Sphere packings, singularities, and statistical mechanics

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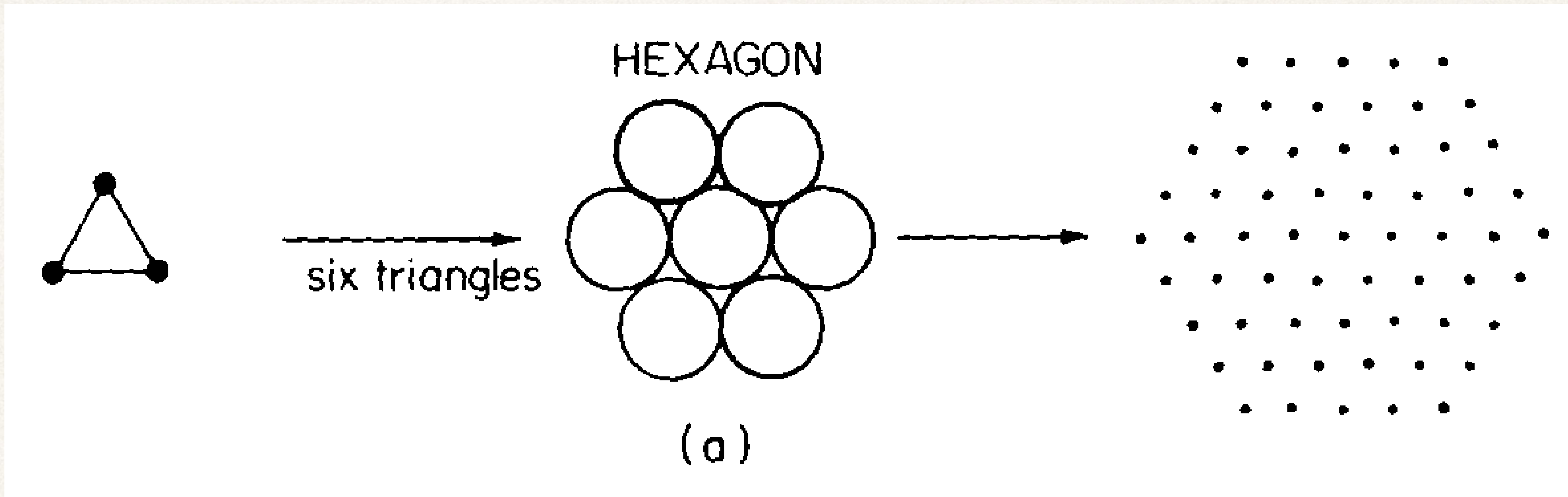
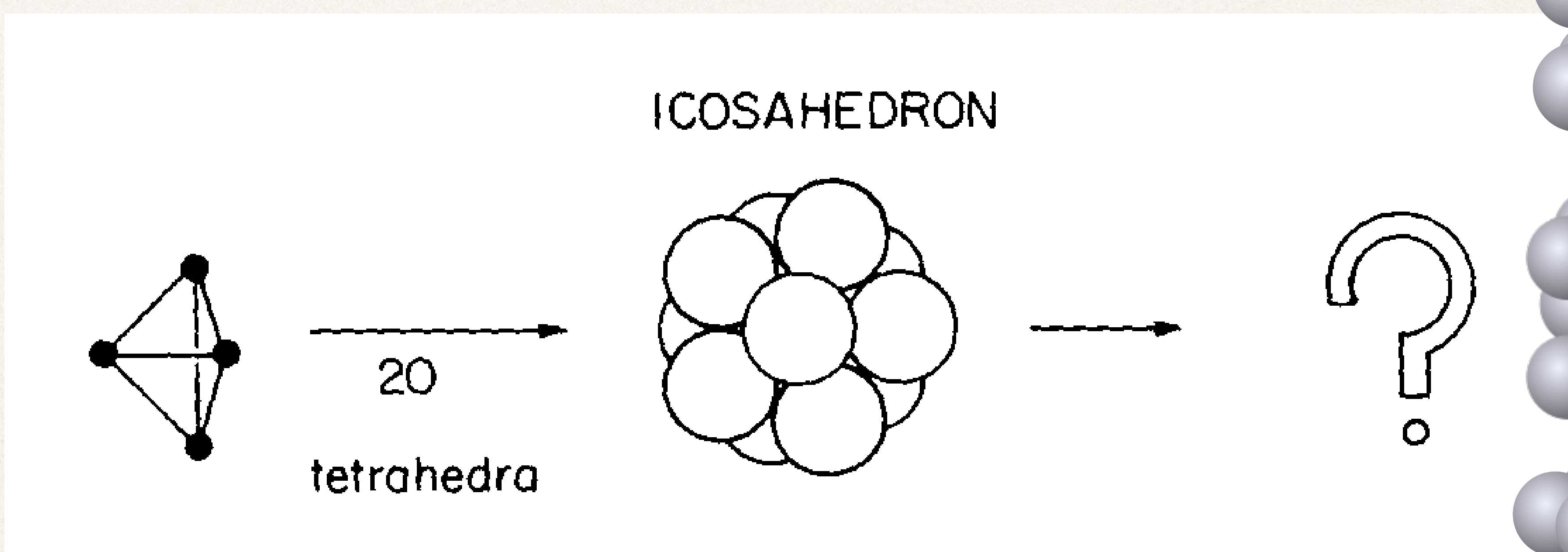
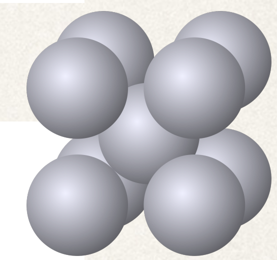
Physics is much richer in 3D —> because of geometrical frustration

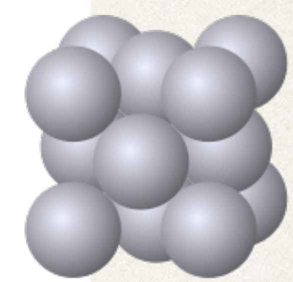
D. Nelson, F. Spaepen, Solid State Phys. 42, 1 (1989)



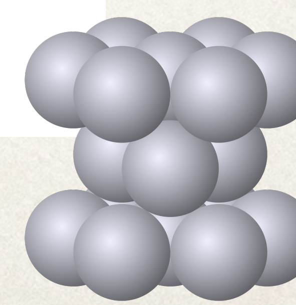




bcc unit cell



fcc unit cell



hcp unit cell

Geometric frustration: locally preferred order ≠ globally preferred order

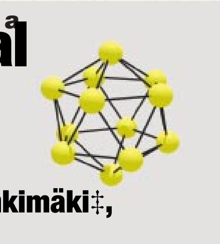
Behaviour of small groups of particles can help understand thermodynamic or dynamic phenomena

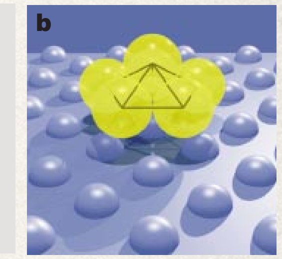
nucleation, phase transitions, glass transition, gel formation, jamming, etc

The theoretical argument is misleading also. Consider the question: 'In how many different ways can one put twelve billiard balls in simultaneous contact with one, counting as different the arrangements which cannot be transformed into each other without breaking contact with the centre ball?' The answer is *three*. Two which come to the mind of any crystallographer occur in the face-centred cubic and hexagonal close-packed lattices. The third comes to the mind of any good schoolboy, and is to put one at the centre of each face of a regular dodecahedron. That body has five-fold axes, which are abhorrent to crystal symmetry: unlike the other two packings, this one cannot be continuously extended in three dimensions. You will find that the outer twelve in this packing do not touch each other. If we have mutually attracting deformable spheres, like atoms, they will be a little closer to the centre in this third type of packing; and if one assumes they are argon atoms (interacting in pairs with attractive and repulsive energy terms proportional to r^{-6} and r^{-12}) one may calculate that the binding energy of the group of thirteen is 8·4 % greater than for the other two packings. This is 40 % of the lattice energy per atom in the crystal. I infer that this will be a very common grouping in liquids, that most of the groups of twelve atoms around one will be in this form, that freezing involves a substantial rearrangement, and not merely an extension of the same kind of order from short distances to long ones; a rearrangement which is quite costly of energy in small localities, and only becomes economical when extended over a considerable volume, because unlike the other packing it can be so extended without discontinuities.

F.C. Frank, Proc. R. Soc. Lond. A Math. Phys. Sci. 215, 43 (1952)

Observation of five-fold local symmetry in liquid lead





H. Reichert*, O. Klein*†, H. Dosch*, M. Denk*, V. Honkimäki‡, T. Lippmann§ & G. Reiter‖

Relchert et al, Nature (2000)

PHYSICAL REVIEW LETTERS 122, 068004 (2019)

Editors' Suggestion

Morphometric Approach to Many-Body Correlations in Hard Spheres

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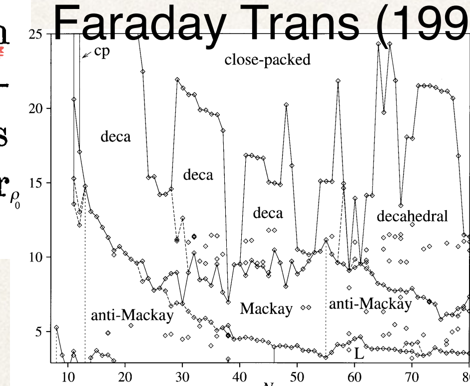
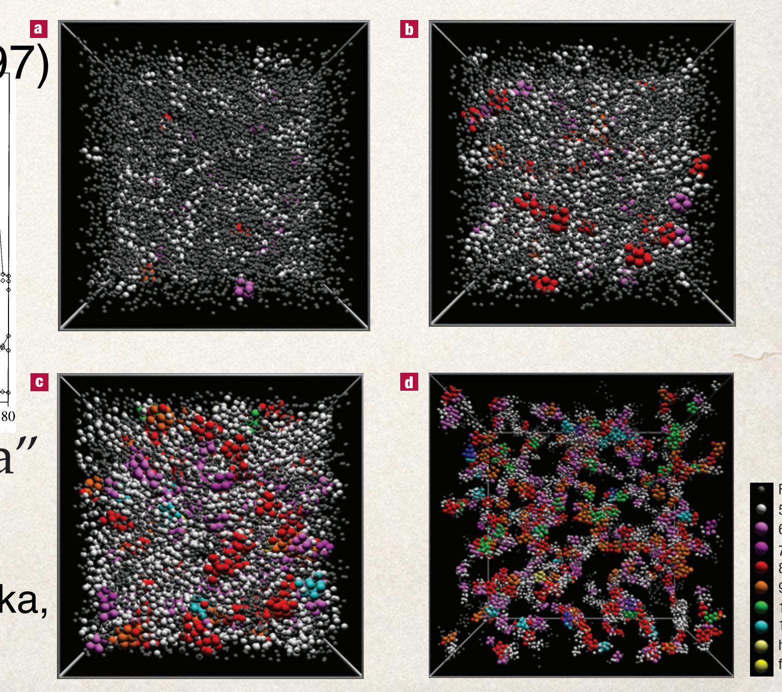
We model the thermodynamics of local structures within the hard sphere liquid at arbitrary volume fractions through the *morphometric* calculation of *n*-body correlations. We calculate absolute free energies of local geometric motifs in excellent quantitative agreement with molecular dynamics simulations across the liquid and supercooled liquid regimes. We find a bimodality in the density library of states where fivefold symmetric structures appear lower in free energy than fourfold symmetric structures and from a single reaction path predict a dynamical barrier which scales linearly in the compressibility factor. The method provides a new route to assess changes in the free energy landscape at volume fractions dynamically inaccessible to conventional techniques.

