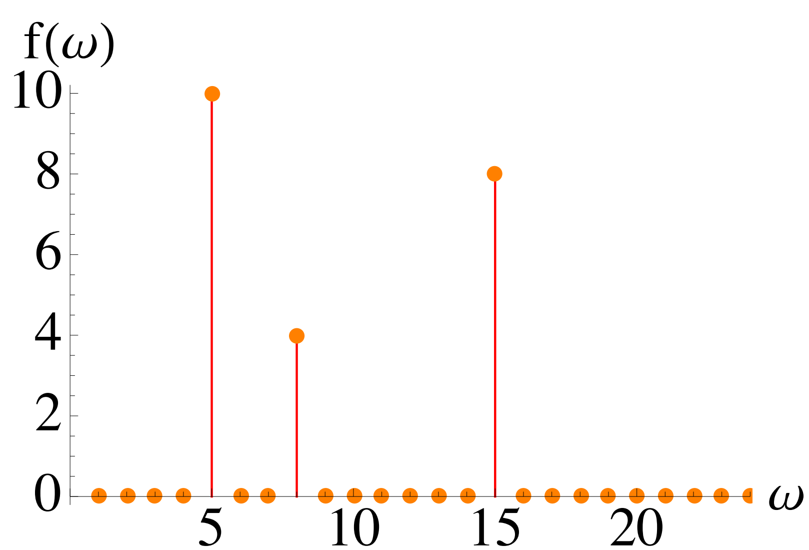




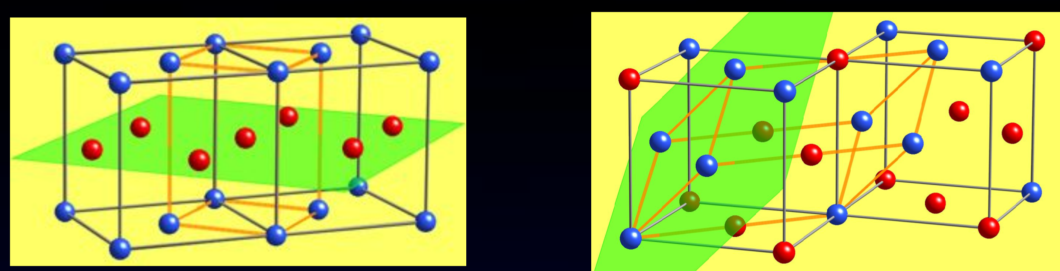






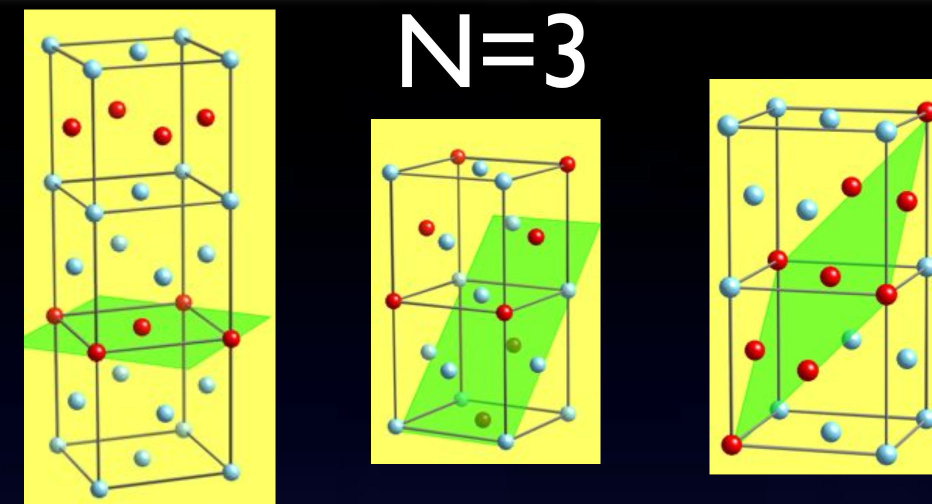


Periodic structures as "cluster" series



[001] N=2 [111]

N=3

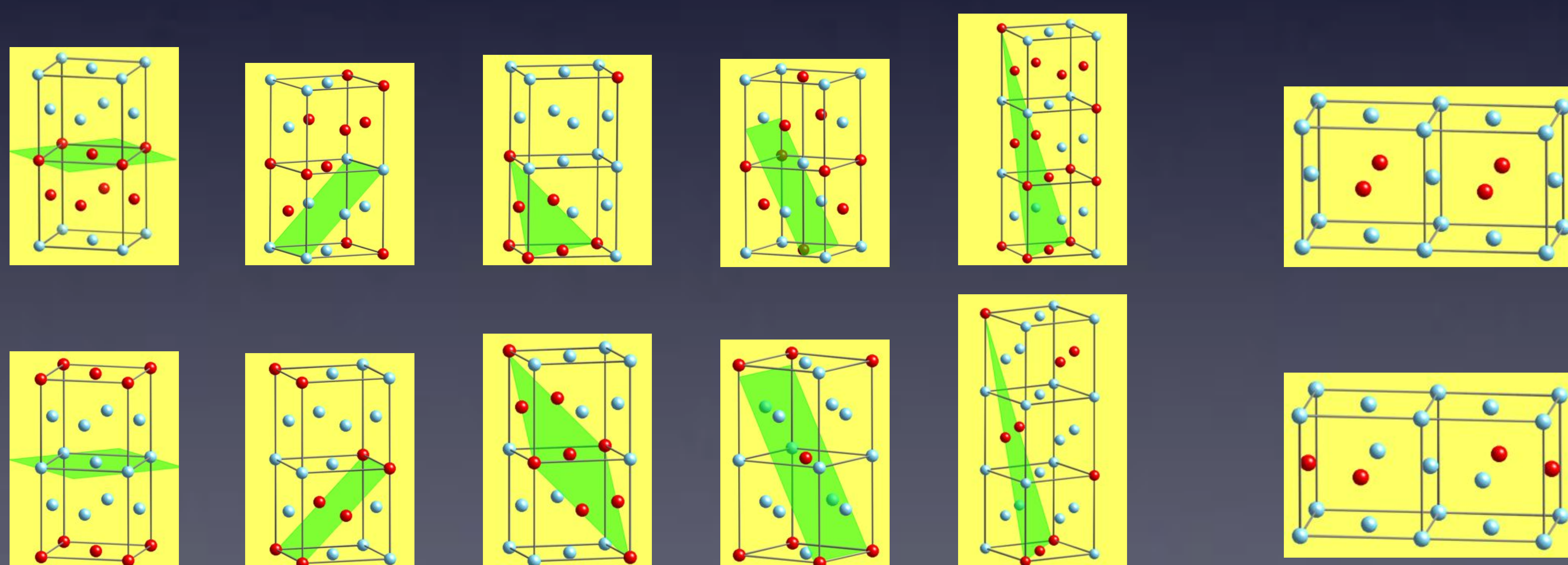


[001] [012] [111]

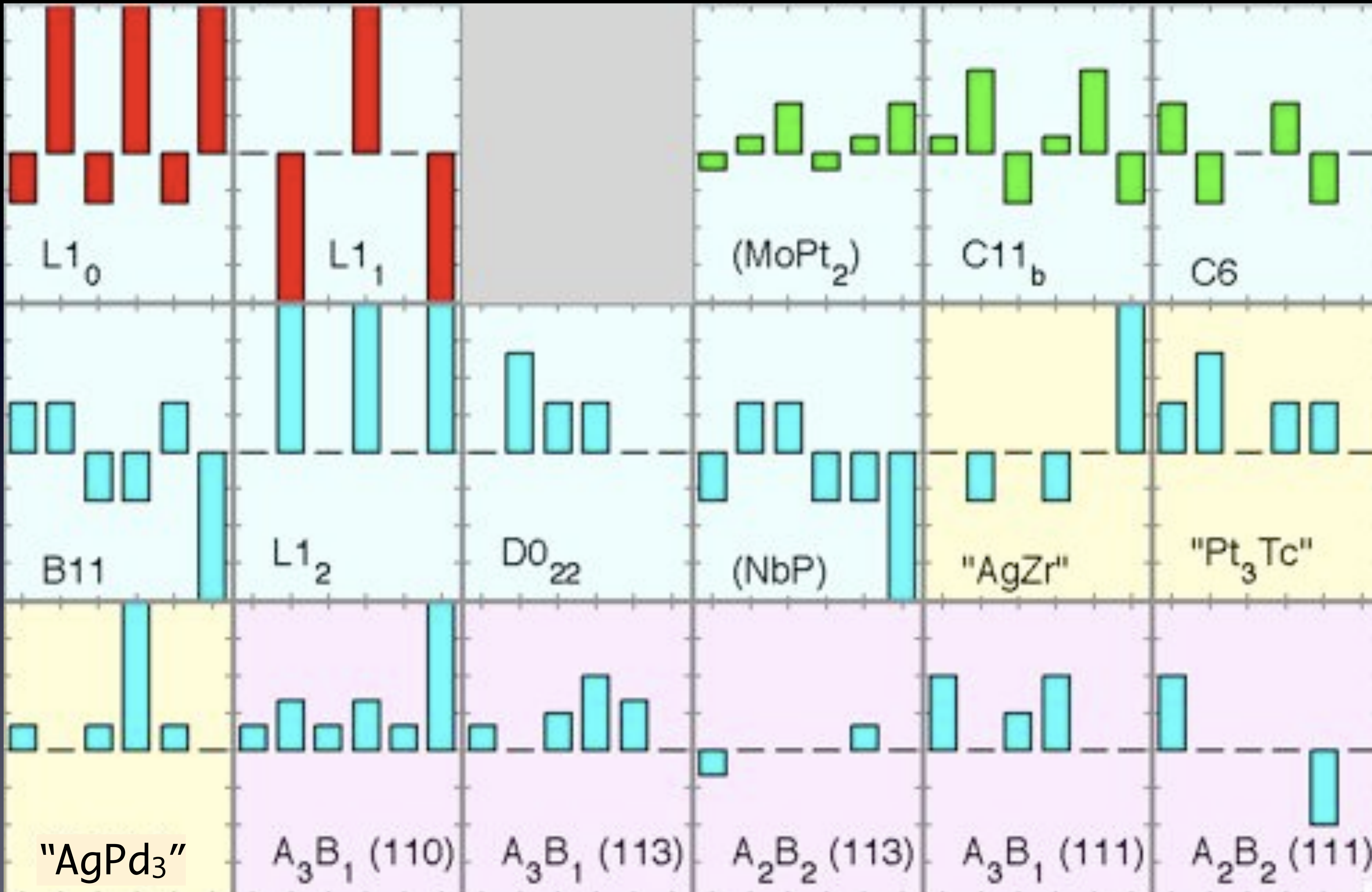
N=4

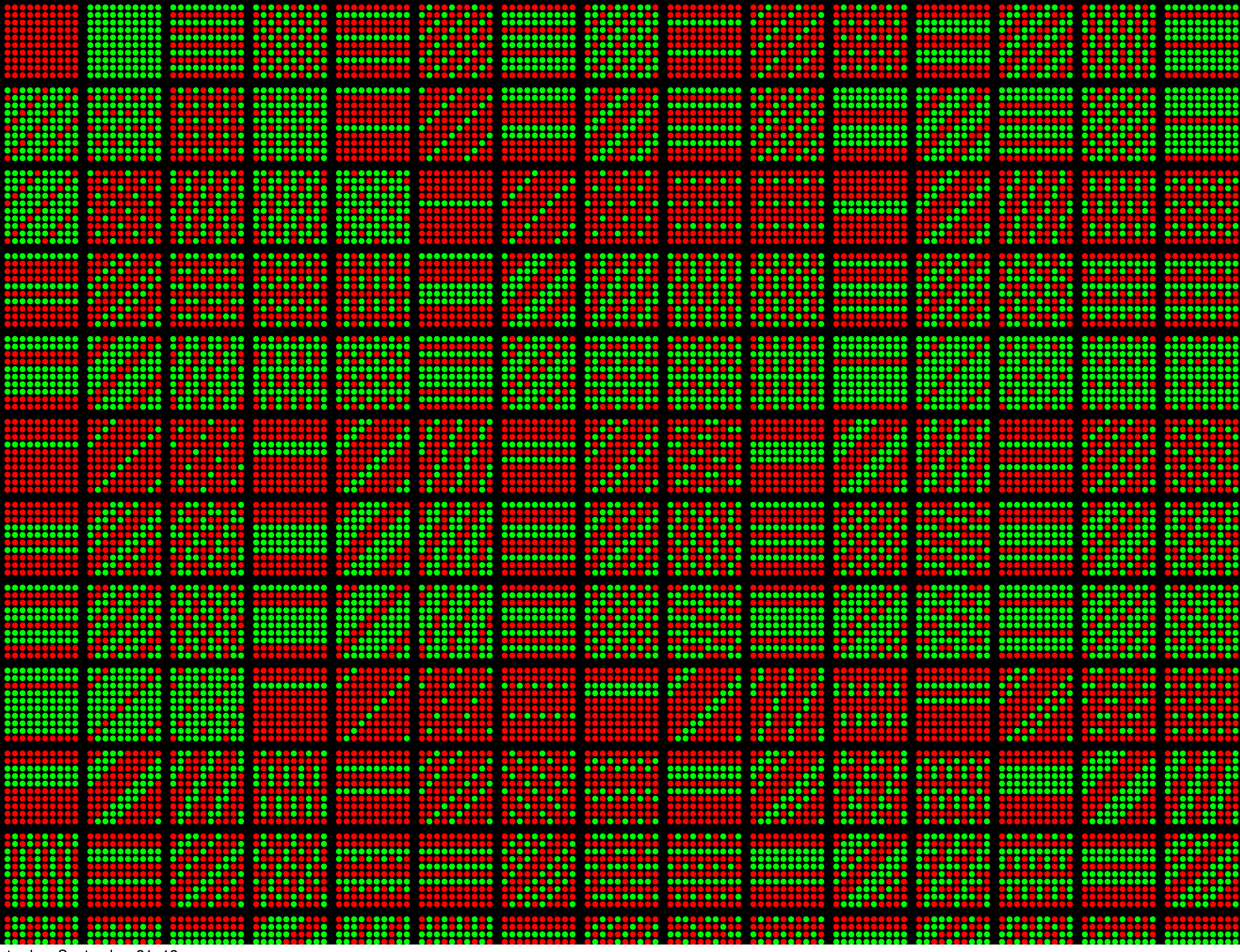
A_2B_2

A_3B_1

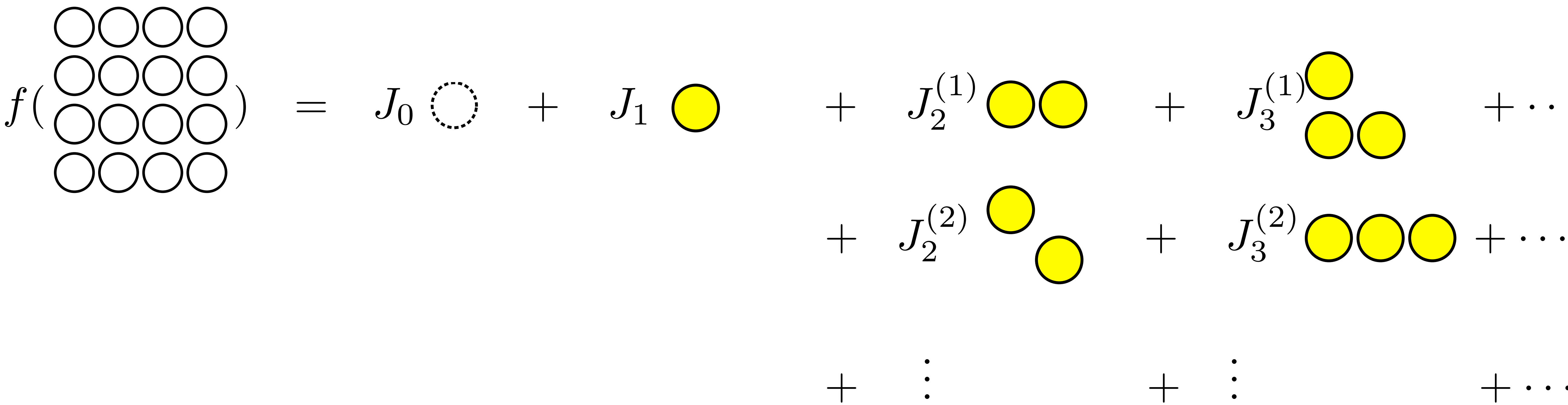


[001] [011] [111] [012] [113]