Doye & Wales, Faraday Trans (1997)



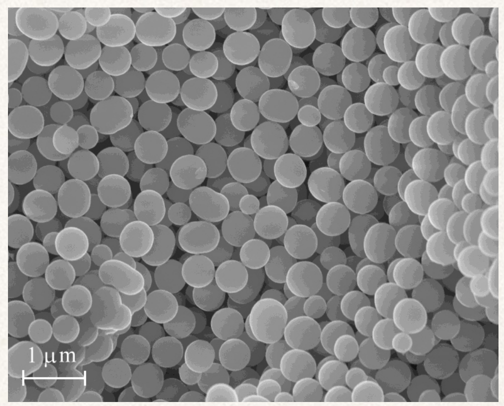


creation of local "global minima" leads to gel formation

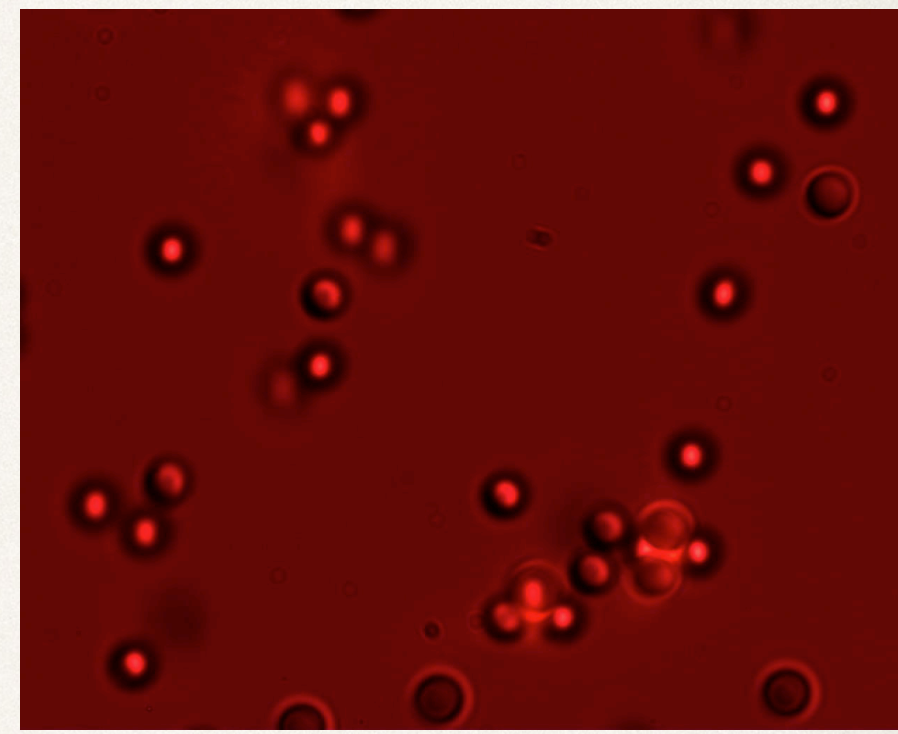
C. Patrick Royall, S. R. Williams, T. Ohtsuka, H. Tanaka, Nat. Mater. 7, 556 (2008)

Colloidal particles (colloids)

- *Colloidal* particles: diameters ~ 10^{-8}-10^{-6} m. (» atoms, « scales of humans)
- Potential to make new materials (∵ size ~ wavelength of light)
- Range of interaction « diameter of particles (unlike atoms)



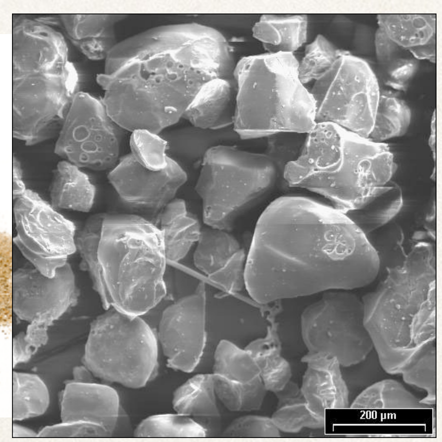
opal

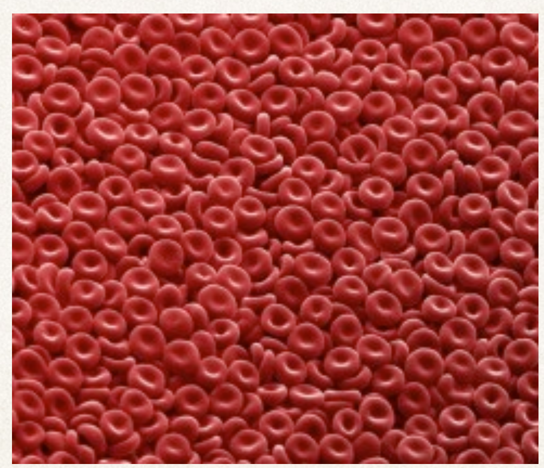


mayonnaise

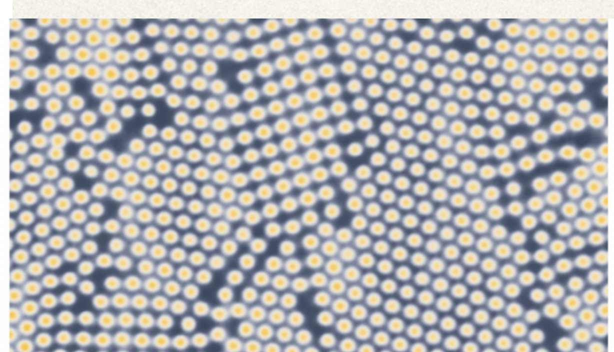
red blood cells

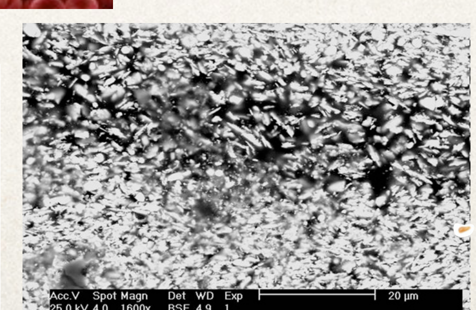
sand





cornstarch



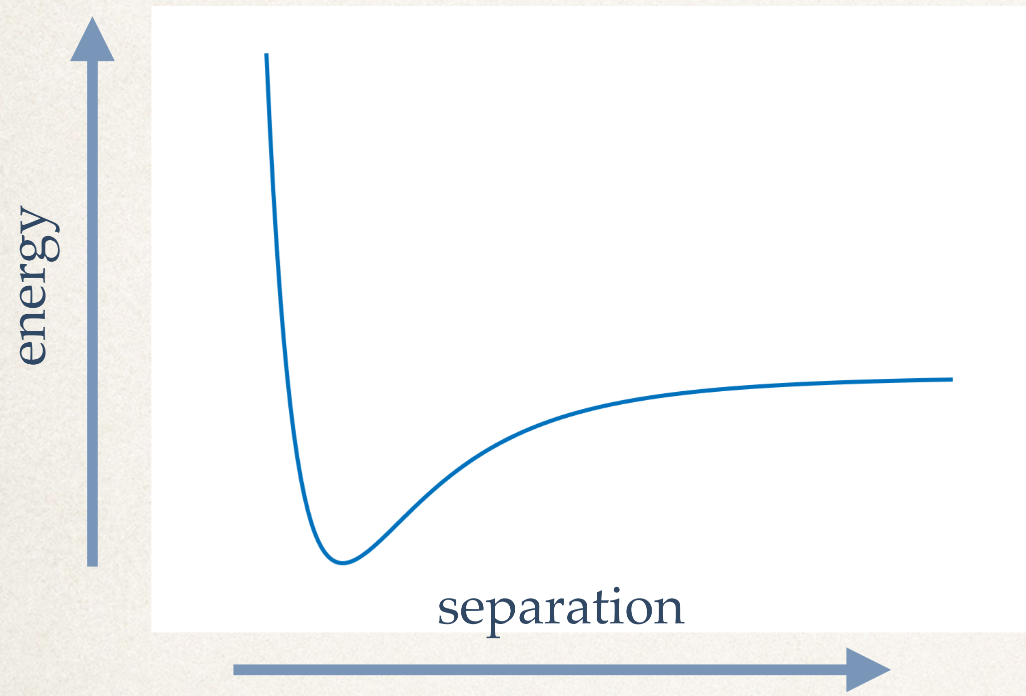


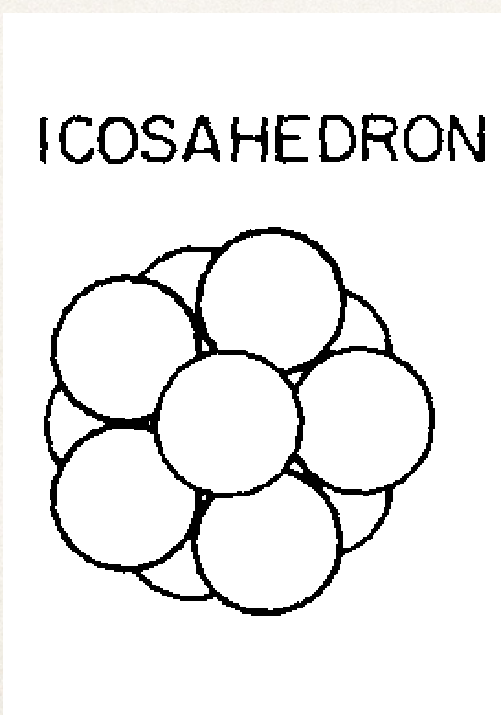
paint

ketchup

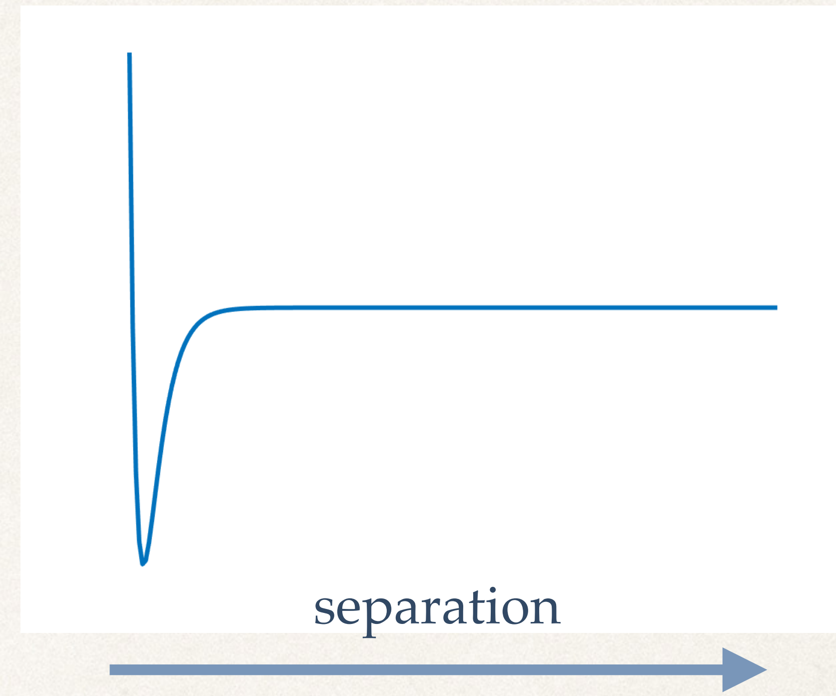
What about frustration in colloids?