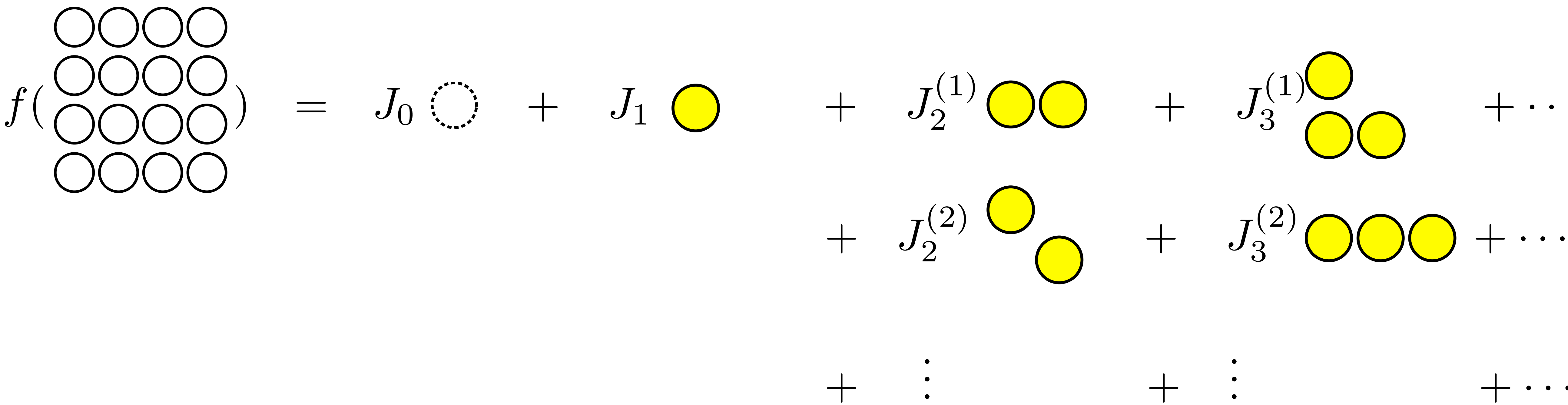

L1_0
L1_1
(MoPt_2)
C11_b
C6
B11
L1_2
D0_22
(NbP)
"AgZr"
"Pt_3Tc"
"AgPd3"
A_3B_1 (110)
A_3B_1 (113)
A_2B_2 (113)
A_3B_1 (111)
A_2B_2 (111)