atoms

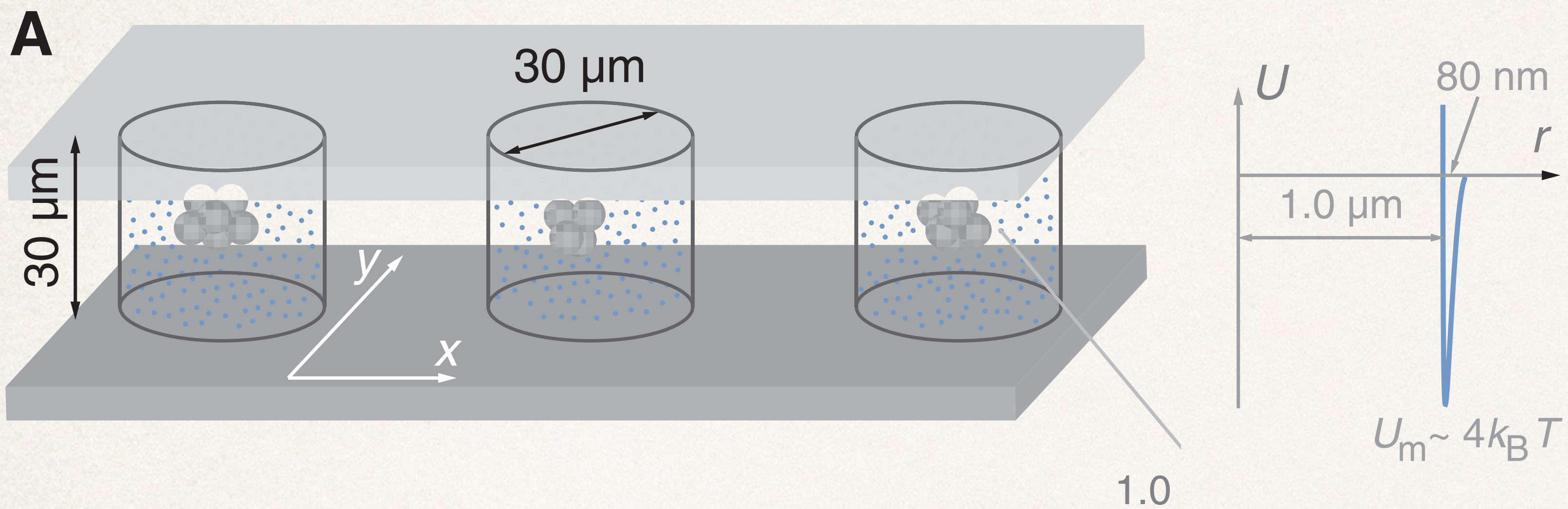


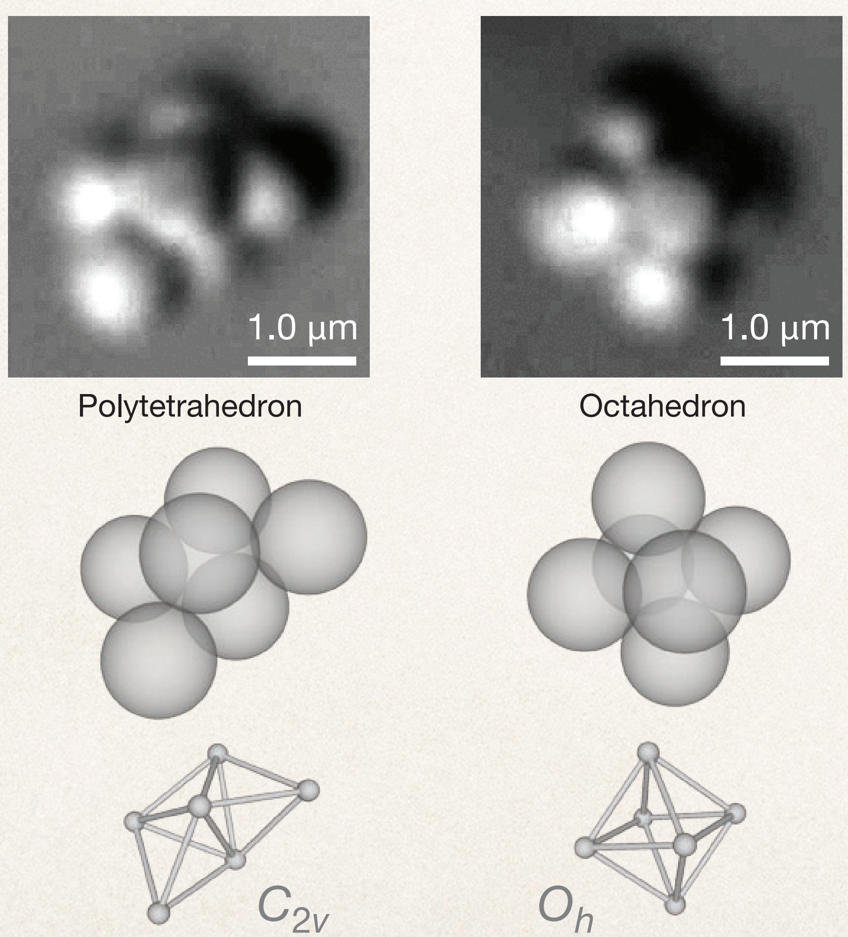


colloids



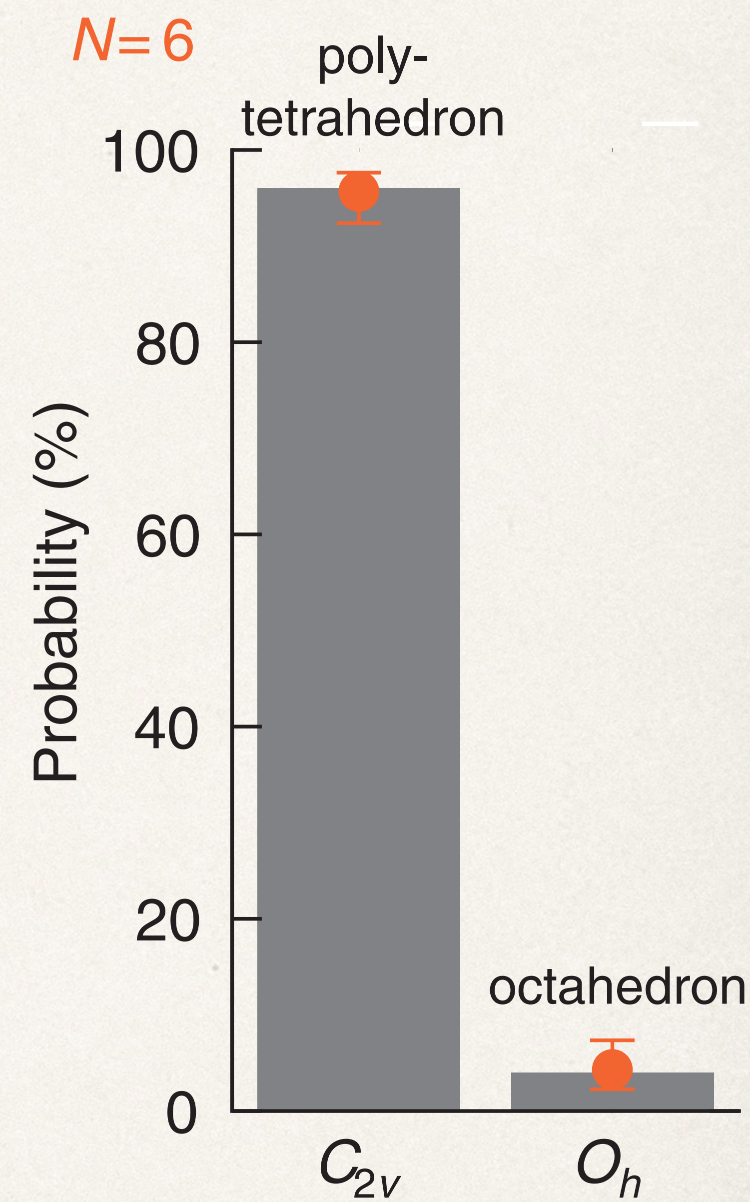
What about frustration in colloids?





sphere packings

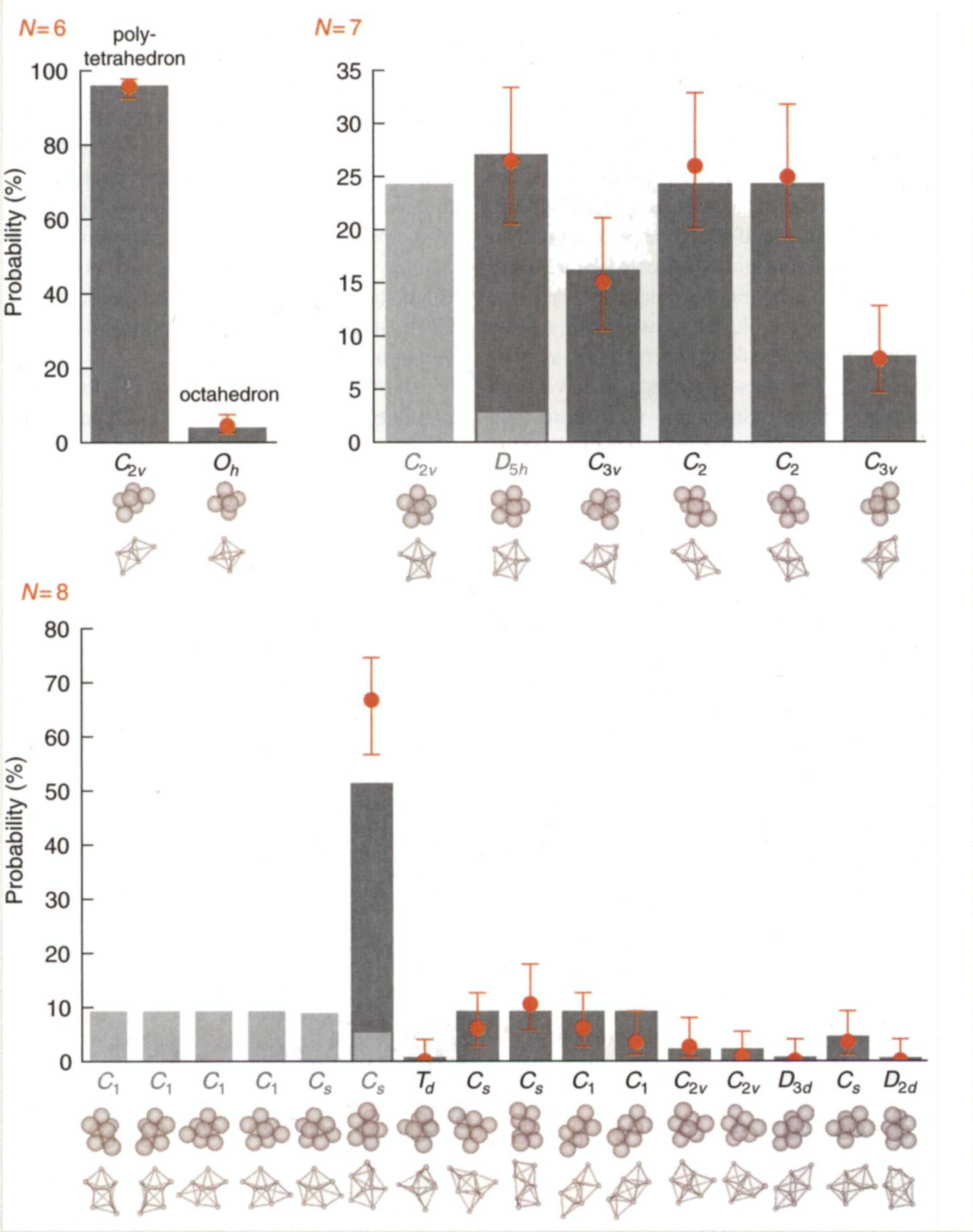
“rigid” graphs



Symmetry number
explains the huge
discrepancy!

G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

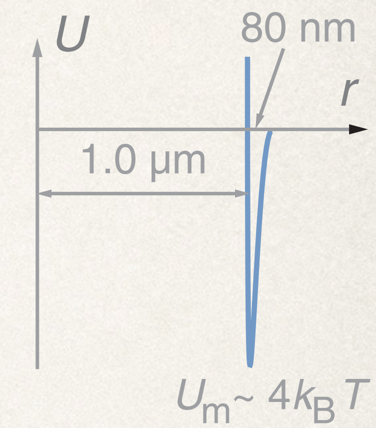
Data for N=6-8



All observed clusters are rigid graphs

Rigid clusters are local minima of the system's energy

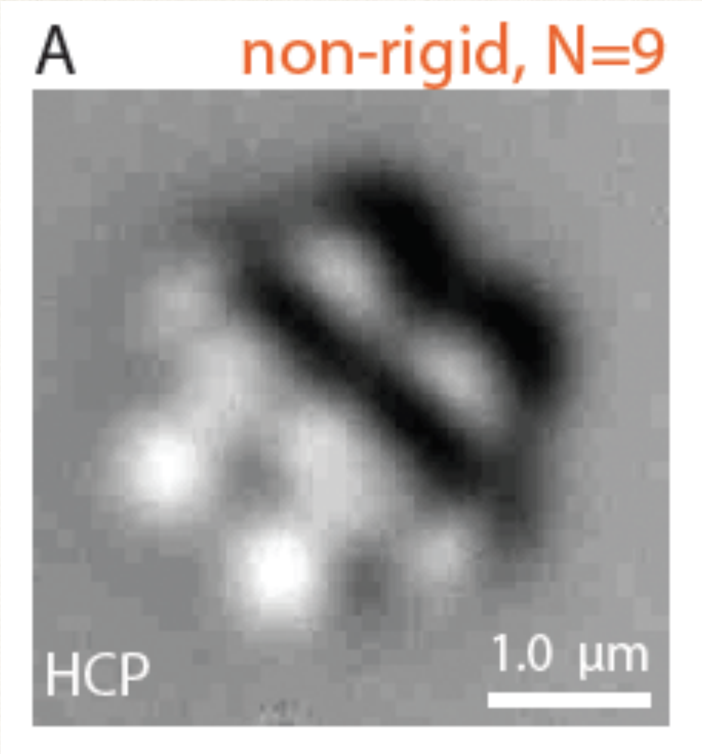
$$\text{Energy}(x) = \sum_{\text{pairs } i,j} U(|x_i - x_j|), \qquad x_i \in \mathbb{R}^3 = \text{sphere centre}$$

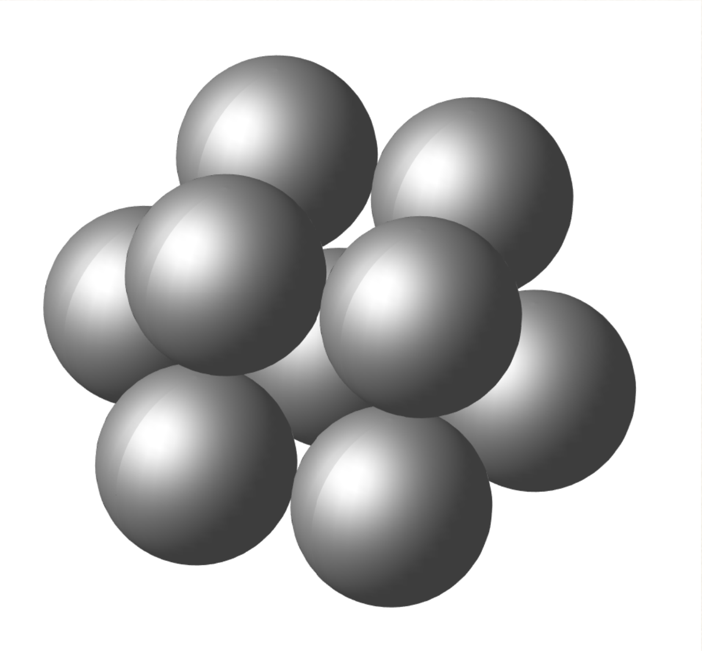


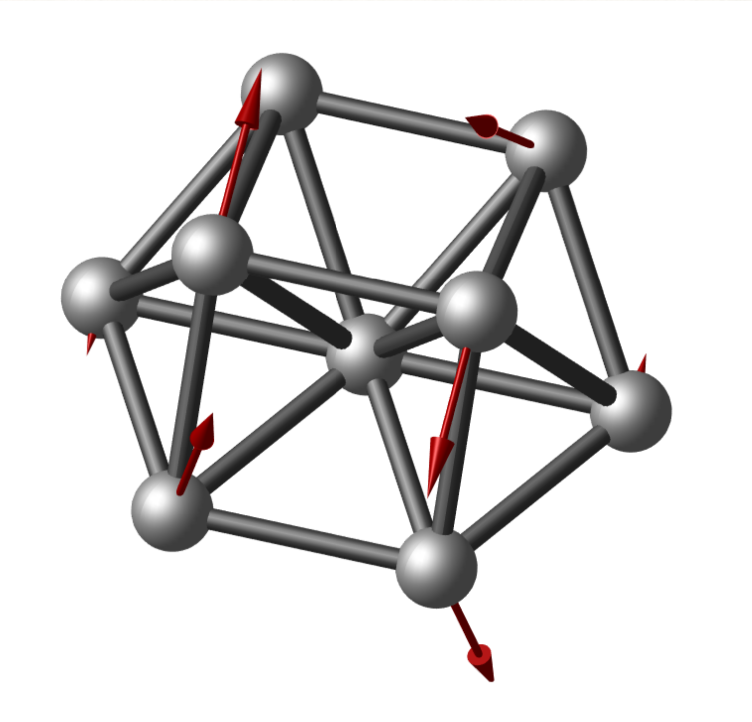
pair potential

- Spheres are either touching, or not
- Energy of cluster of N spheres ∝ # of contacts
- Lowest-energy clusters = those with maximal number of contacts
- These are (typically) **rigid**: they cannot be continuously deformed without breaking a contact (=crossing an energy barrier.)
- More generally: energetic local minima have a locally maximal number of contacts, so are (typically) rigid.

Data for N=9



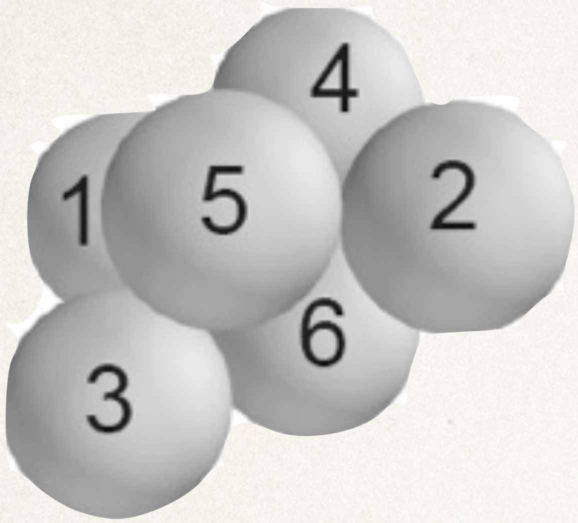


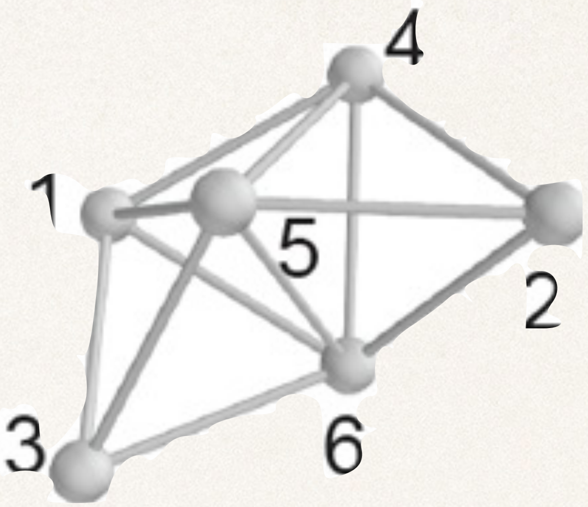


G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

- One cluster dominated — probability = 11%! (out of 52 clusters total)
- It has a fair amount of symmetry —> symmetry cannot be that important…
- Seems to be "floppy" — has an infinitesimal zero mode.
- *Important property* — it's not actually floppy — it's rigid!

What is rigid?





adjacency matrix A

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

- Each adjacency matrix corresponds to a system of quadratic equations and inequalities ($x_i \in \mathbb{R}^3$):

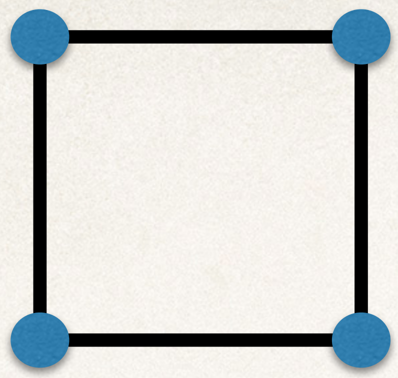
$$|x_i - x_j|^2 = d^2 \qquad \text{if } A_{ij} = 1$$
$$|x_i - x_j|^2 \geq d^2 \qquad \text{if } A_{ij} = 0$$

- A cluster (x,A) with $x = (x_1, x_2, \ldots, x_N)$ is *rigid* if it is an isolated solution to this system of equations (modulo translations, rotations)   (e.g. Asimow&Roth 1978)
  $\Longleftrightarrow$ There is no finite continuous deformation of the cluster that preserves all edge lengths.

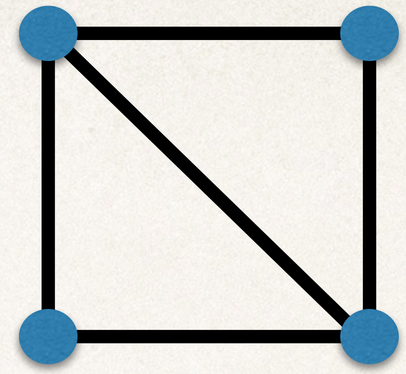
Generically, expect 3N-6 contacts: from 3N variables, 6 dof in SE(3).

- It is *first order rigid* if it is rigid and the equations above are linearly independent $\Longleftrightarrow$ rigid and there are no infinitesimal zero-modes in the above equations

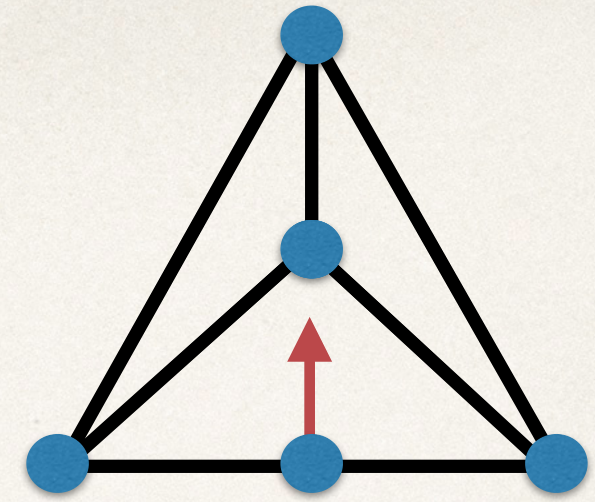
Quiz!



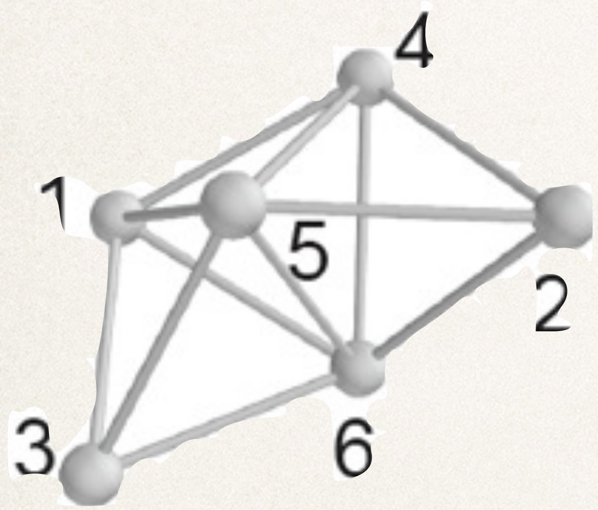
floppy (in R^2,R^3)



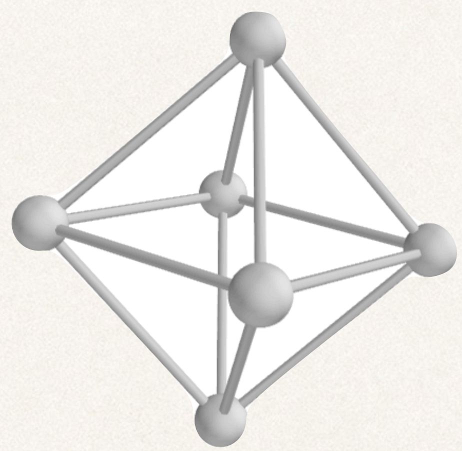
first-order rigid (in R^2)
floppy (in R^3)



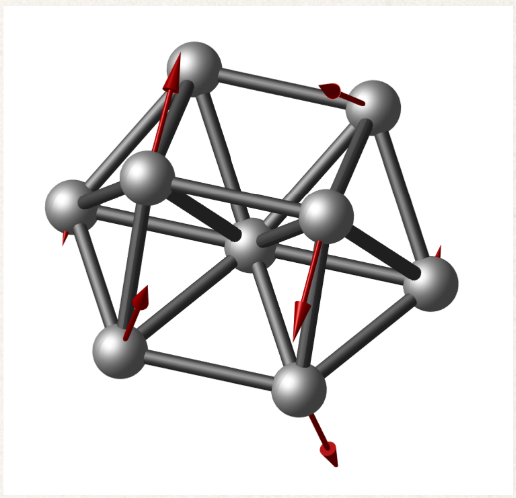
rigid (R^2)
not first-order rigid (R^2)



first-order rigid (in R^3)



first-order rigid (in R^3)



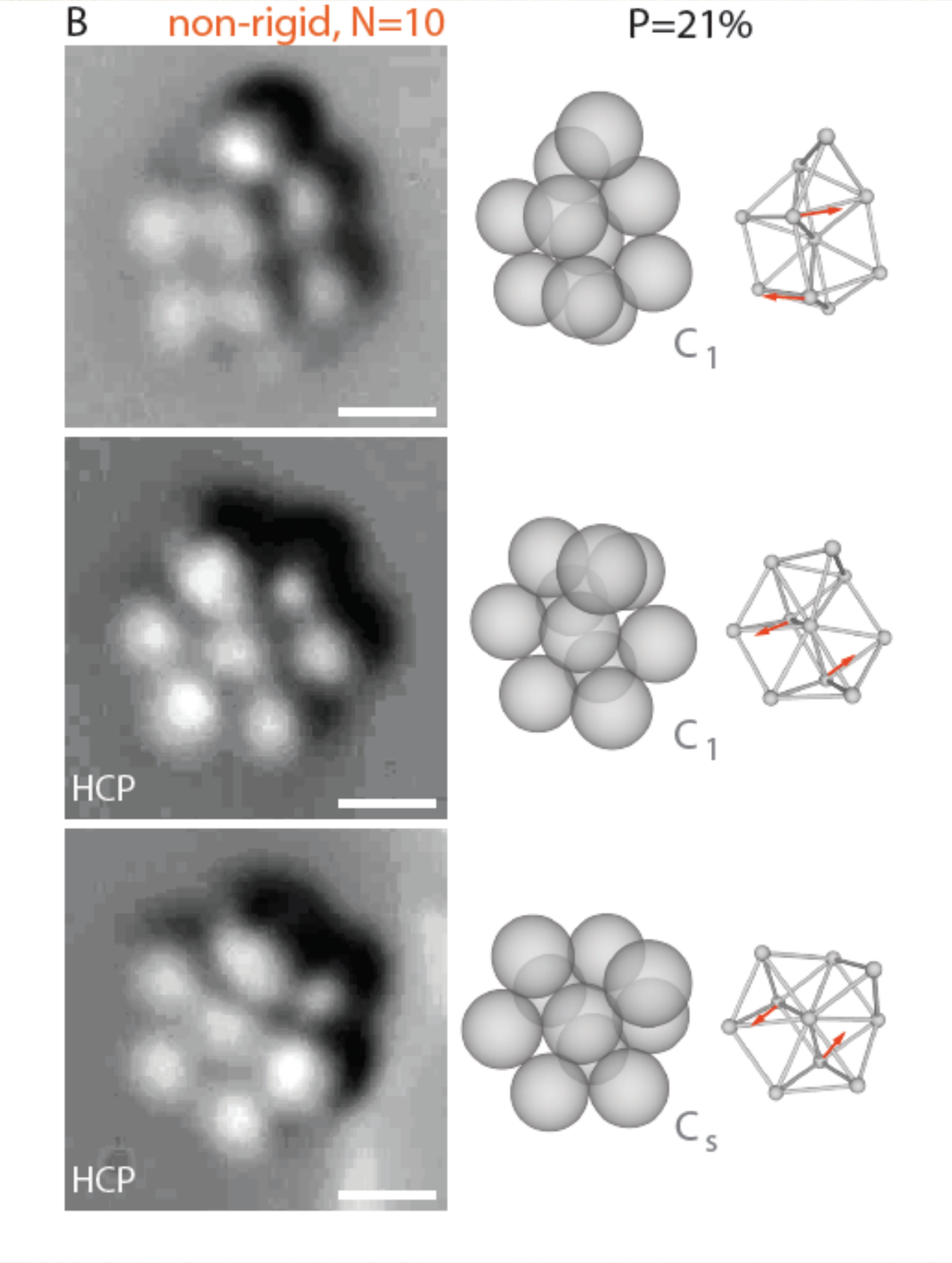
rigid (R^3)
not first-order rigid (R^3)