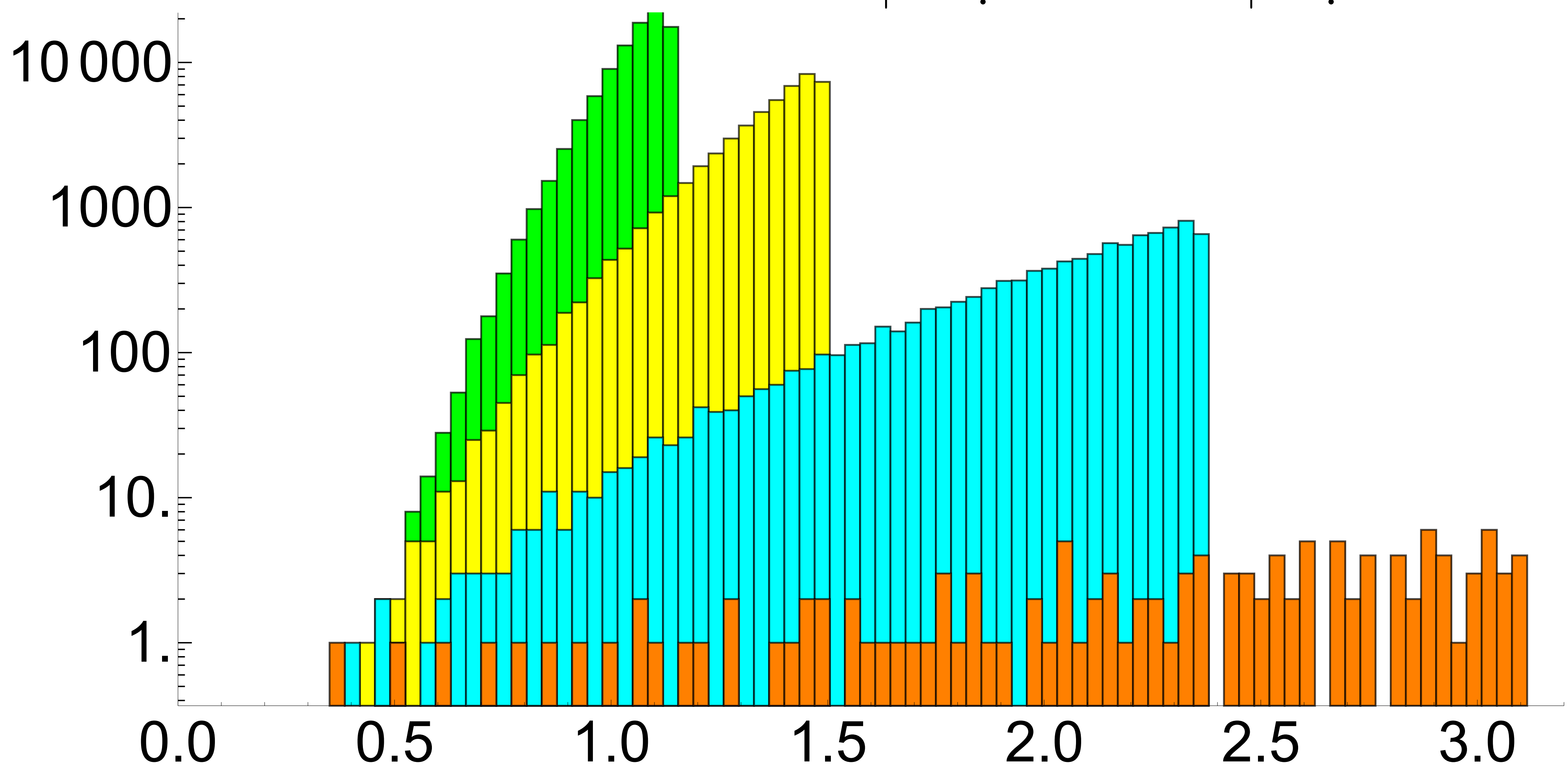


Cluster expansion: 2D

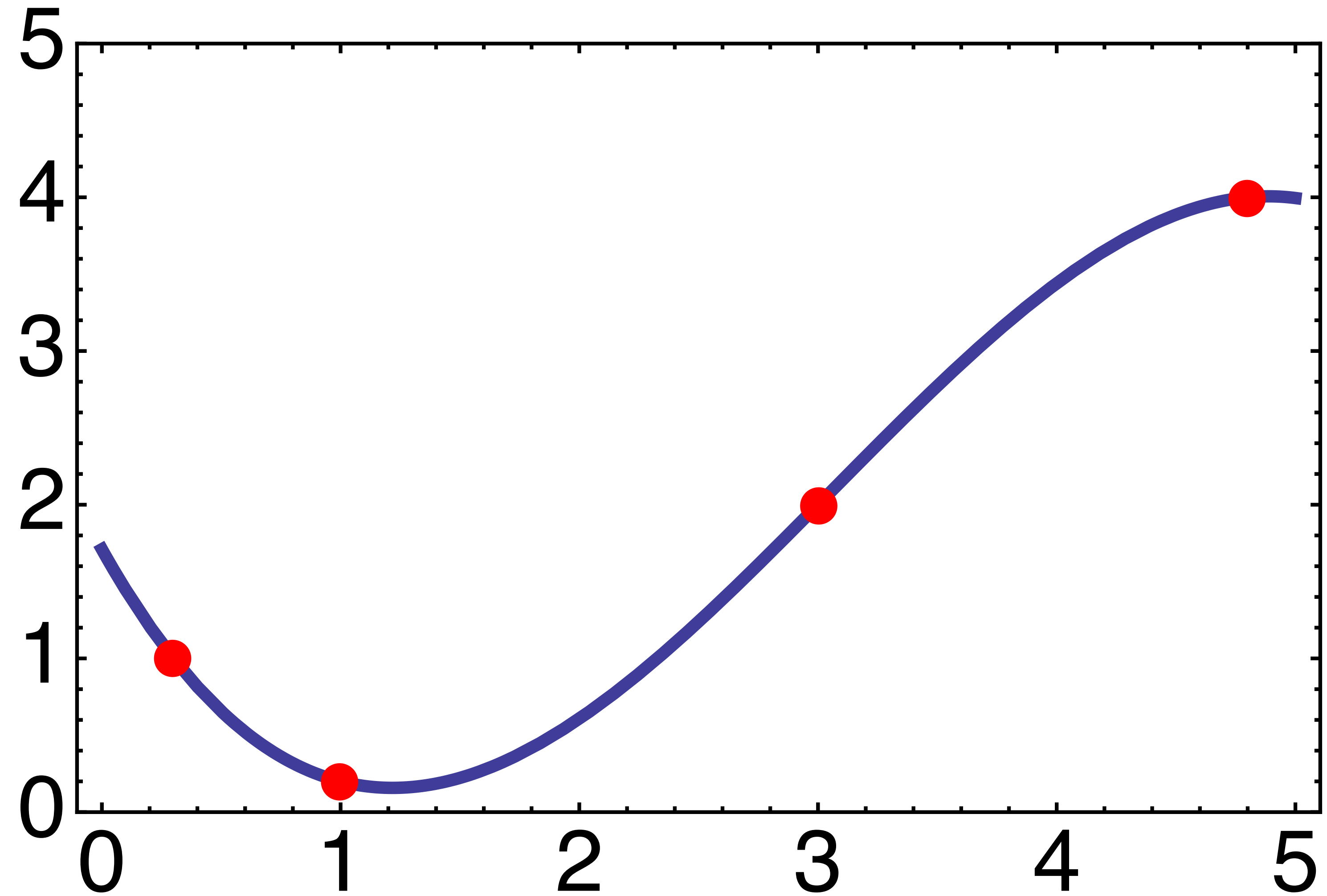


Cluster expansion: 2D





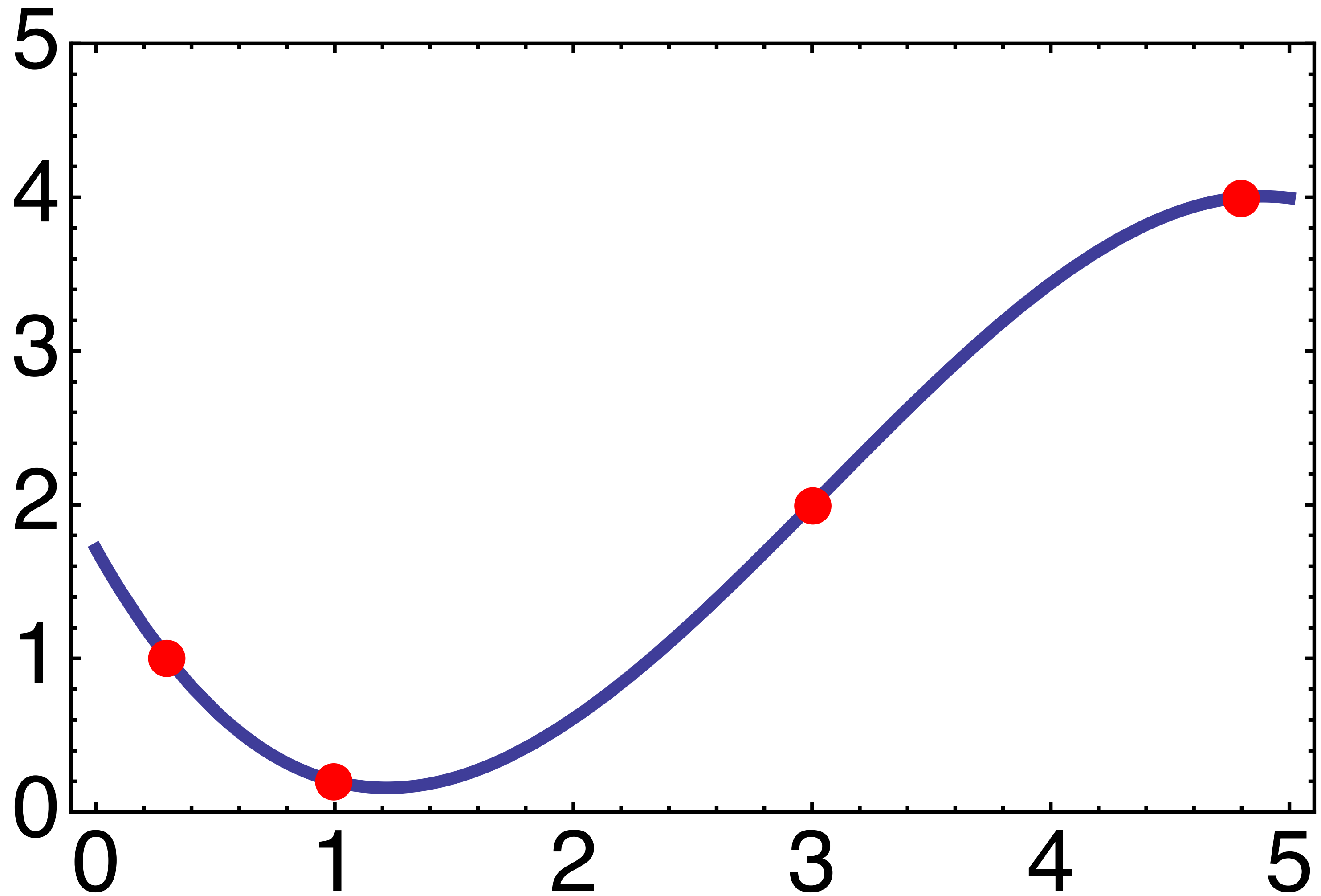
Expanding in a power series



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

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

Expanding in a power series

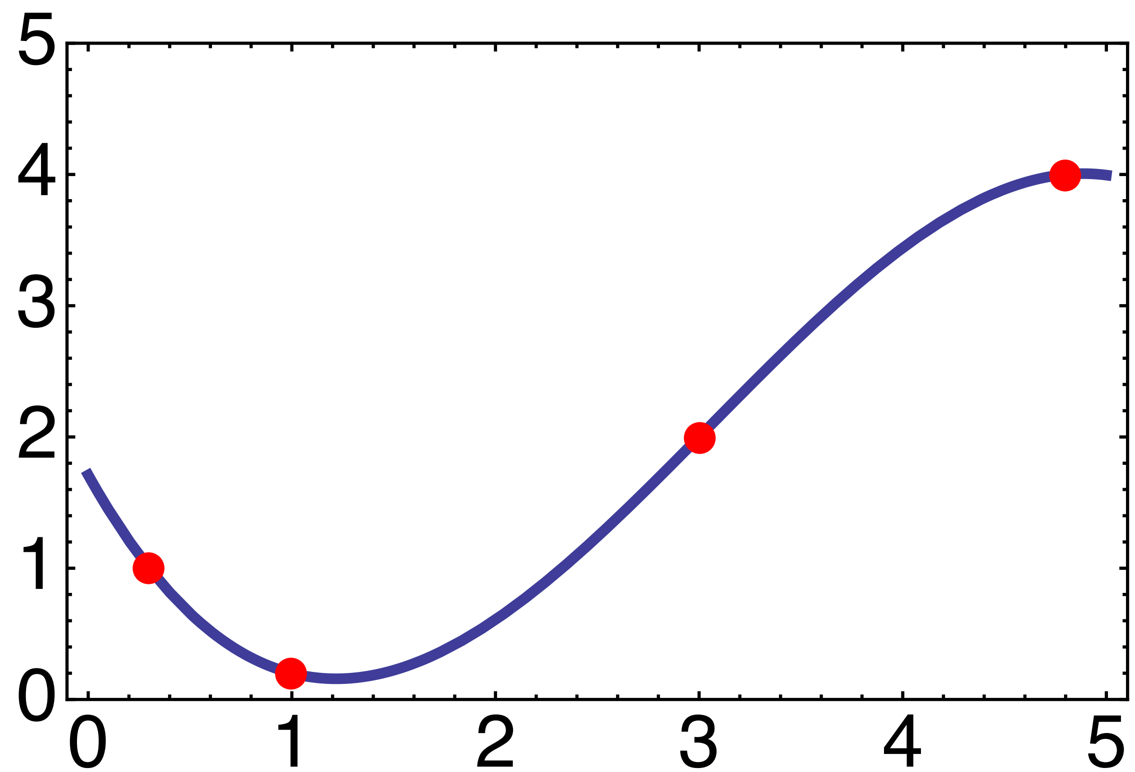


$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots$$

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

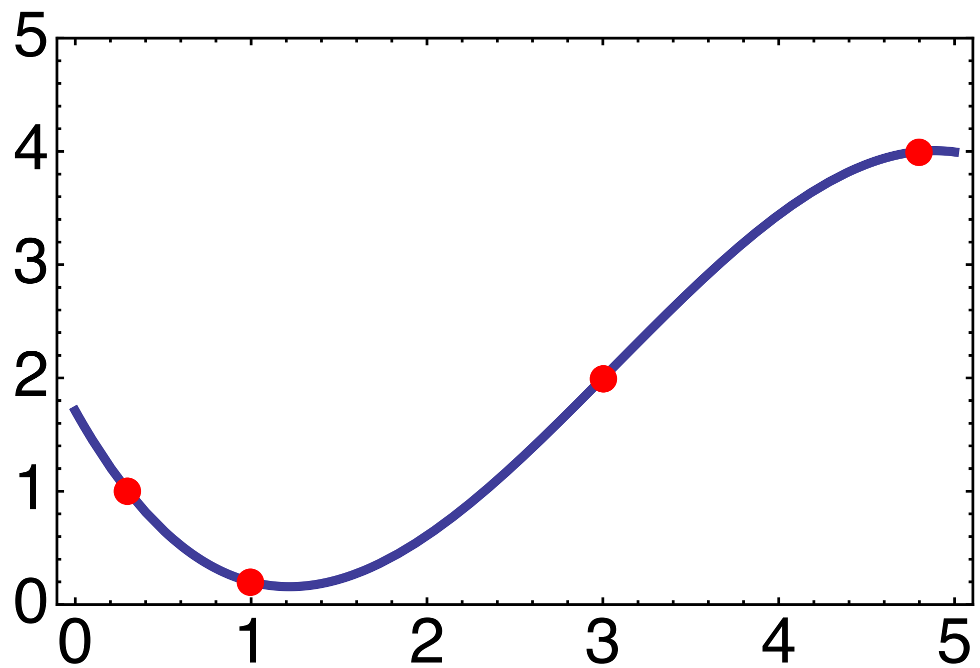
How do we find the coefficients?

Expanding in a power series



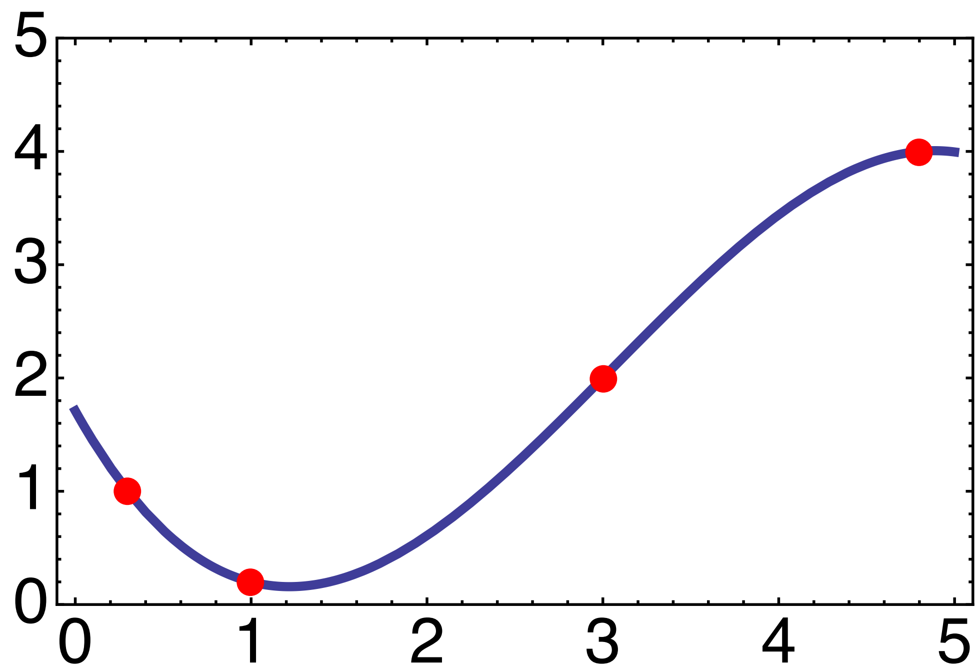
$$
\begin{aligned}
f(x_1) &= a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3 \\
f(x_2) &= a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3 \\
f(x_3) &= a_0 + a_1 x_3 + a_2 x_3^2 + a_3 x_3^3 \\
f(x_4) &= a_0 + a_1 x_4 + a_2 x_4^2 + a_3 x_4^3
\end{aligned}
$$