Singular: rigid but NOT first-order rigid

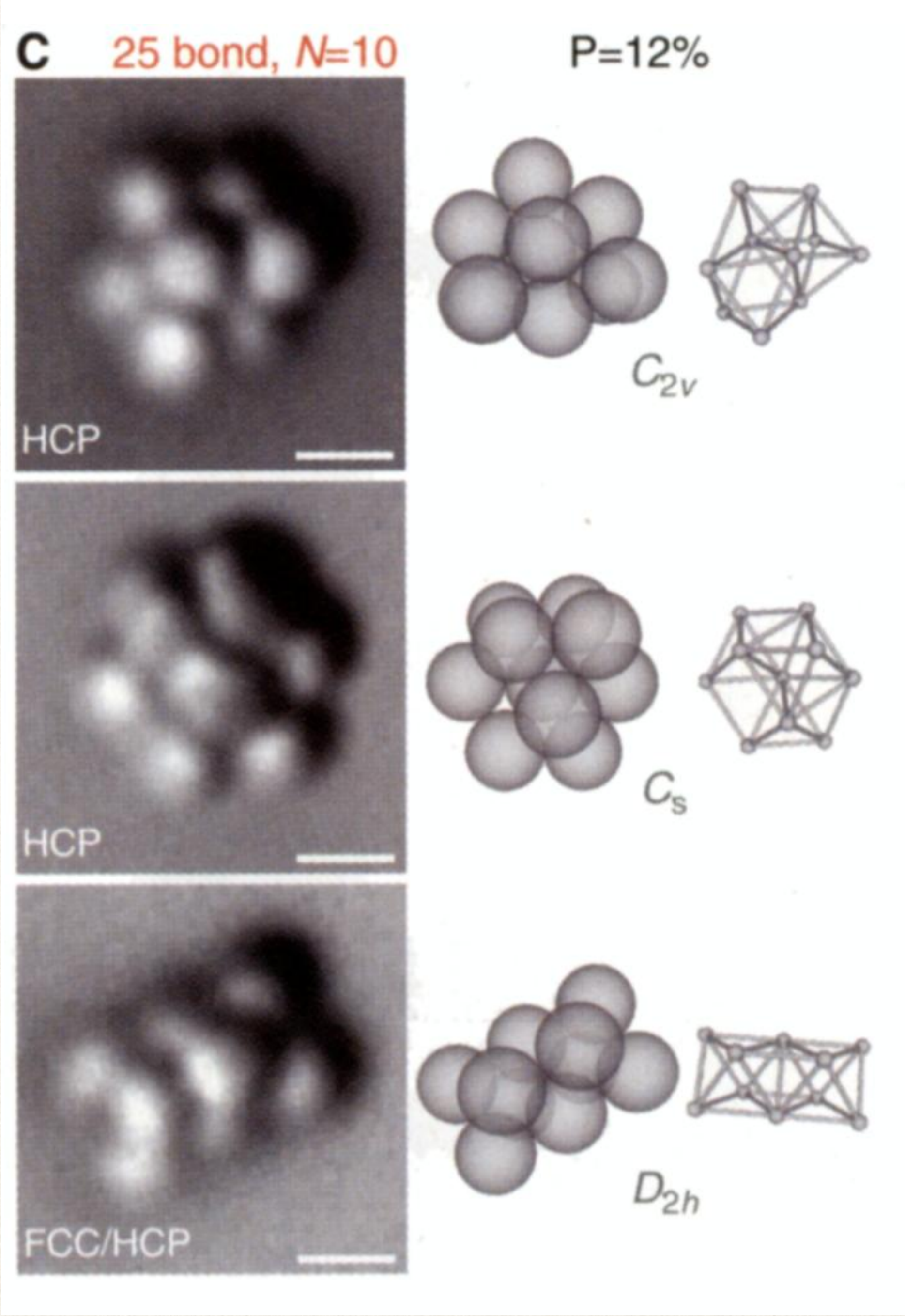
Regular: rigid AND first-order rigid

N=10

Singular clusters:



Hyperstatic (>3N-6 edges) clusters:



Singular 21%, Hyperstatic 12%, > 250 total rigid clusters!

Question:
Is there a competition between singular & hyperstatic clusters as N increases?
What can we say about this competition mathematically?

Strategy

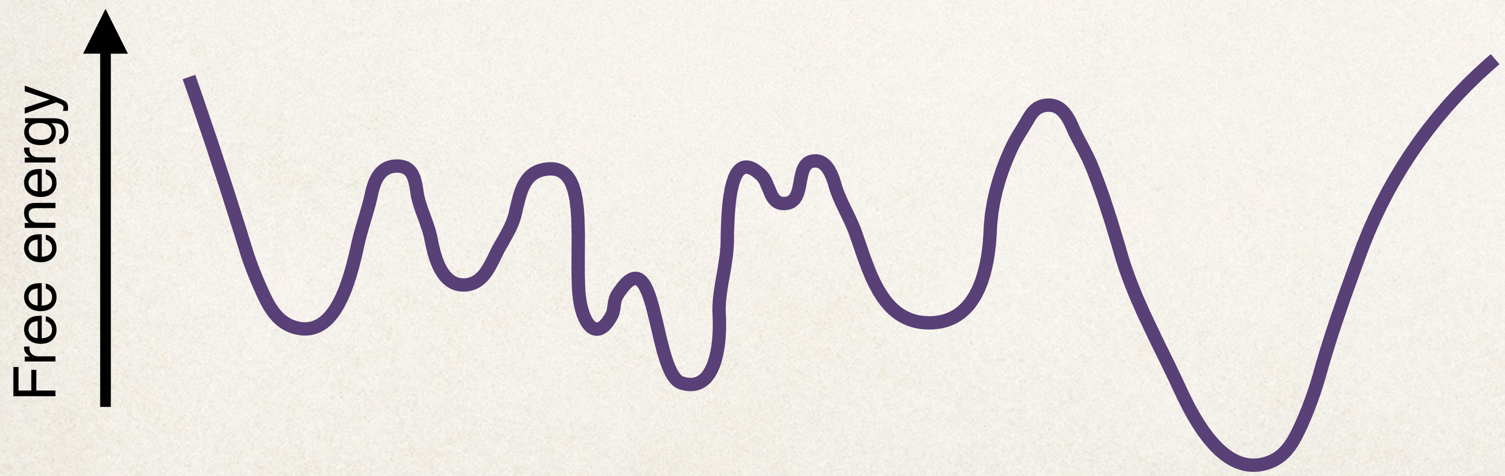
- Enumerate all rigid clusters of N sticky spheres
- Evaluate their probabilities (equilibrium)

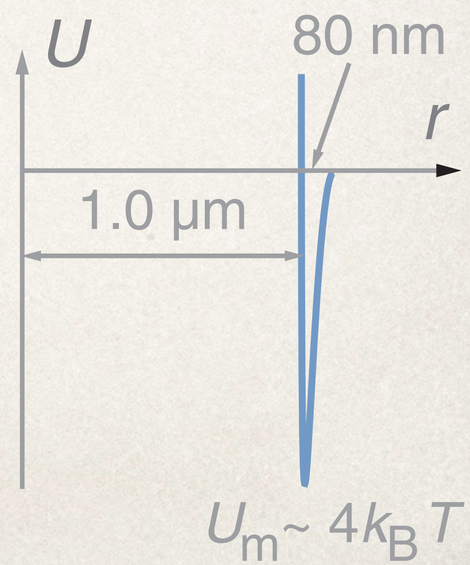
***Sticky*:** interacting with infinitestimally short-ranged (&deep) pair potential

i.e.

range —> 0

depth—> ∞





What are all the rigid clusters of N identical spheres?

H.-C. (2016) *SIAM Review*

Previous approaches

(1) List all adjacency matrices with 3N-6 contacts

(2) For each adjacency matrix, solve for the positions of the particles, or argue that no solution exists.

Analytical (to N=10)

- N. Arkus, V. N. Manoharan, M. P. Brenner. *Phys. Rev. Lett., 103 (2009)*
- N. Arkus, V. N. Manoharan, M. P. Brenner. *SIAM J. Disc. Math., 25 (2011)*

Numerical (to N=13, though many were missed)

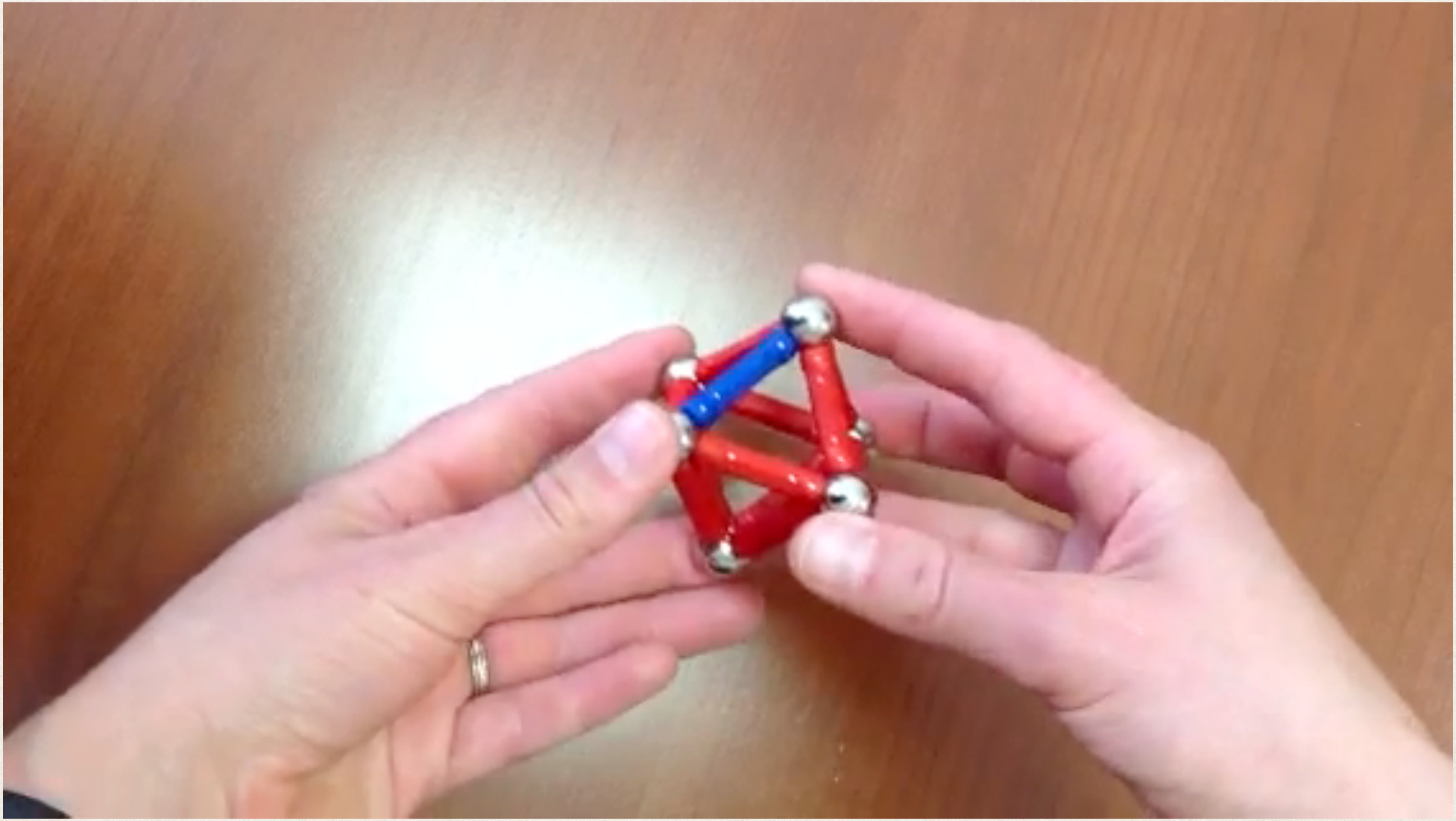
- R. S. Hoy, J. Harwayne-Gindansky, C. O'Hern, *Phys. Rev. E*, 85 (2012)
- R. S. Hoy, *Phys. Rev. E*, 91 (2015)

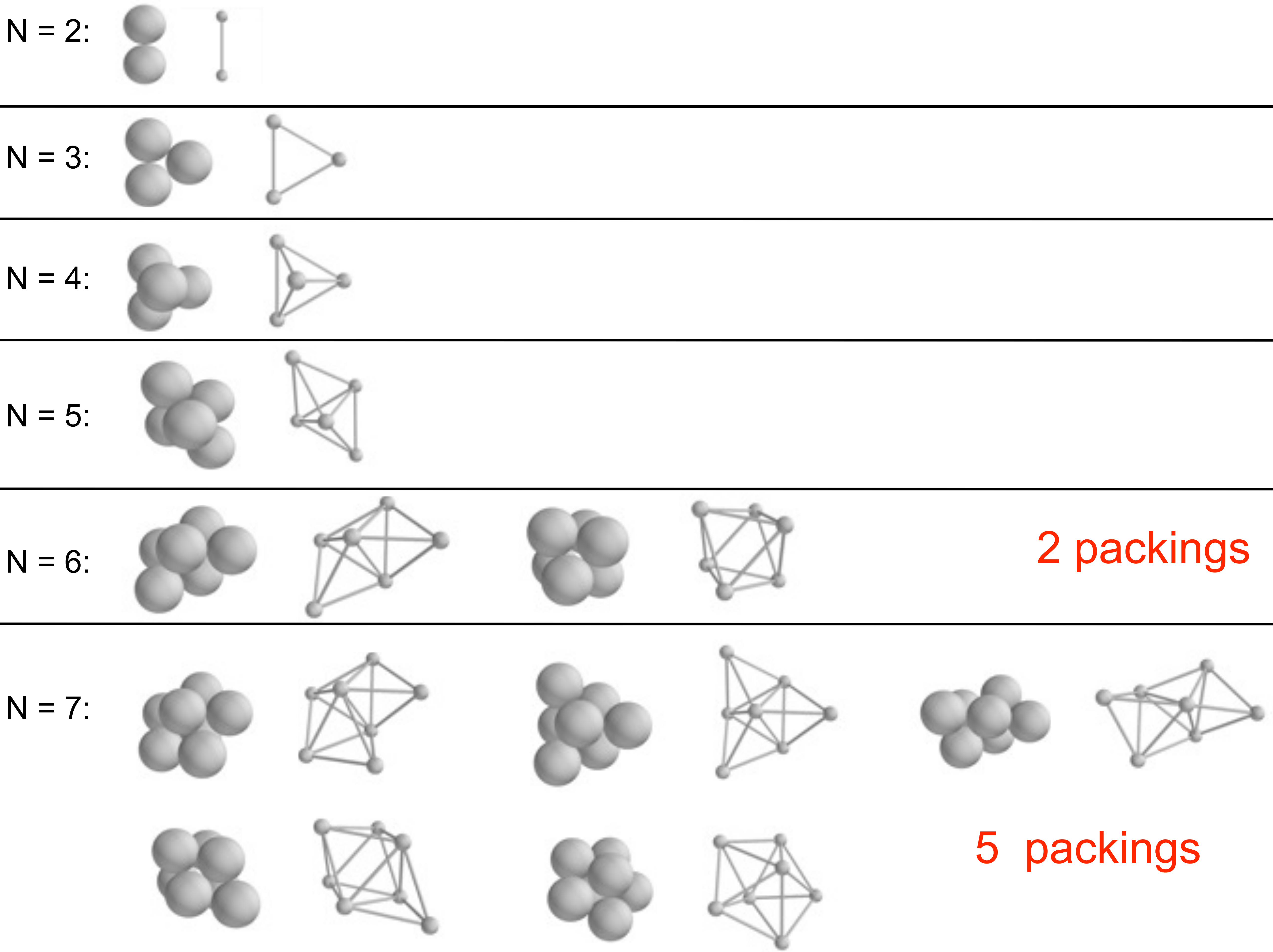
Problems:

- LOTS of adjacency matrices: $\approx 2^{n(n-1)/2}$
- How to solve equations?
  - ✦ analytical — really hard
  - ✦ computer — can't guarantee found solutions
  - ✦ Degree of equations is VERY high ($\approx 2^{3N-6}$!)

A different algorithm

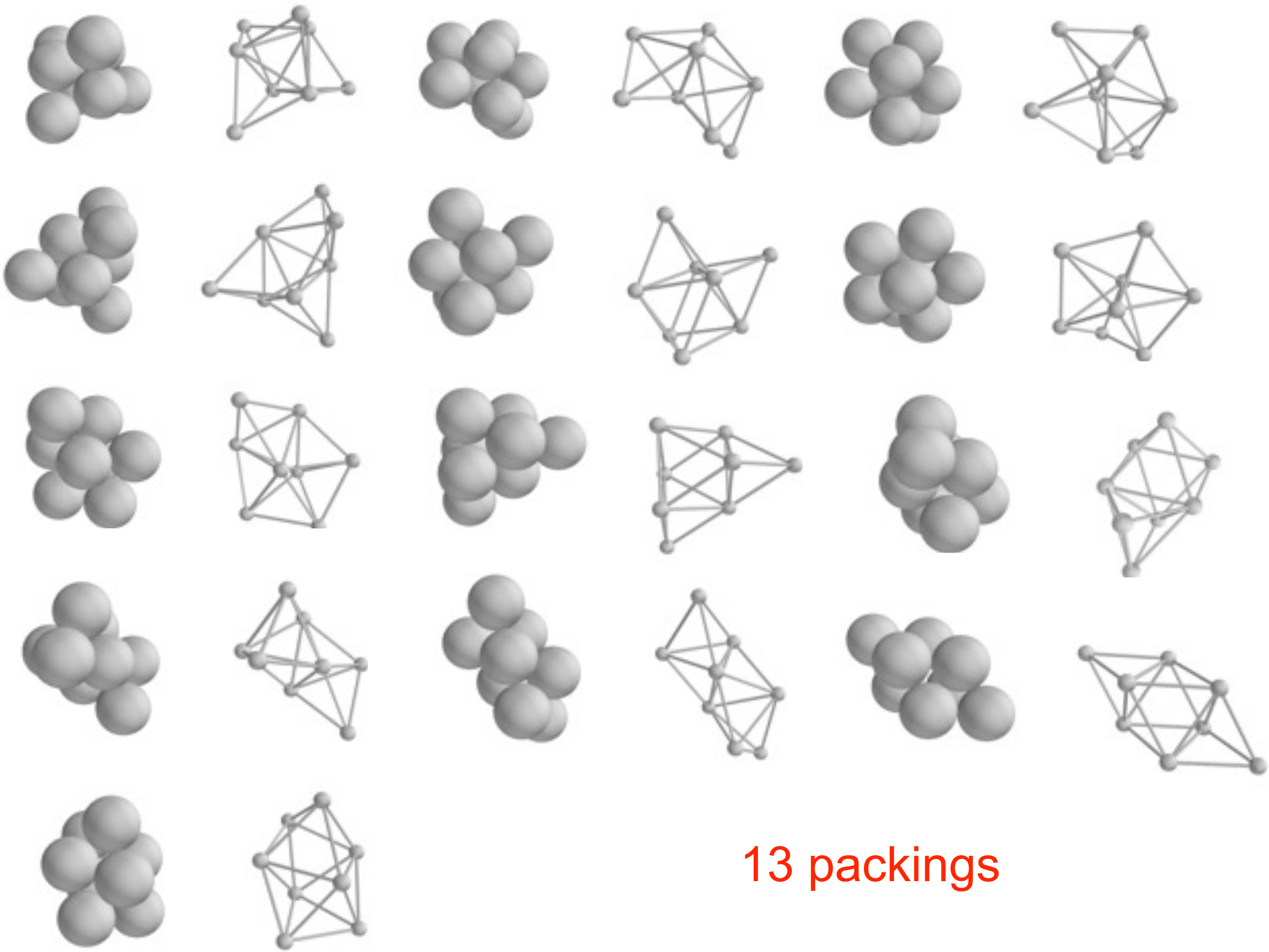
Move from cluster to cluster dynamically





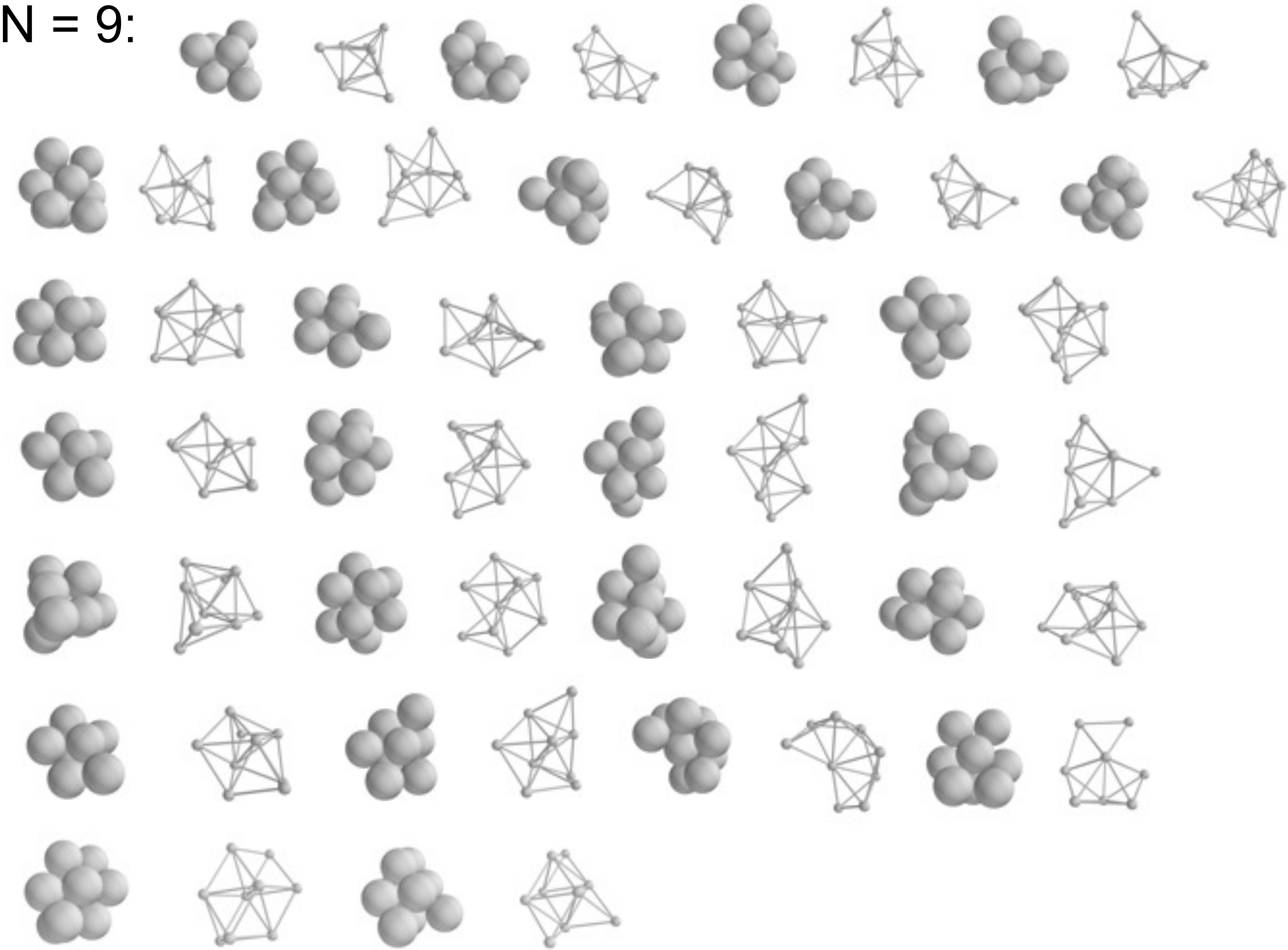
N = 2:
N = 3:
N = 4:
N = 5:
N = 6:
2 packings
N = 7:
5 packings