Expanding in a power series



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

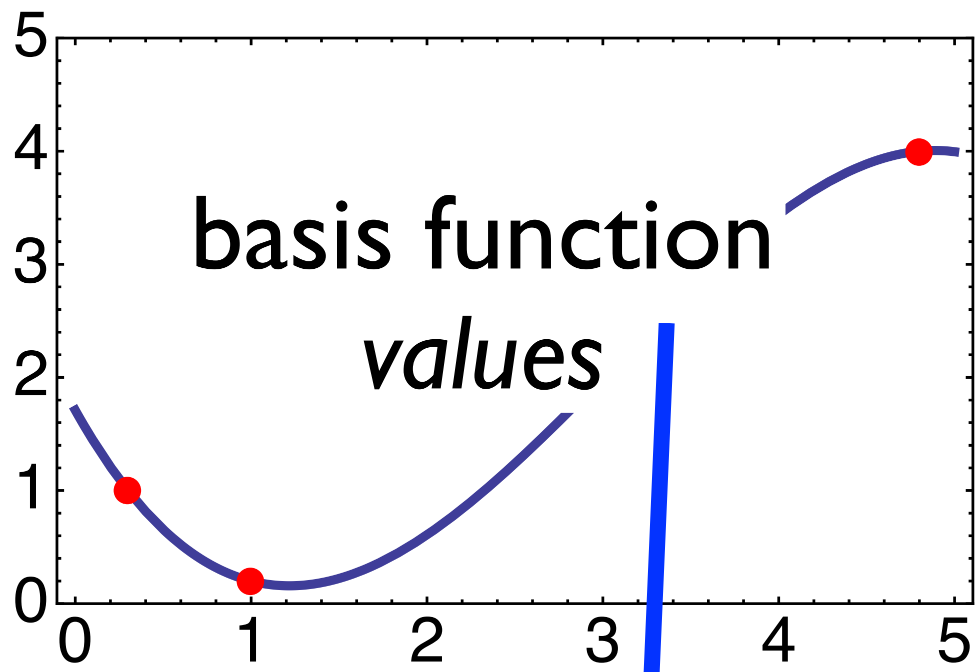
Expanding in a power series



Data

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

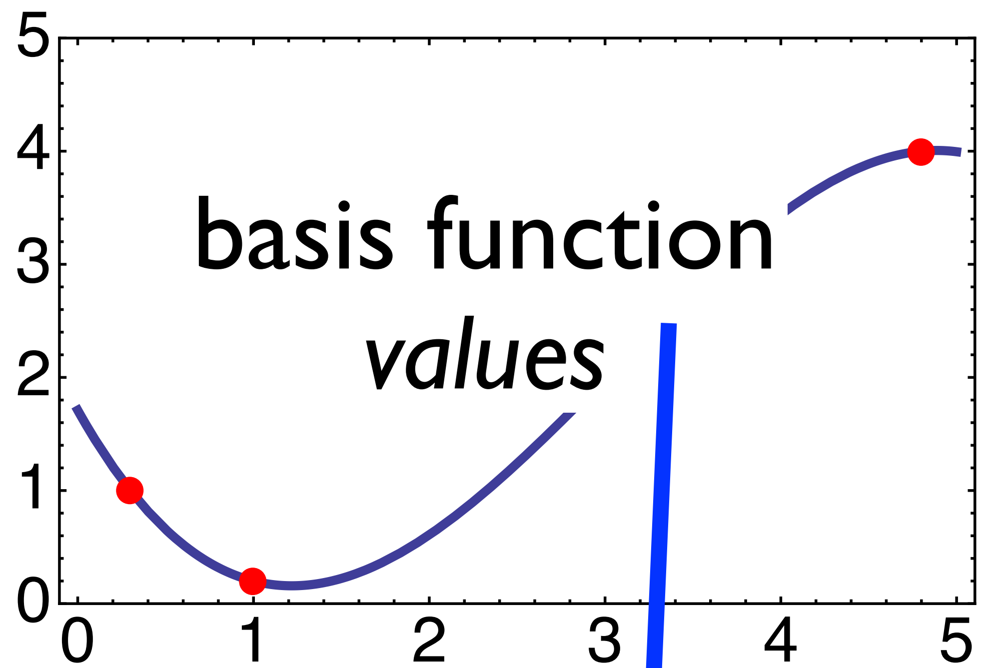
Expanding in a power series



Data

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

Expanding in a power series



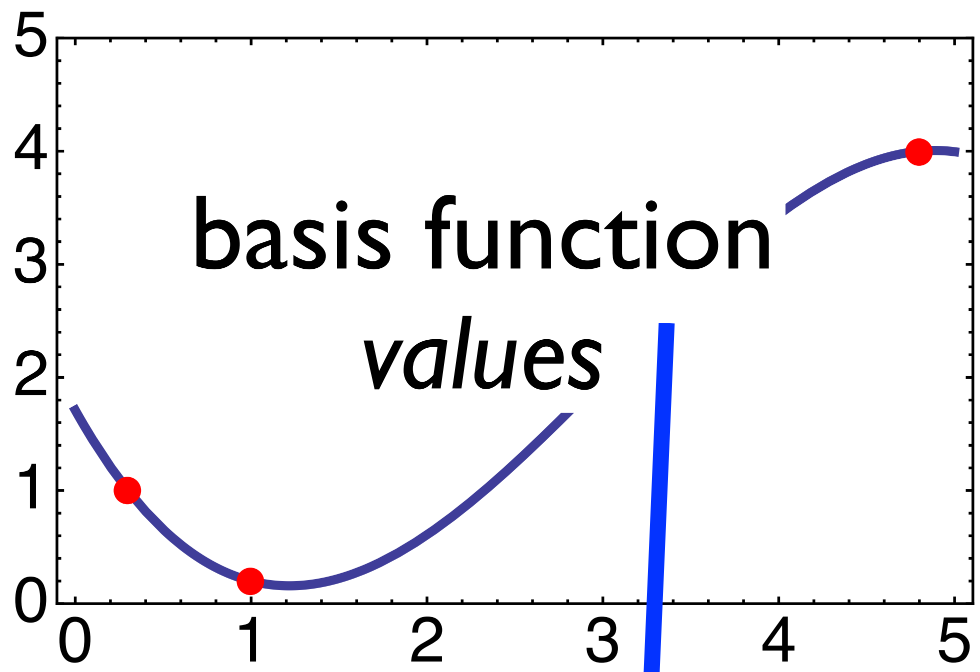
Data

basis function *values*

coefficients of the model

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

Expanding in a power series



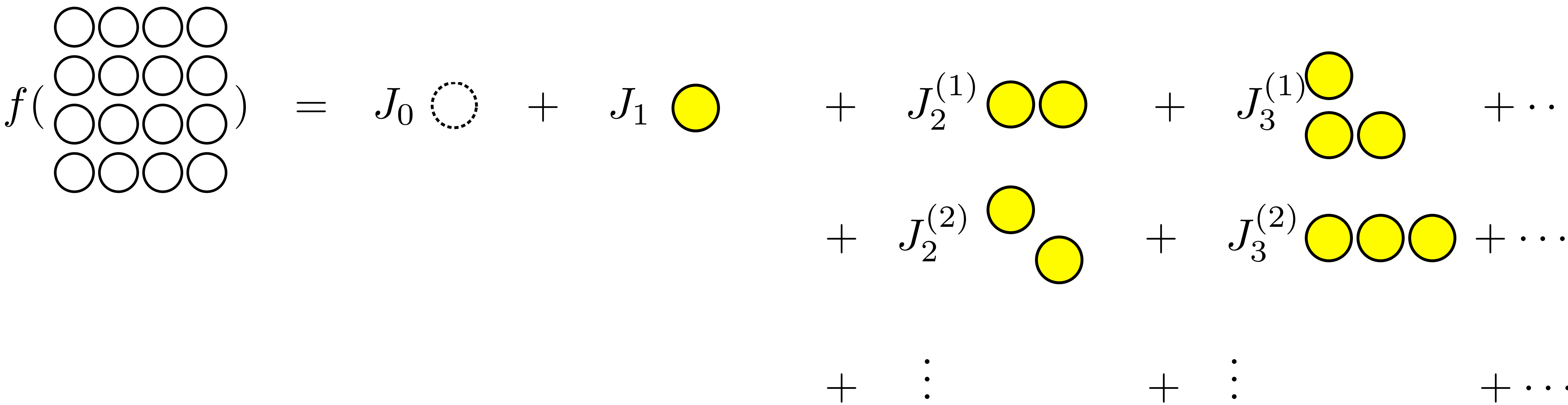
Data

basis function *values*

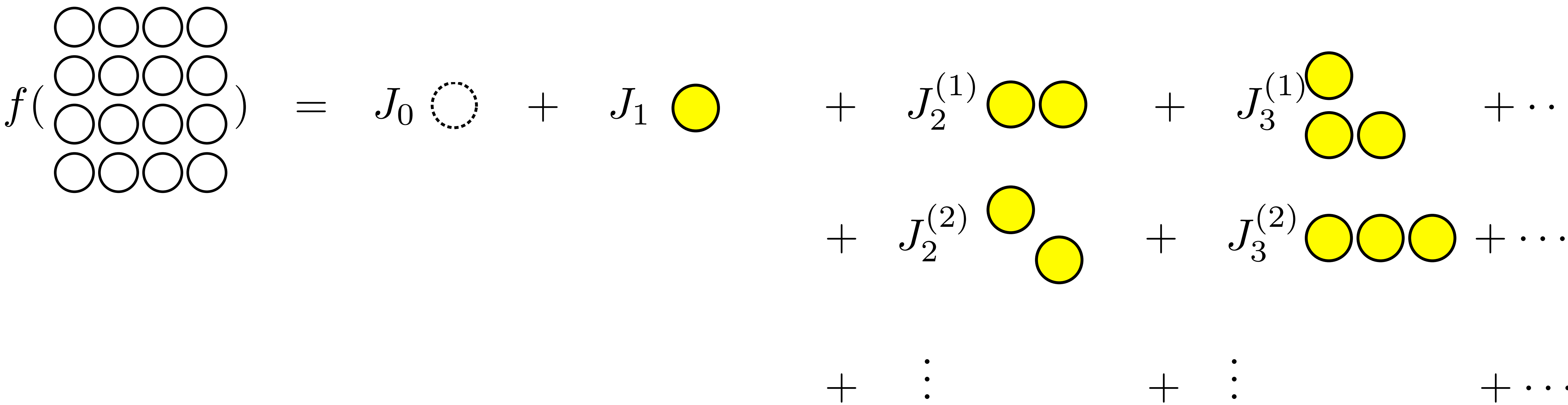
coefficients of the model

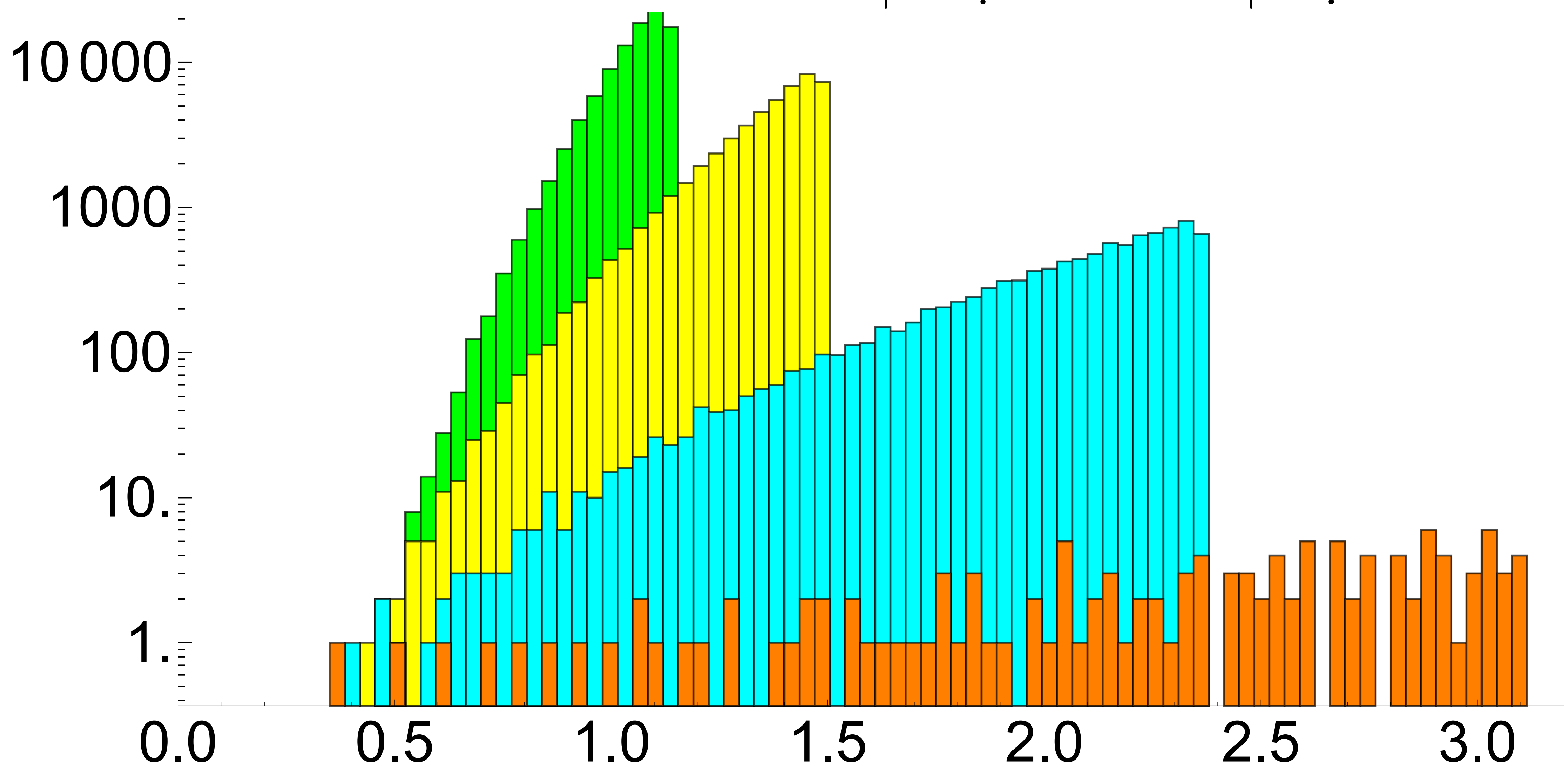
$$\begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

Cluster expansion



Cluster expansion





Model building with compressive sensing

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)

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

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

Going beyond a linear model fit (adding terms)

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

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

$$\mathbb{M}\vec{a} = \vec{f}$$

Going beyond a linear model fit (adding terms)

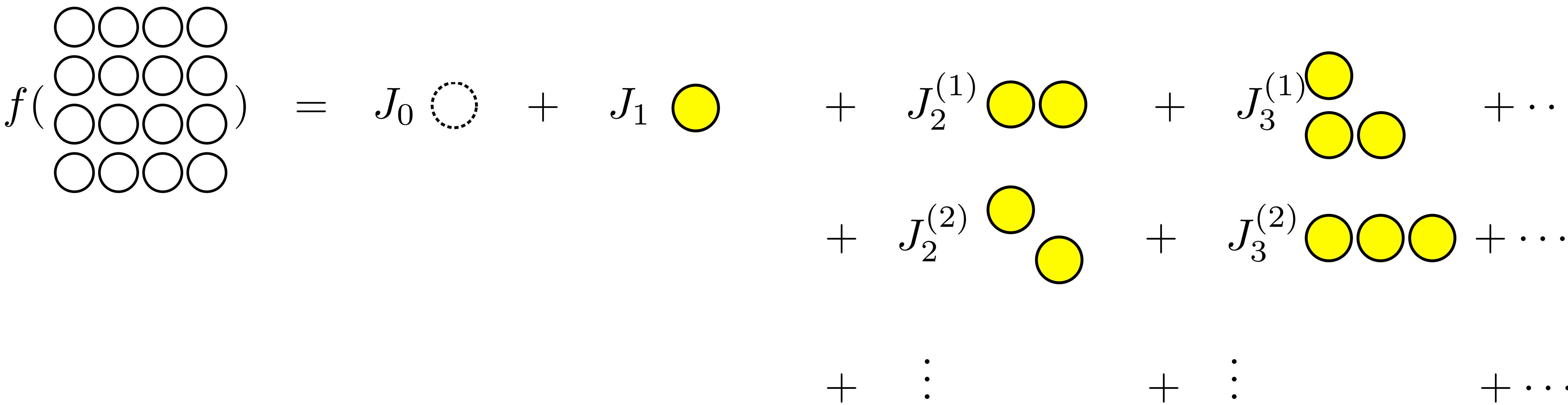
$$f(x,y) = \boxed{a_0 + a_1 x + a_2 y + a_3 xy + a_4 x^2 + a_5 y^2} + \cdots$$

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

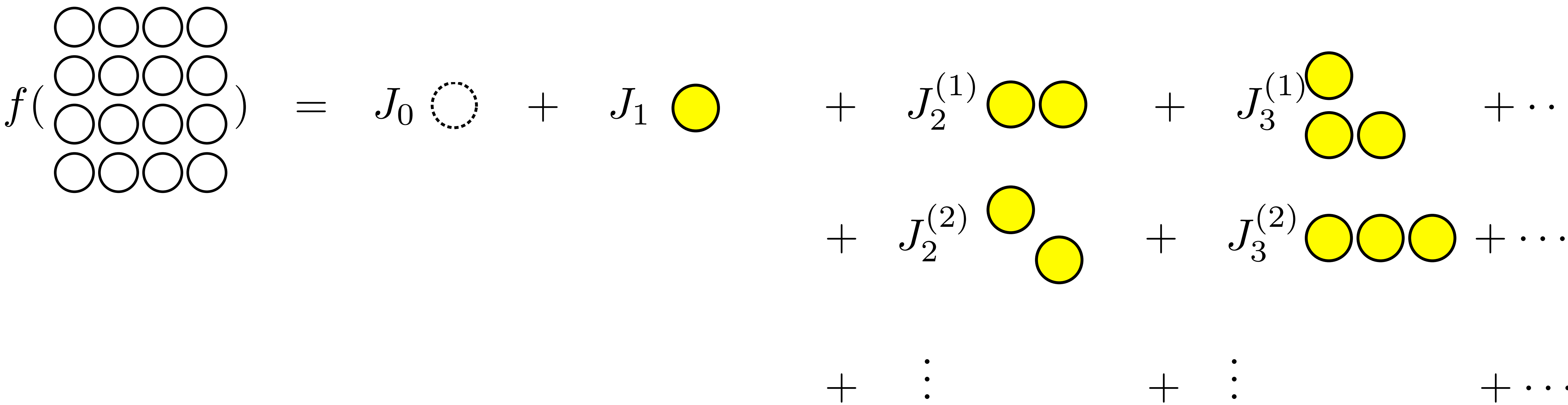
$$\mathbb{M}\vec{a} = \vec{f}$$

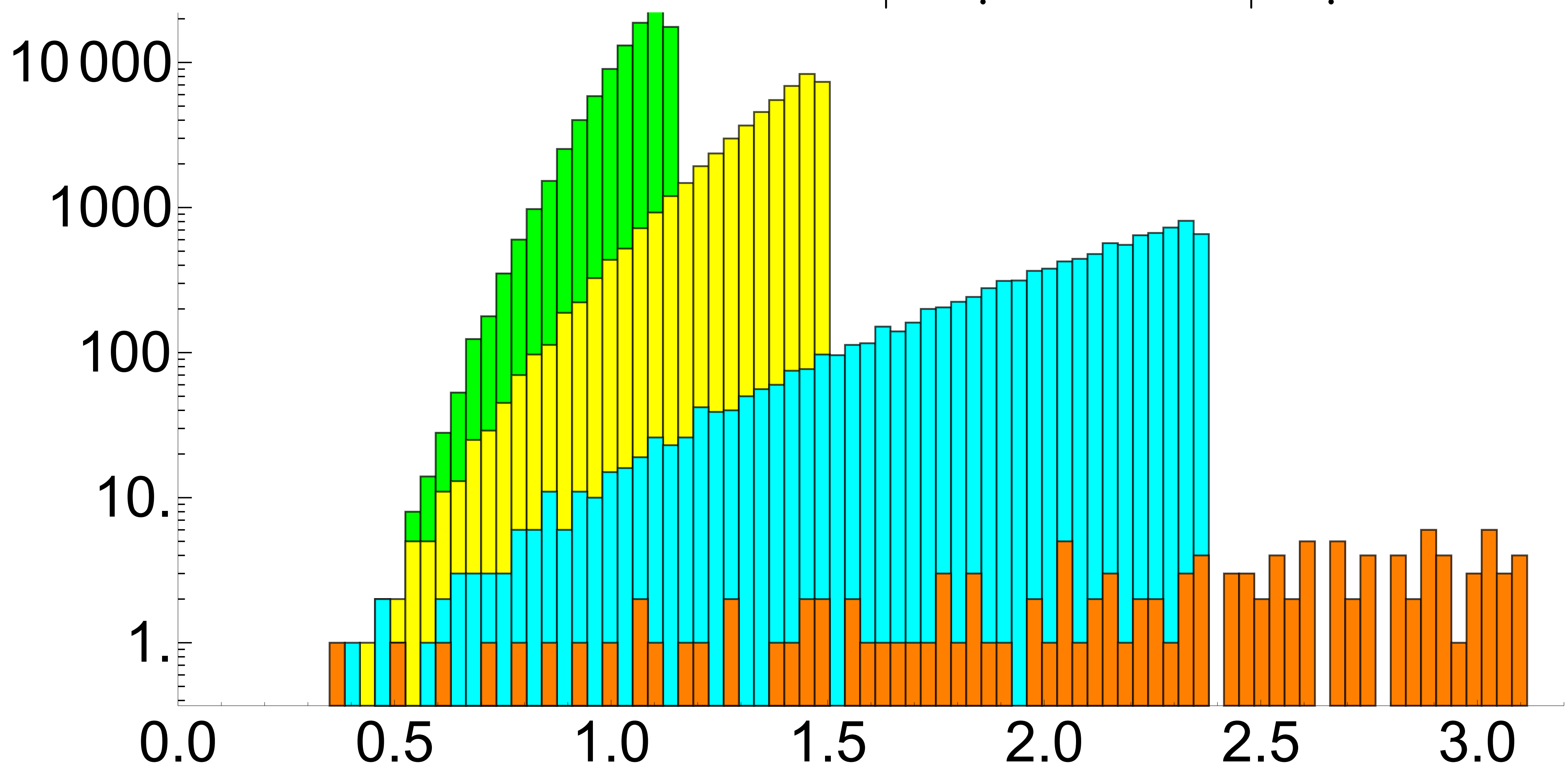
But the matrix isn't square!