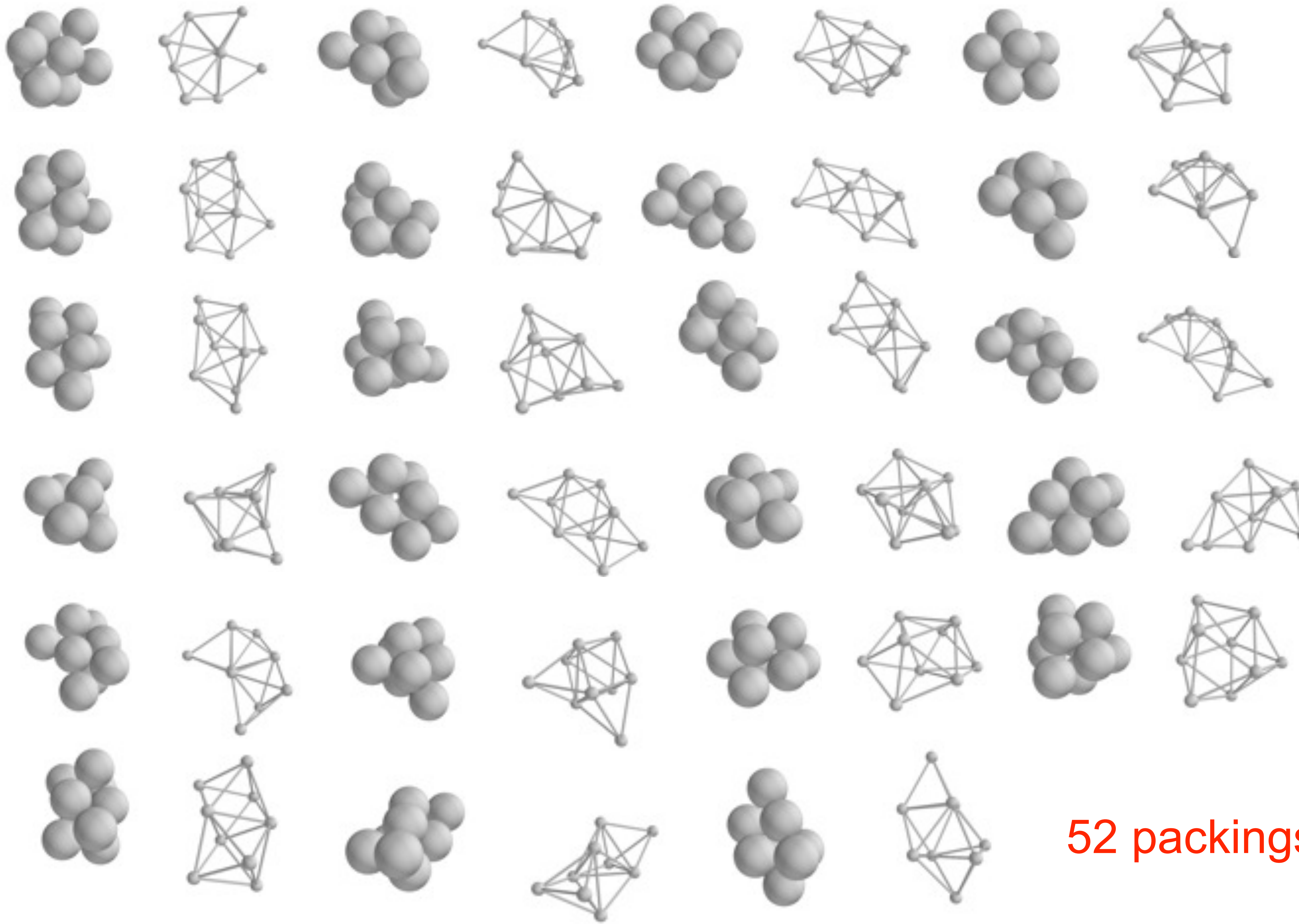
N = 8:



13 packings

N = 9:





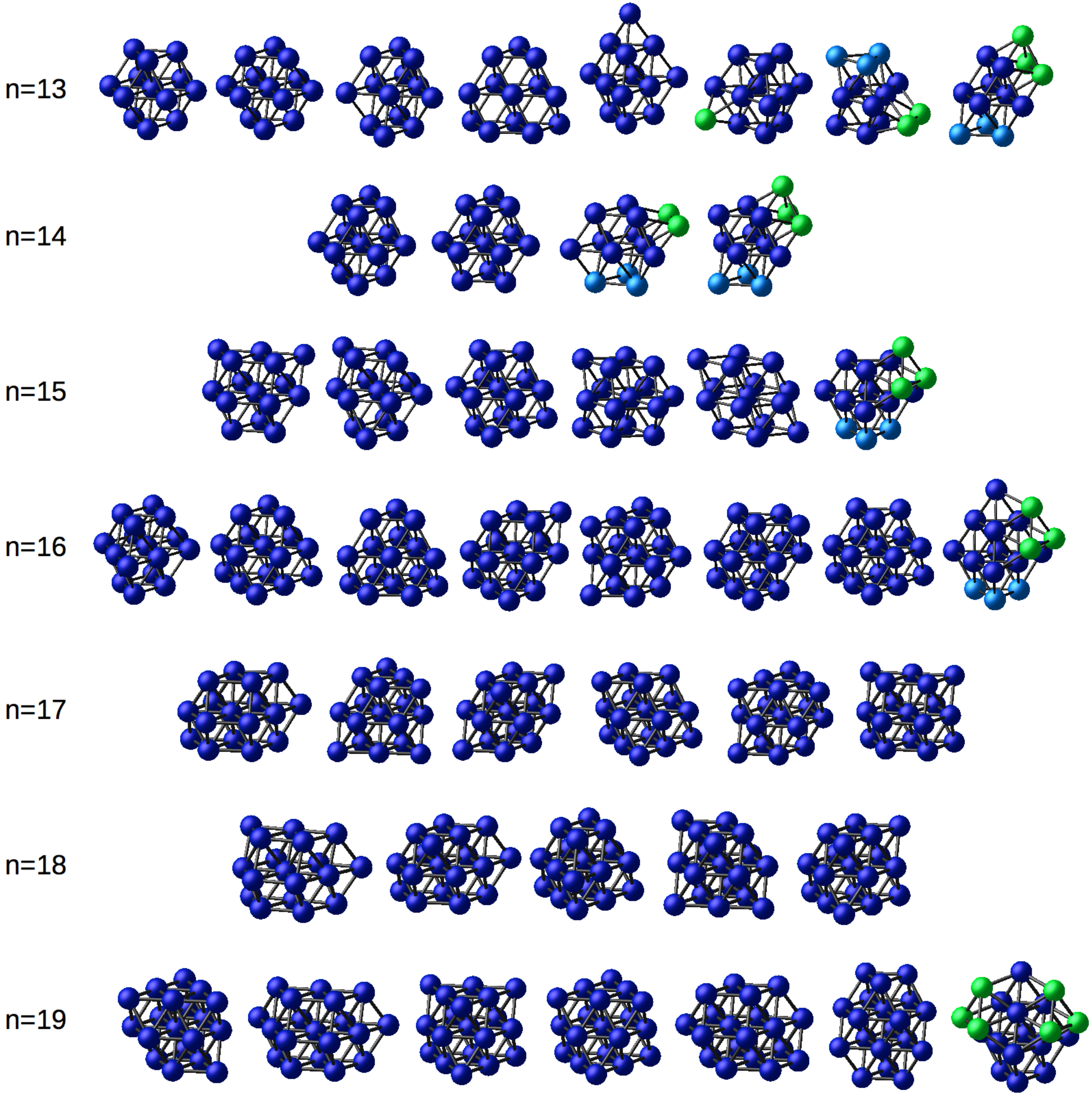
52 packings

Total number of clusters computed

n	number of contacts								Total
	$3n-9$	$3n-8$	$3n-7$	$3n-6$	$3n-5$	$3n-4$	$3n-3$	$3n-2$	Total
5				1					1
6				2					2
7				5					5
8				13					13
9				52					52
10			1	259	3				263
11		2	18	1618	20	1			1659
12		11	148	11,638	174	8	1		11,980
13		87	1221	95,810	1307	96	8		98,529
14	1	707	10,537	872,992	10,280	878	79	4	895,478
	$3n-4$	$3n-3$	$3n-2$	$3n-1$	$3n$	$3n+1$	$3n+2$		
15	7675	782	55	6					(9×10^6 est.)
16		7895	664	62	8				(1×10^8 est.)
17			7796	789	85	6			(1.2×10^9 est.)
18				9629	1085	91	5		(1.6×10^{10} est.)
19					13,472	1458	95	7	(2.2×10^{11} est.)

(N=20,21 also; data not shown)

hyperstatic


n=13
n=14
n=15
n=16
n=17
n=18
n=19

H.-C. (2016) *SIAM Review*

Total number of clusters computed

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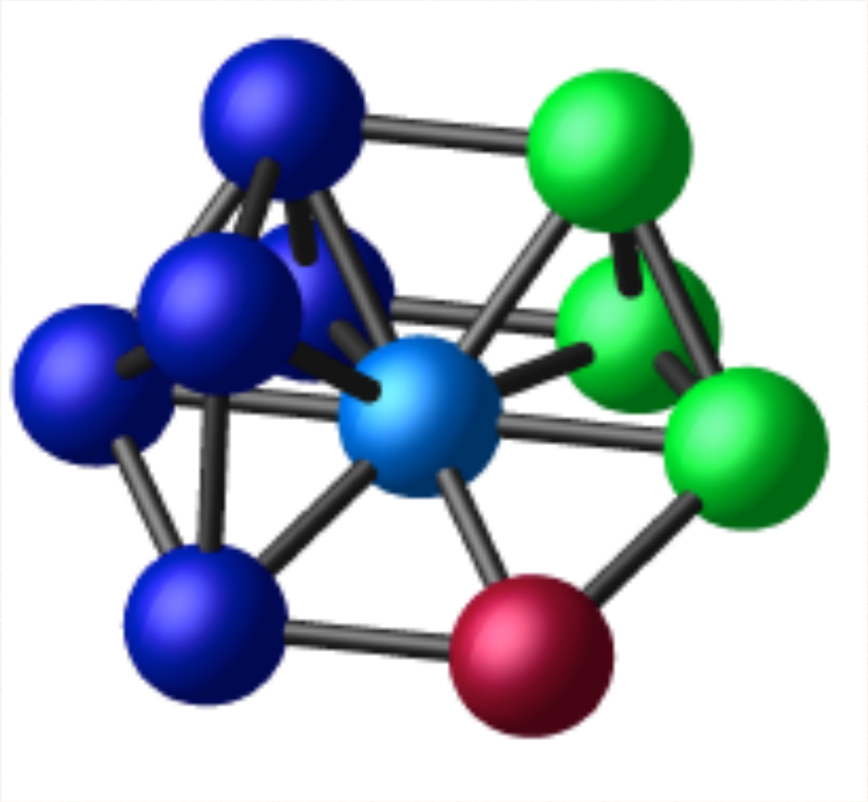
19					13,472	1458	95	7	(2.2×10^{11} est.)