Cluster expansion



Cluster expansion





“Solving” an under-determined problem

“Solving” an under-determined problem

$$\mathbb{M}\vec{a} = \vec{f}$$

“Solving” an under-determined problem

$$\mathbb{M}\vec{a} = \vec{f}$$

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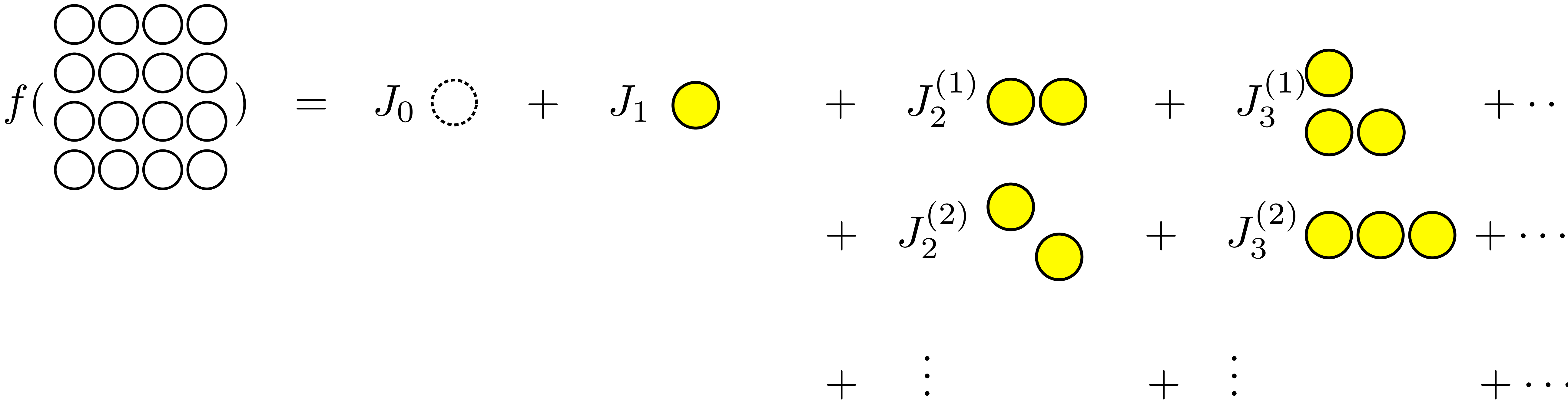
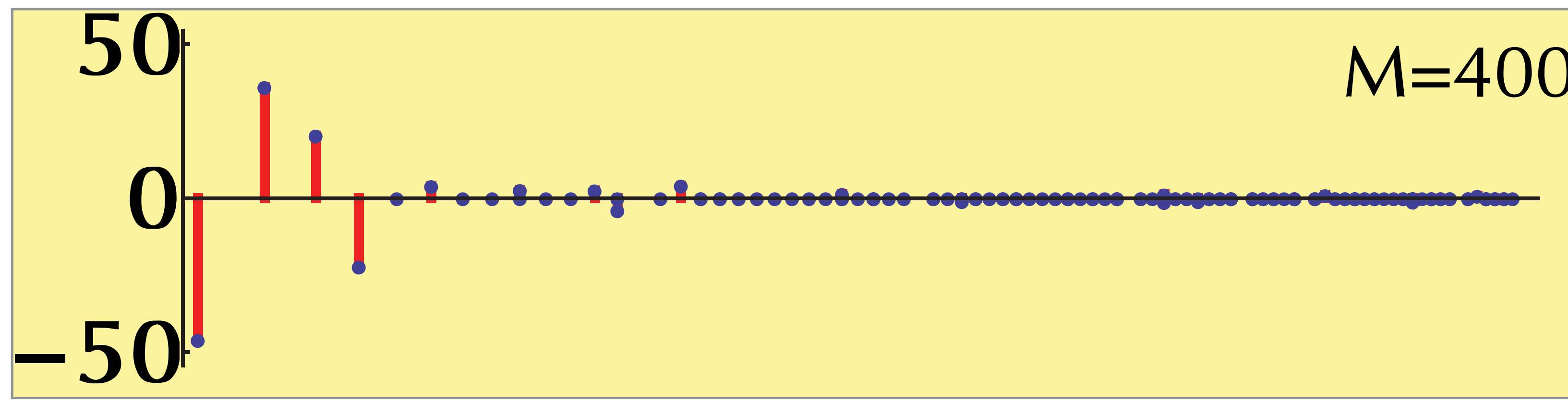
Models built via Compressive Sensing



Models built via Compressive Sensing

$$f(\ \cdot\ ) = J_0 + J_1 + J_2^{(1)} + J_3^{(1)} + \cdots$$
$$+ J_2^{(2)} + J_3^{(2)} + \cdots$$

Pair



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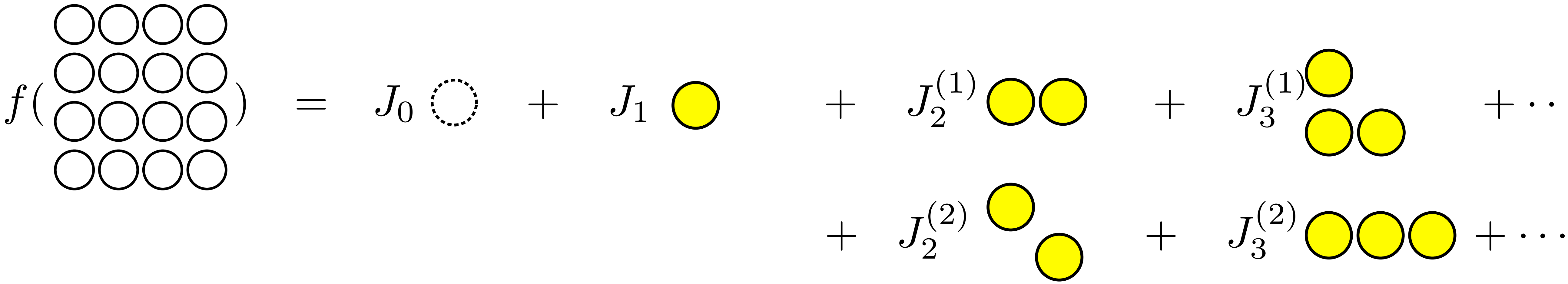

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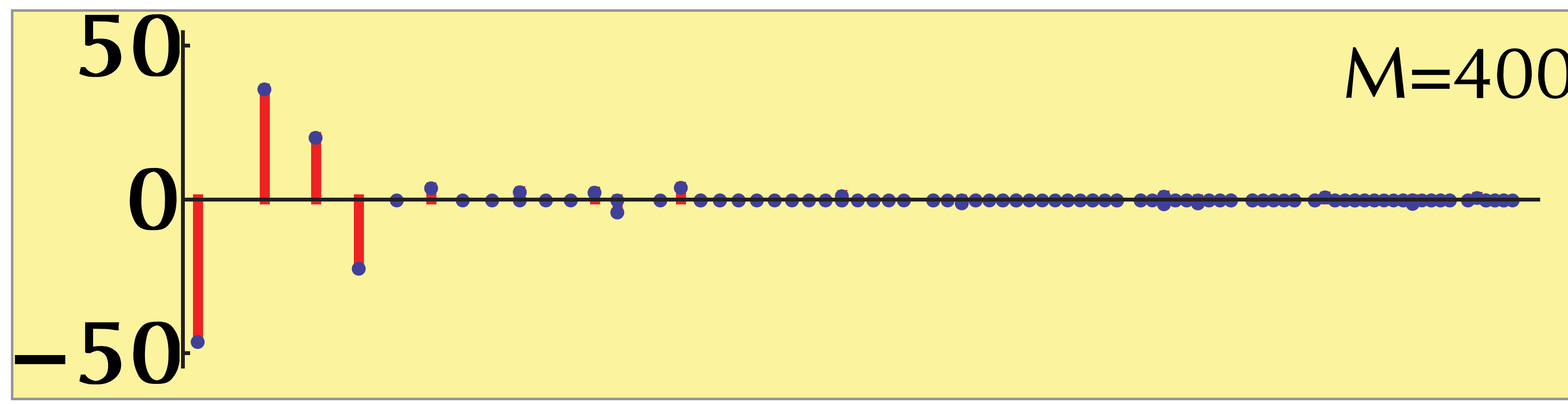
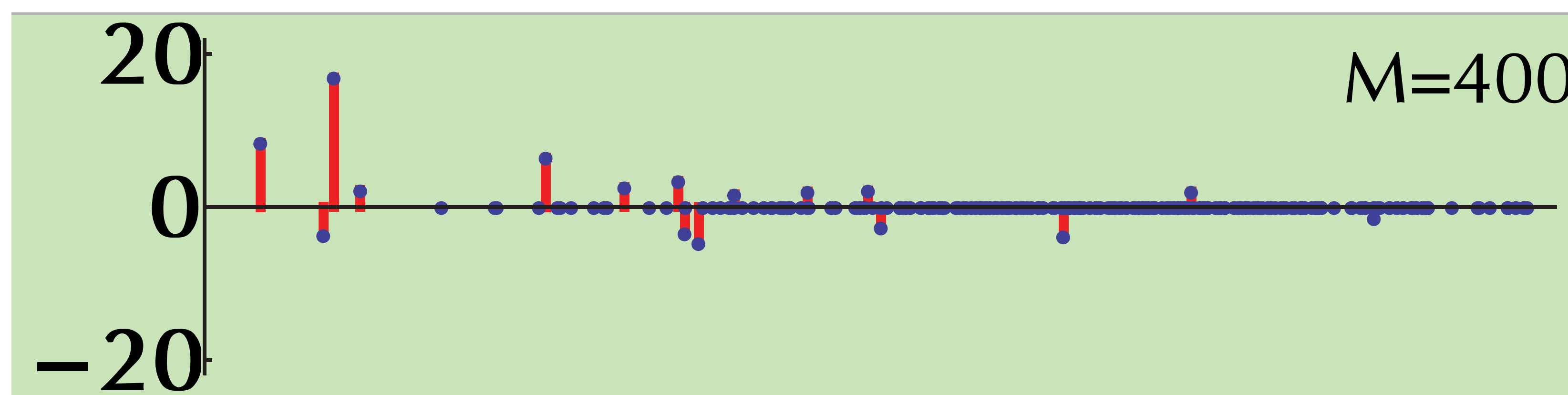


Triplet



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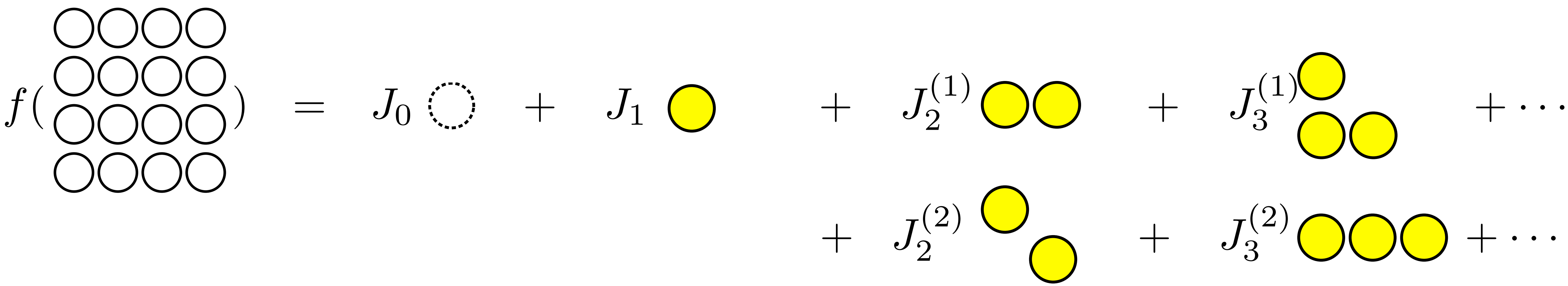

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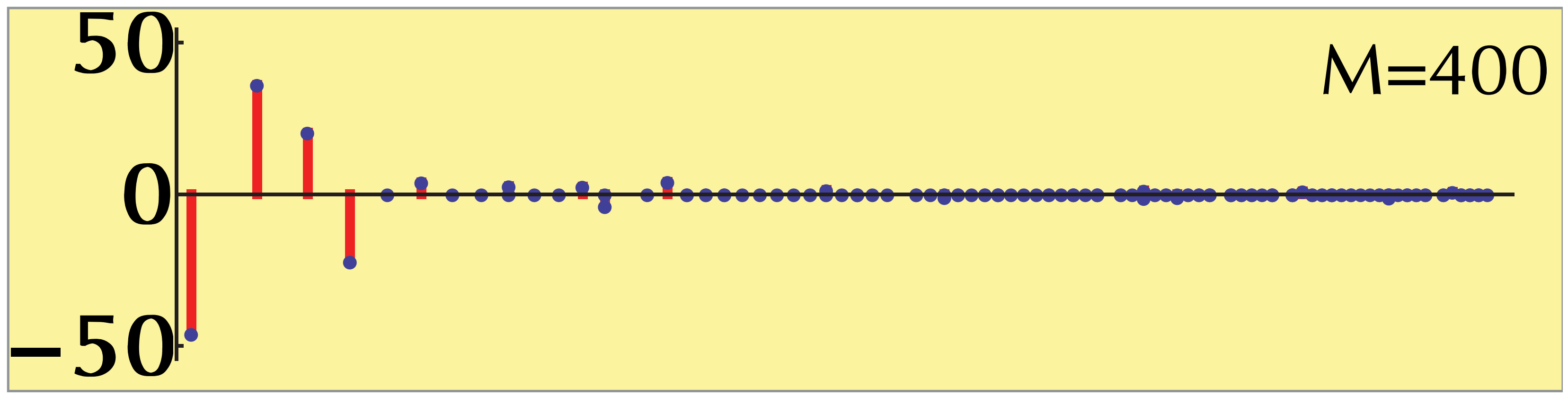
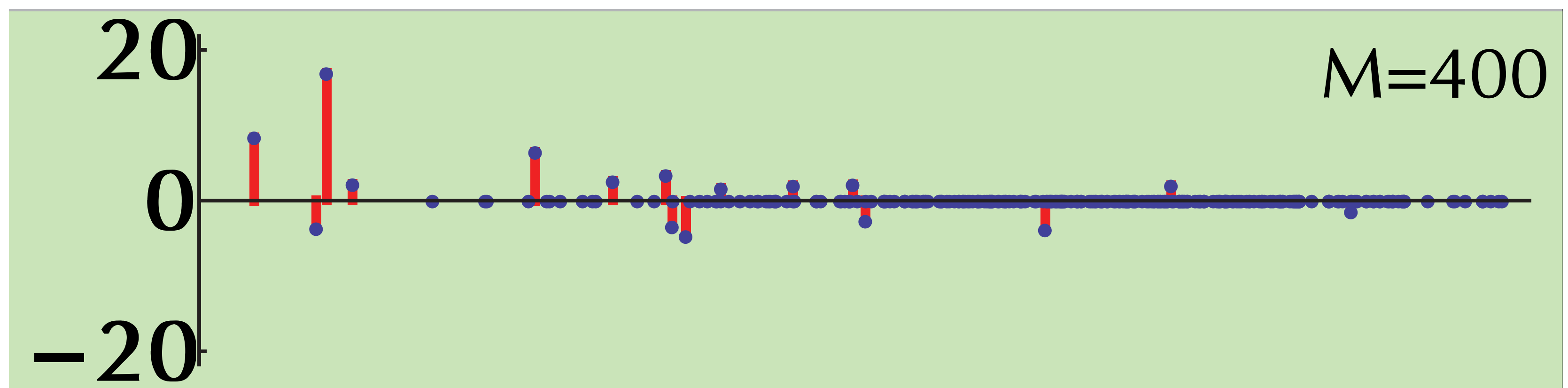
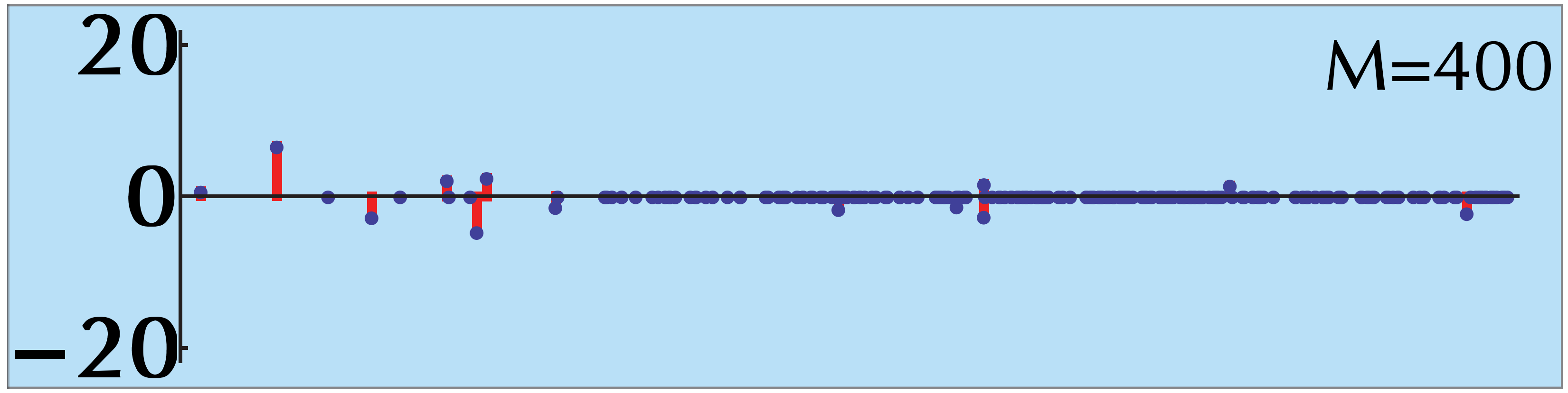


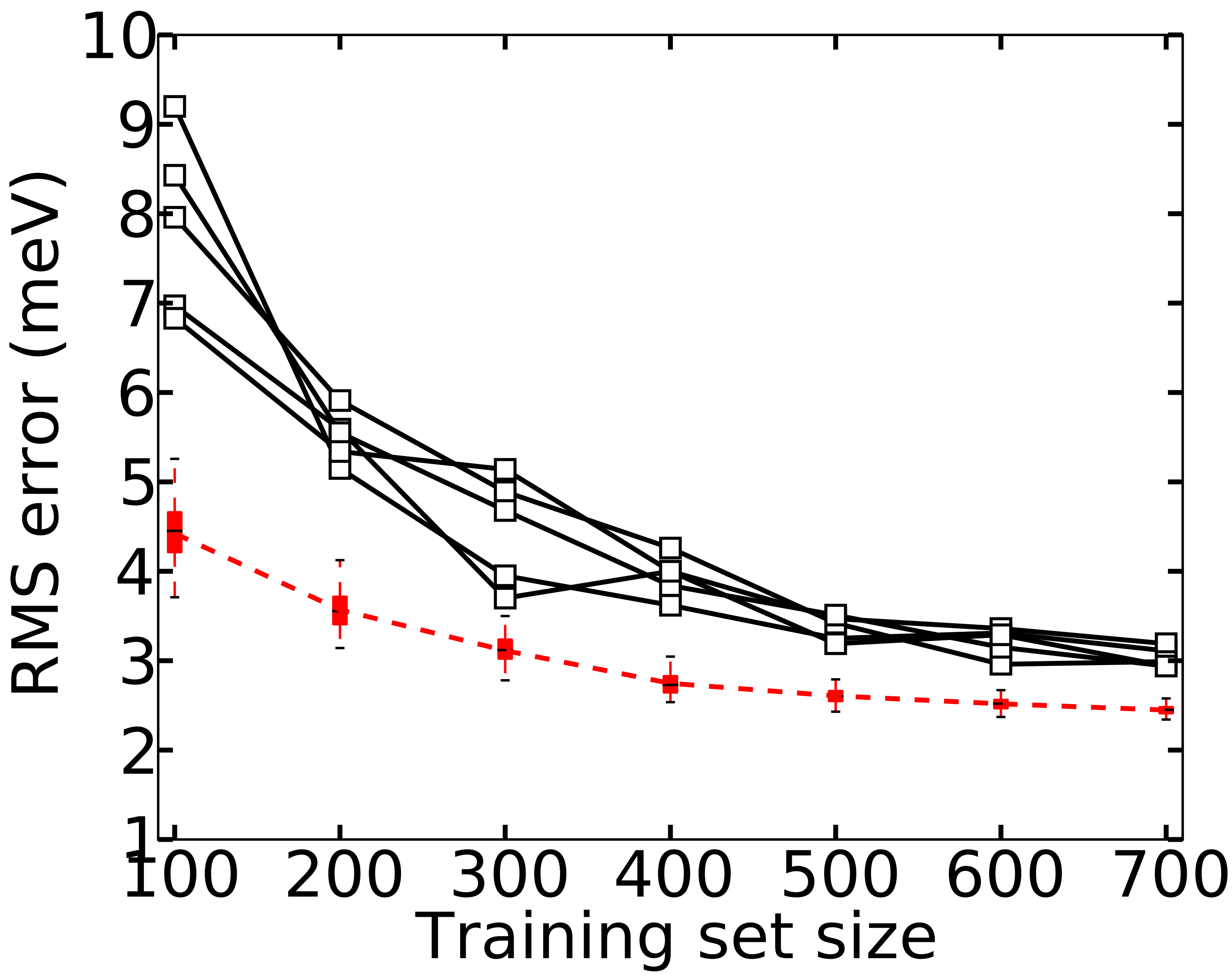
Triplet



Quadruplet



Bayesian Compressive Sensing vs. GA



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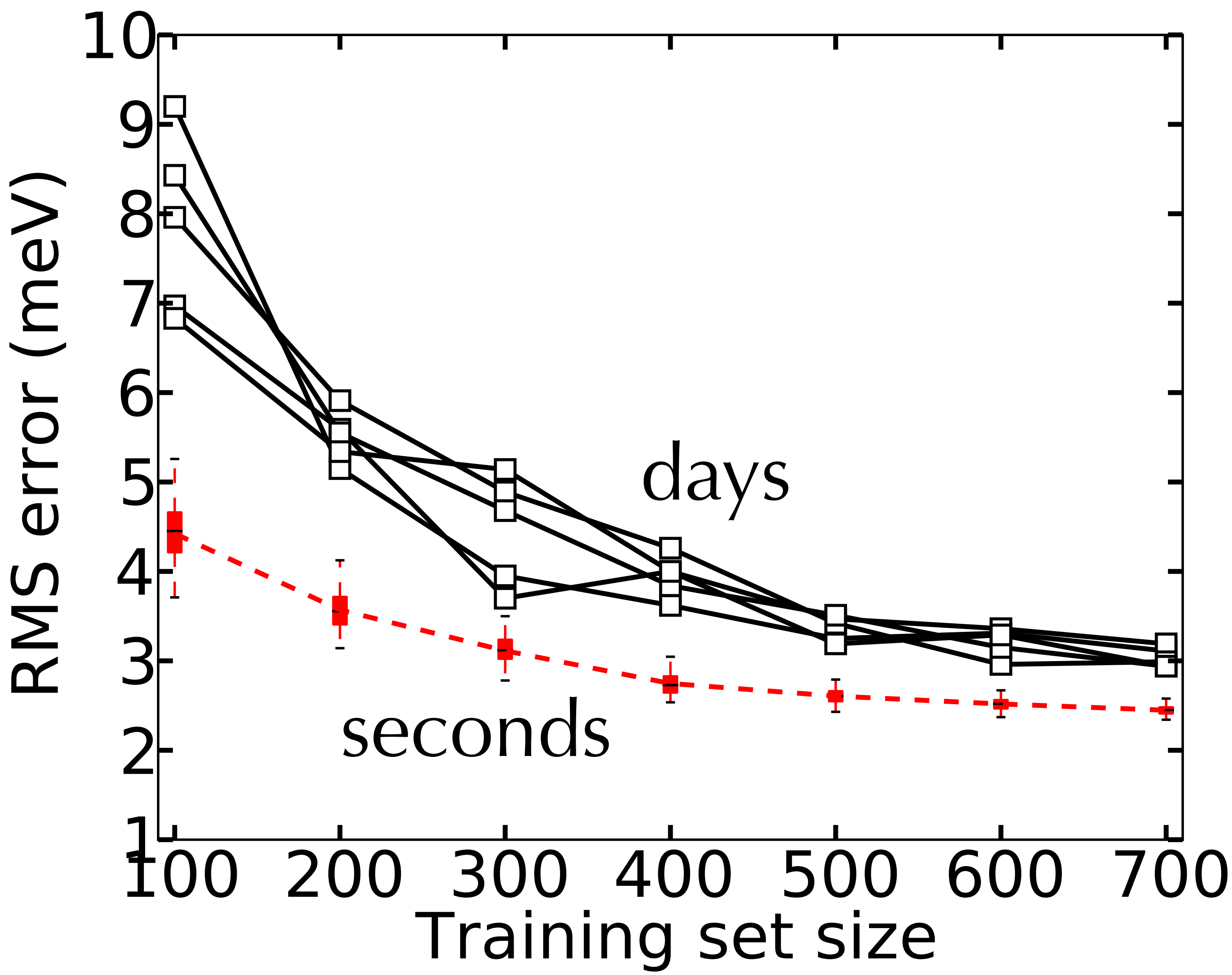

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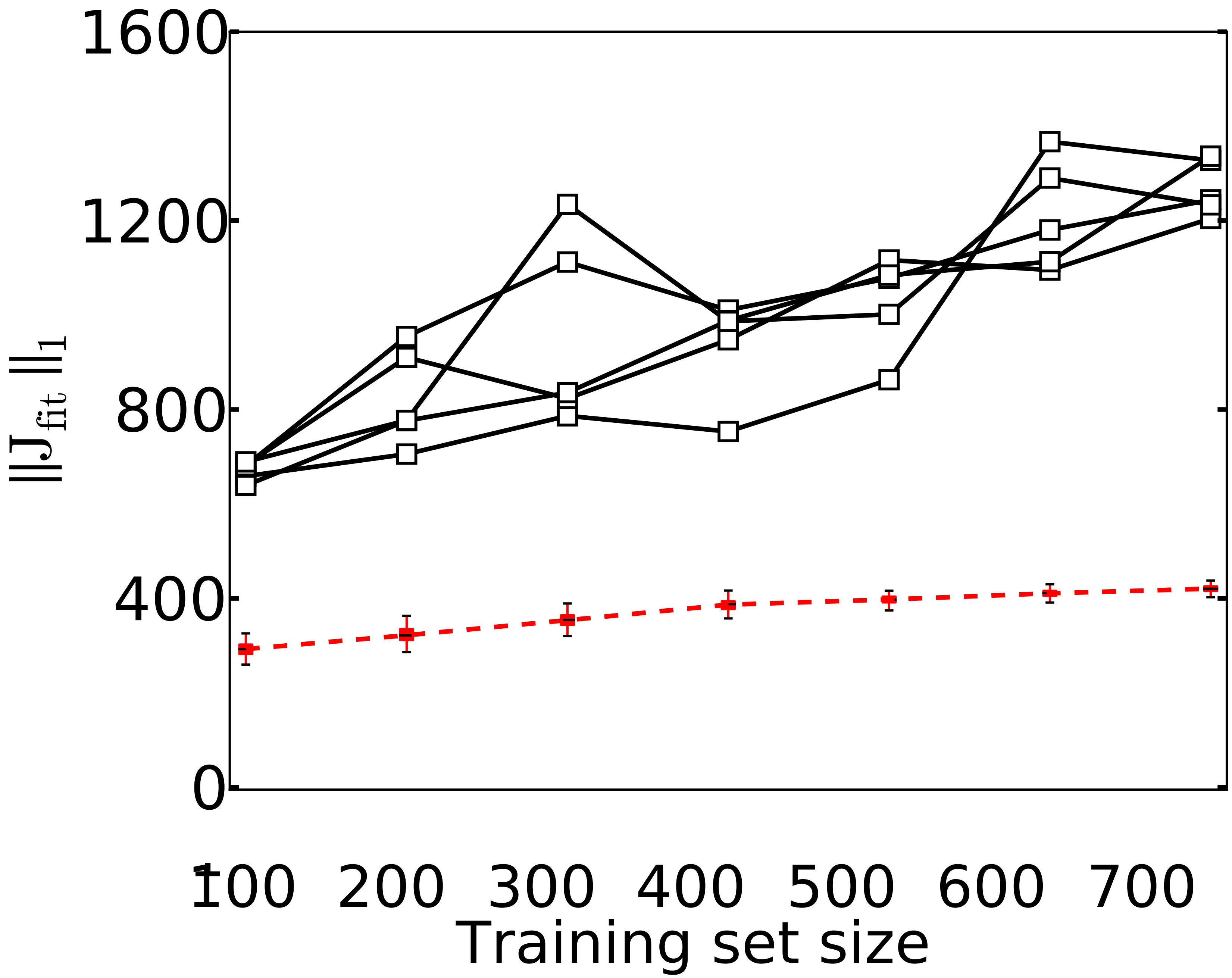

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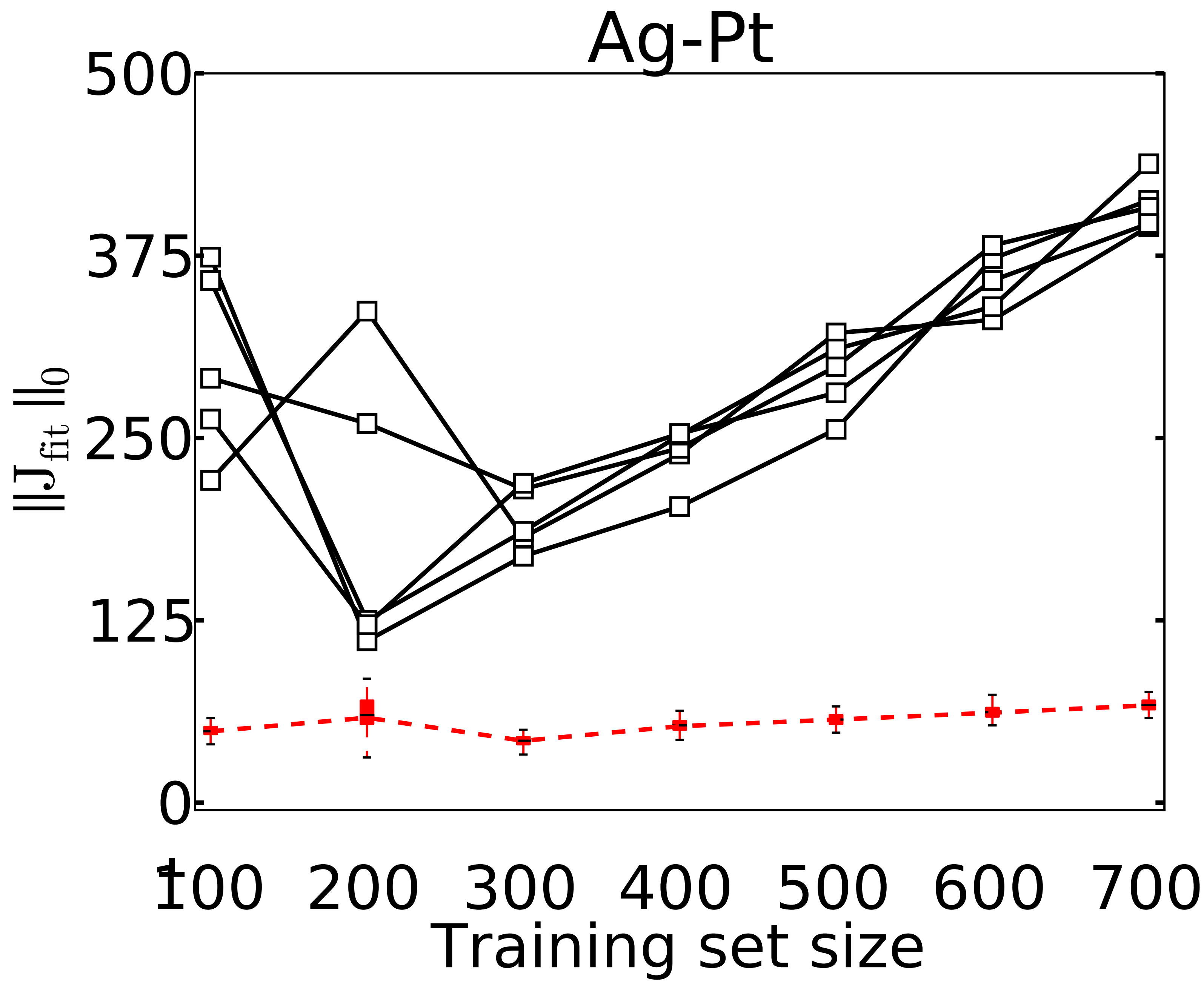
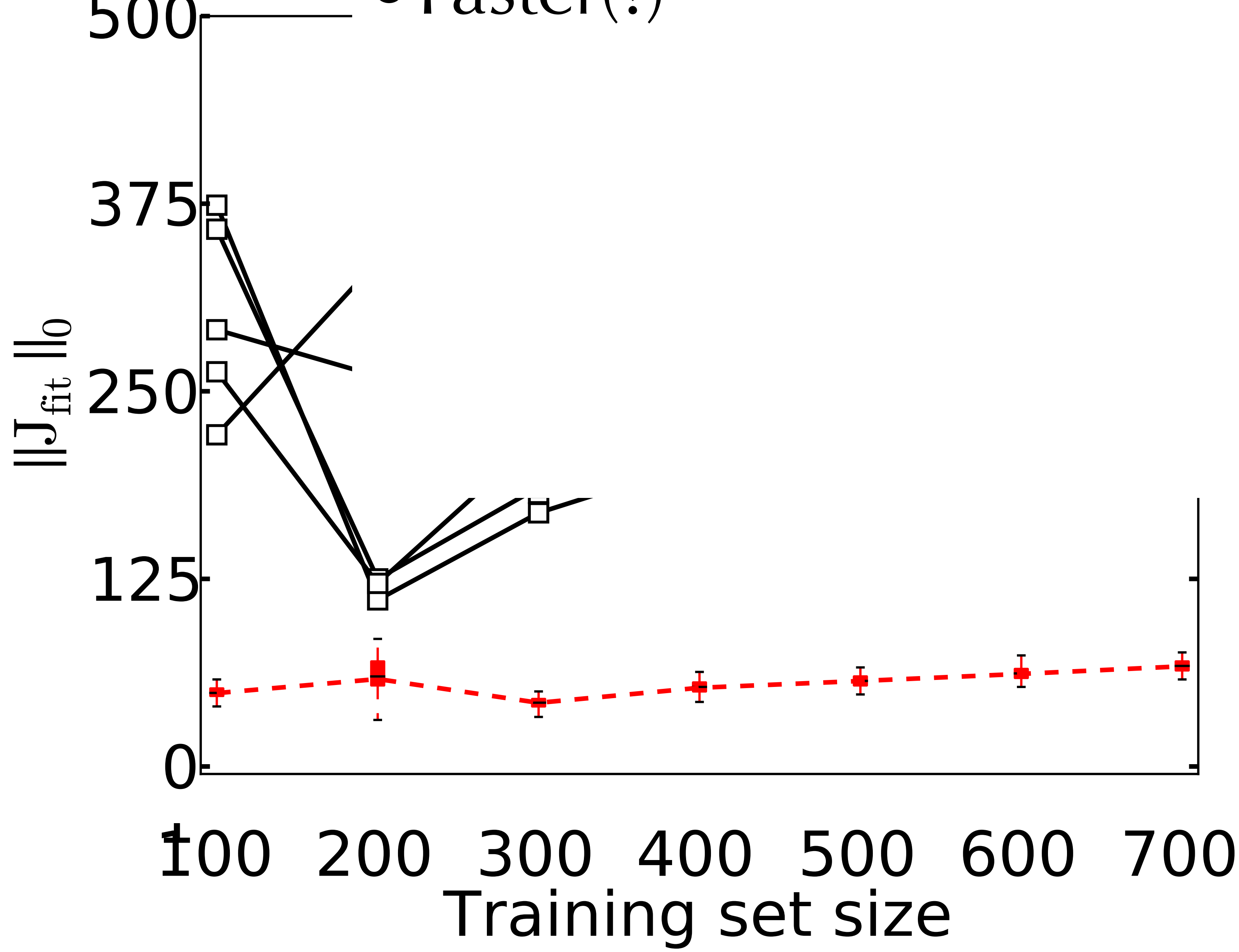


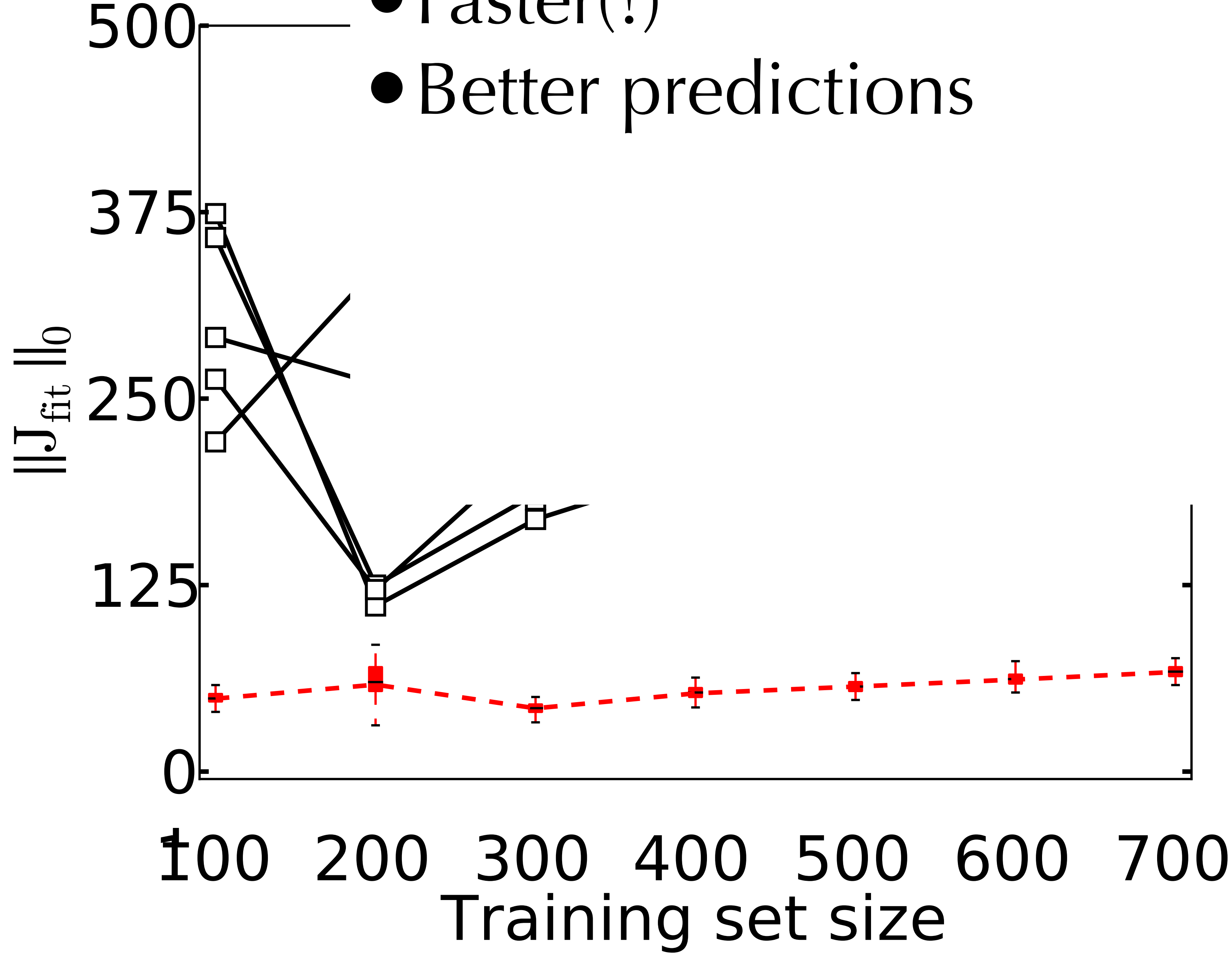
Bayesian Compressive Sensing vs. GA

- Faster(!)



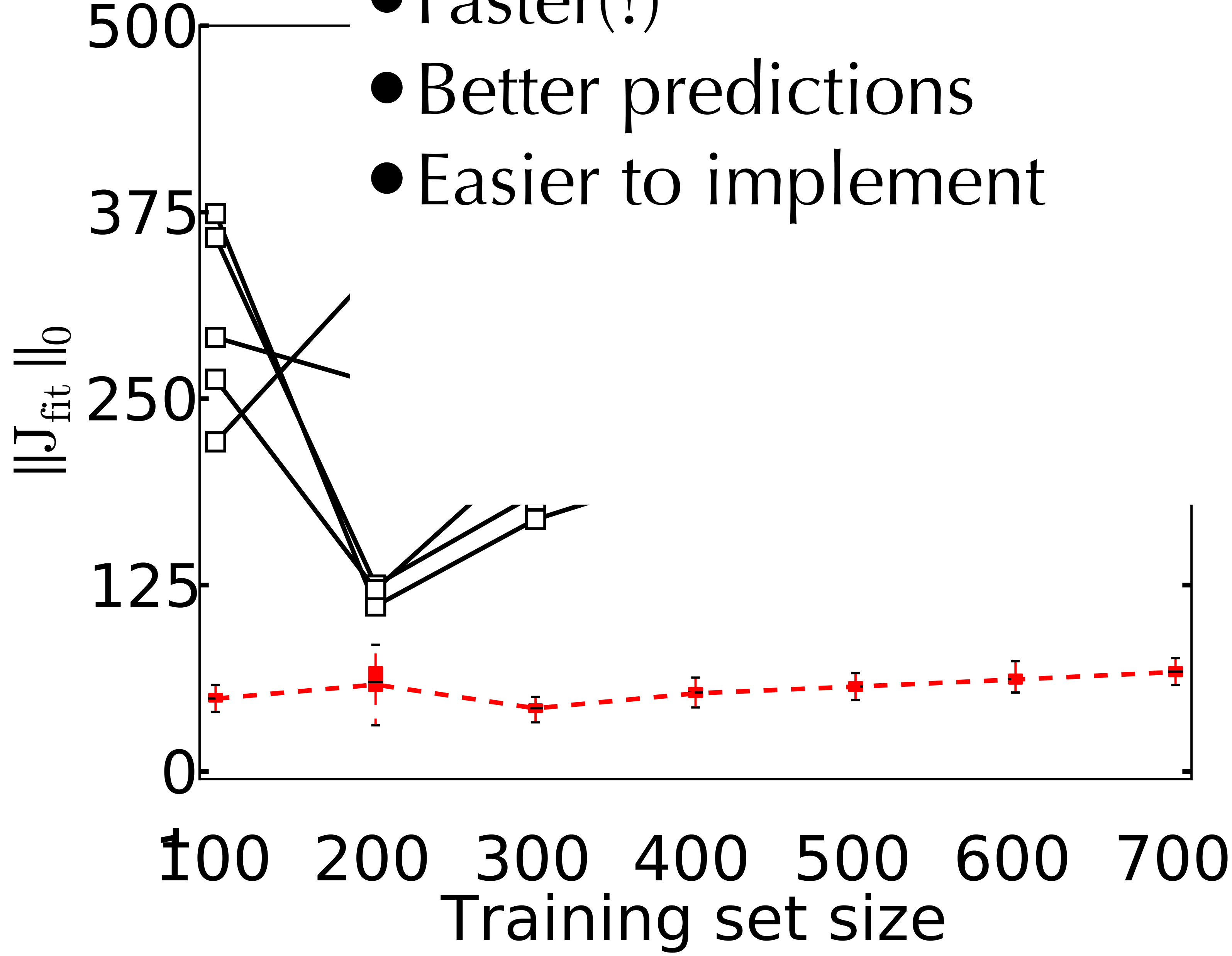
Bayesian Compressive Sensing vs. GA

- Faster(!)
- Better predictions



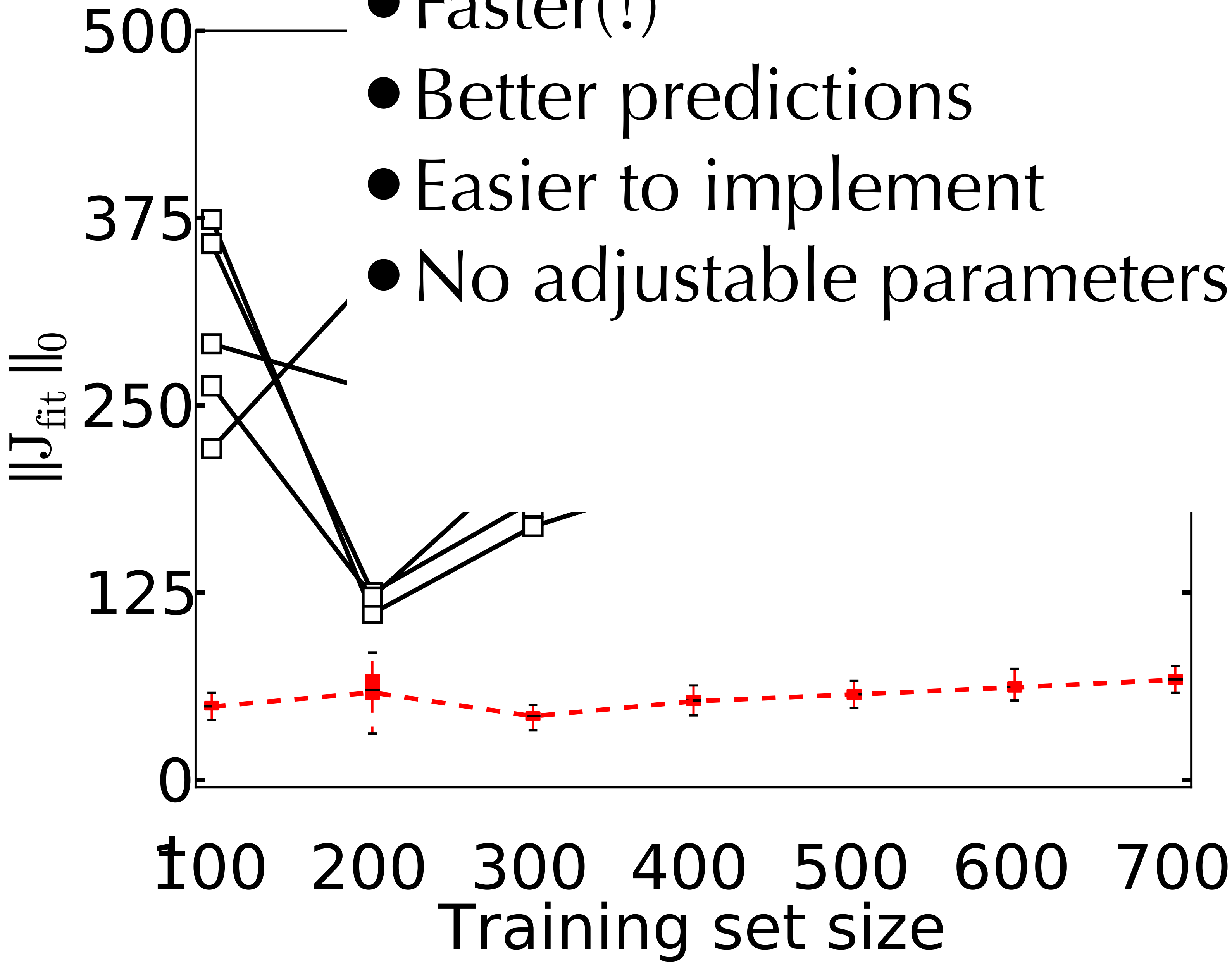
Bayesian Compressive Sensing vs. GA

- Faster(!)
- Better predictions
- Easier to implement



Bayesian Compressive Sensing vs. GA

- Faster(!)
- Better predictions
- Easier to implement
- No adjustable parameters (hands free!)



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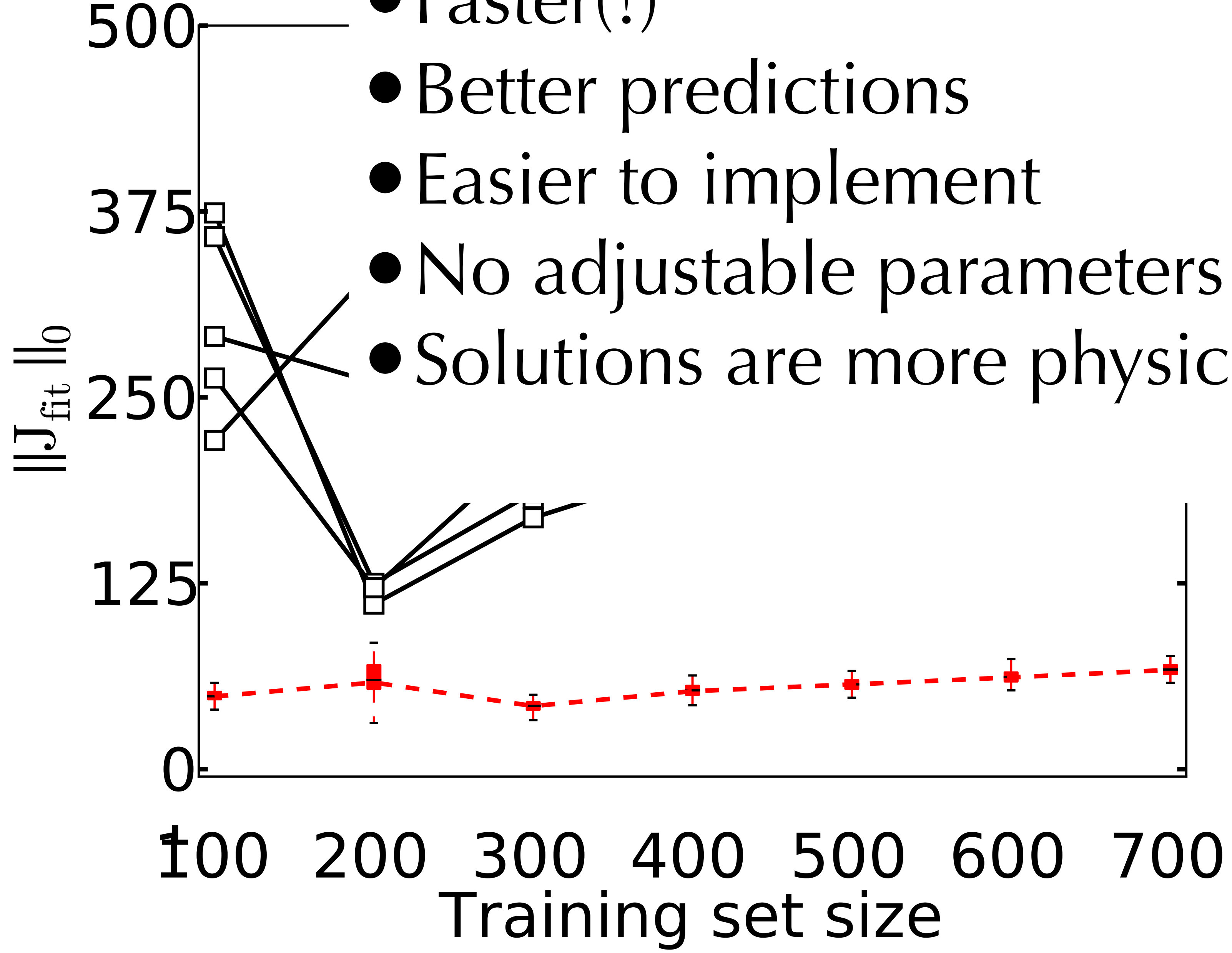

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Bayesian Compressive Sensing vs. GA

- Faster(!)
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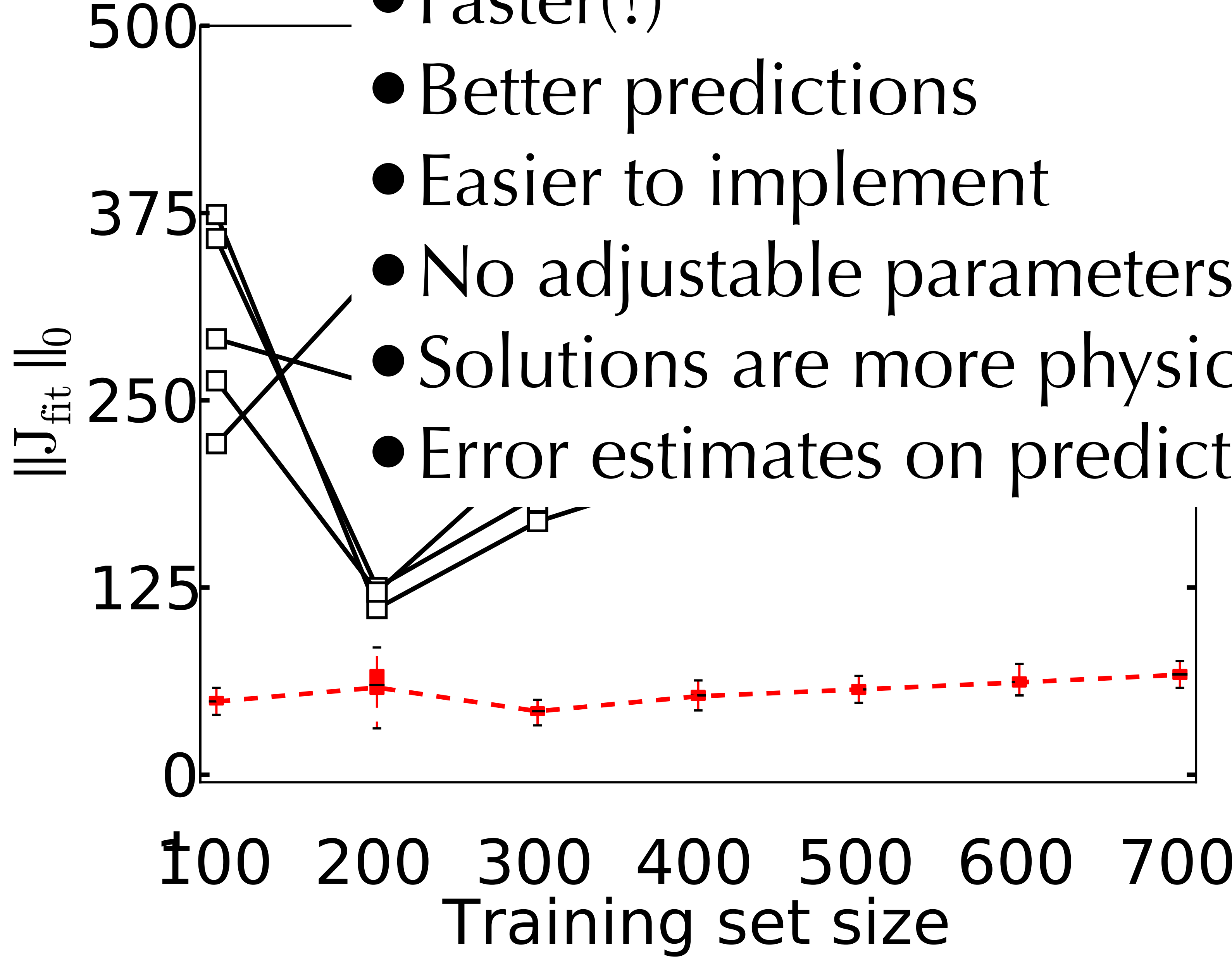
- Solutions are more physical
- Error estimates on predictions



Further reading

Lance J. Nelson, Gus L. W. Hart, Fei Zhou, and Vidvuds Ozolins, "*Cluster expansion made easy with Bayesian compressive sensing*," arXiv:1307.2938 [cond-mat.mtrl-sci]

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, vol. 25, no. 2, pp. 21–30 (2008).

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

Outstanding challenges and outlook...

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Lose the lattice!

The most important question is “how can we coarse grain materials properties without using a lattice gas model?” Fitting classical potentials is time consuming and unreliable. Can it be automated and improved? Or is there another coarse grained approach that we can invent that will be better?