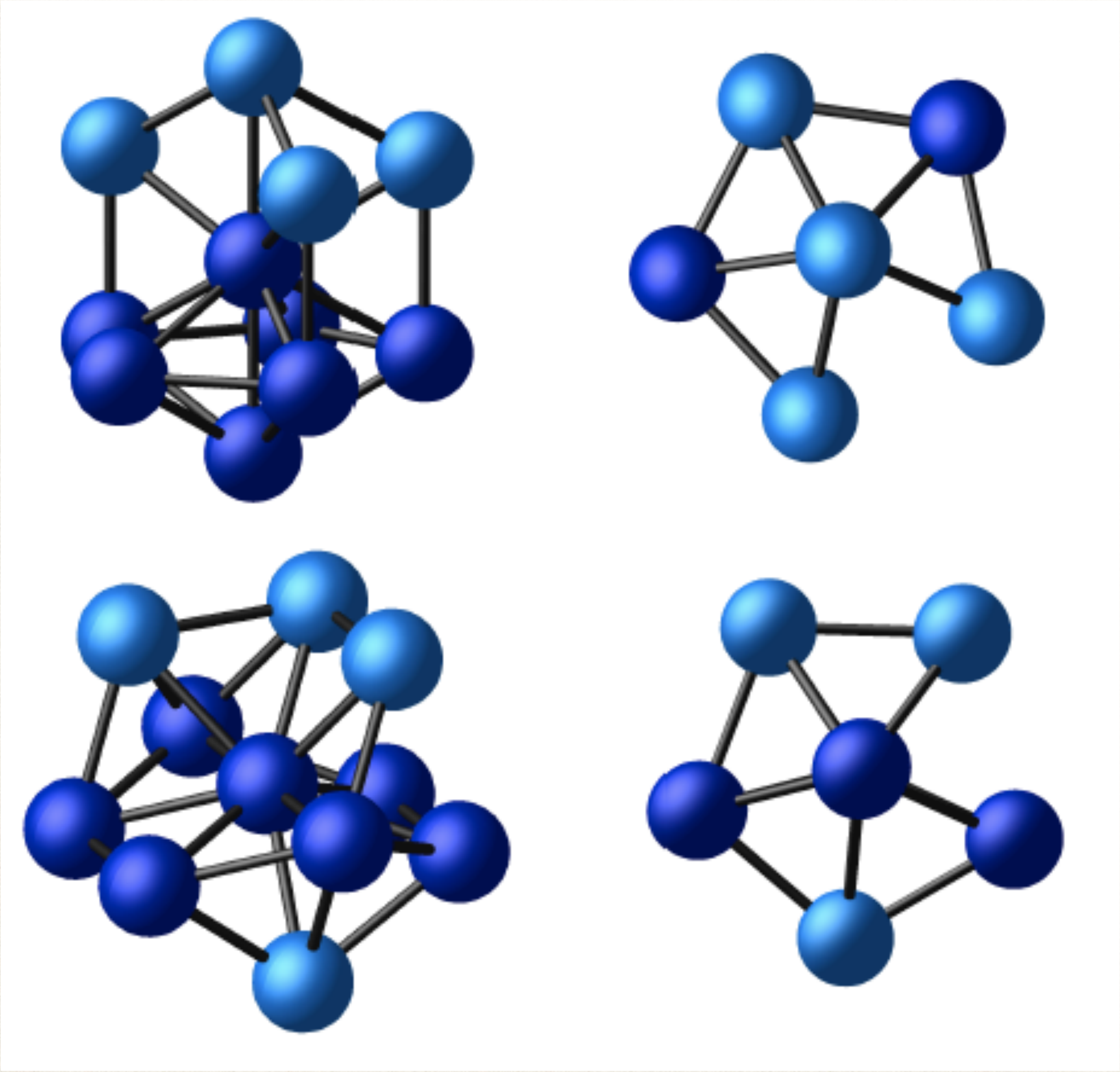
(N=20,21 also; data not shown)

hypostatic

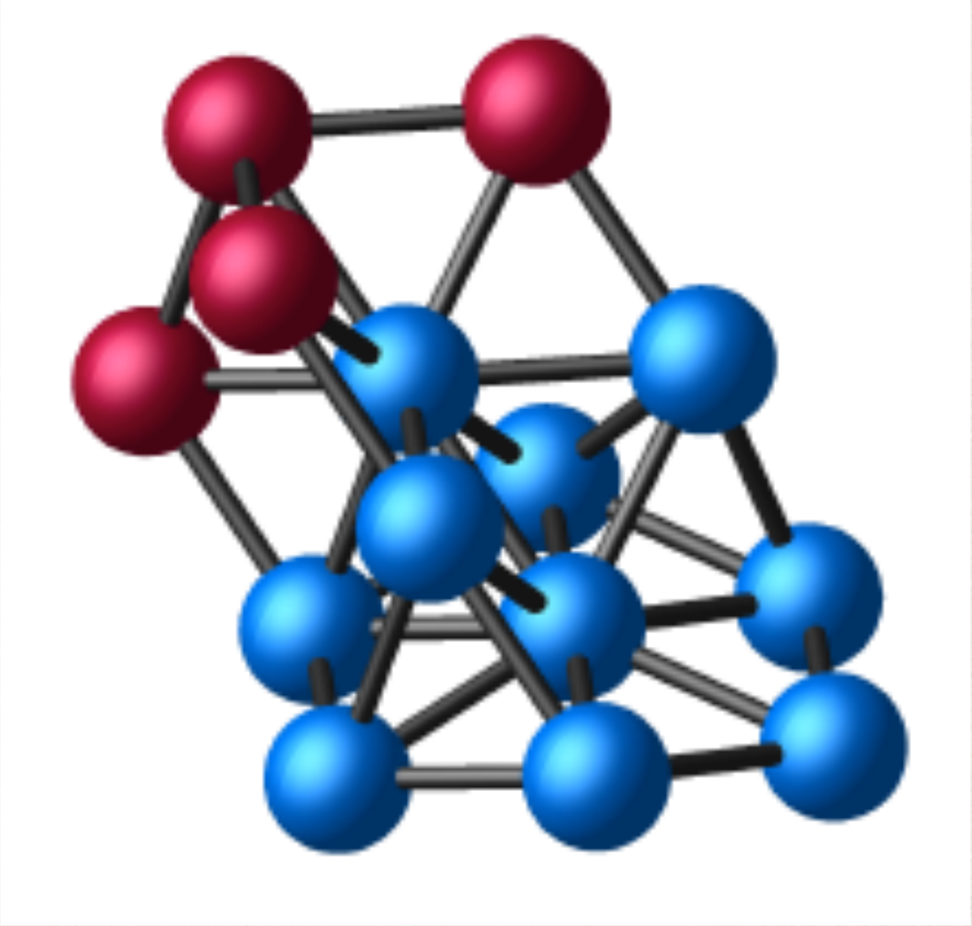
A cluster “missing” one contact, N=10



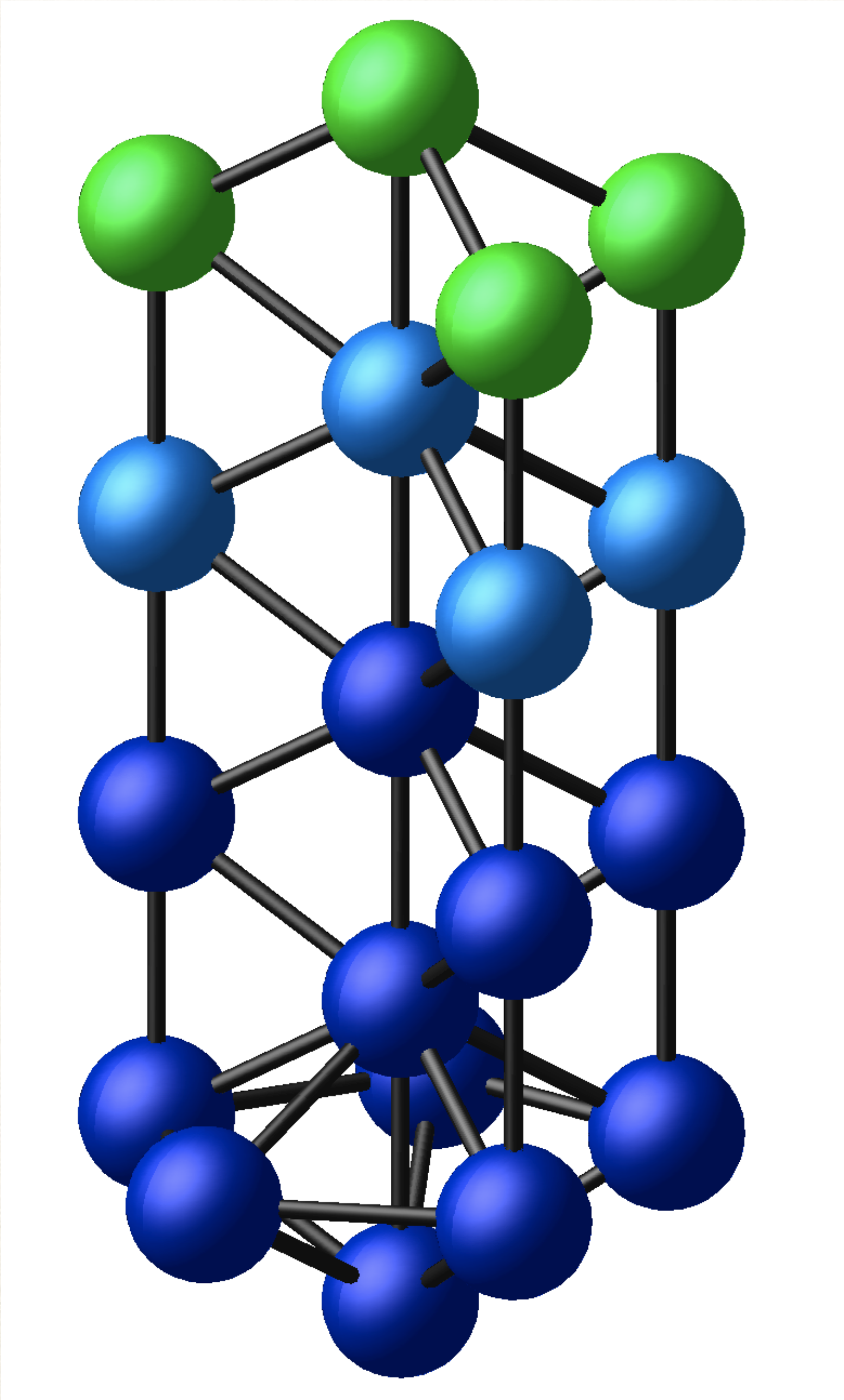
clusters missing two contacts, N=11



cluster missing three contacts, N=14

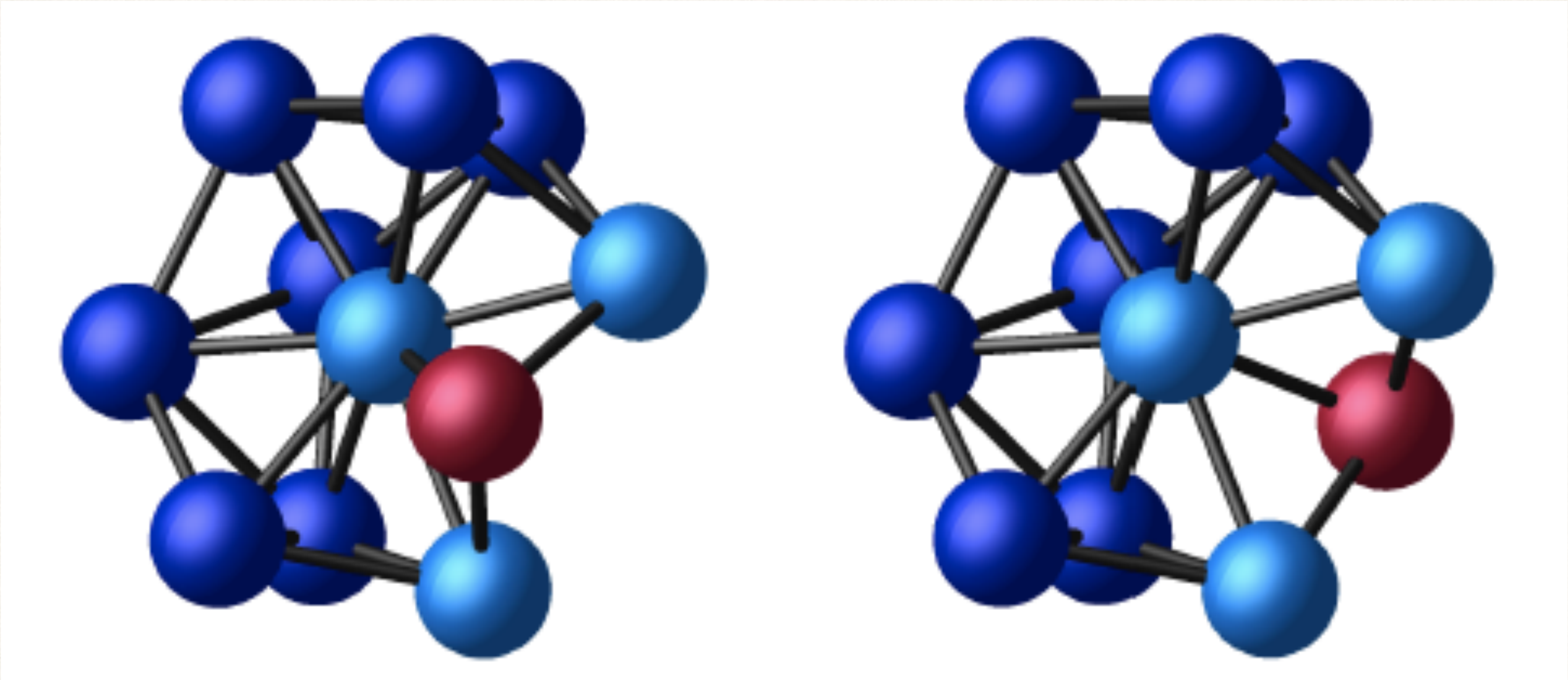


cluster missing arbitrarily many contacts

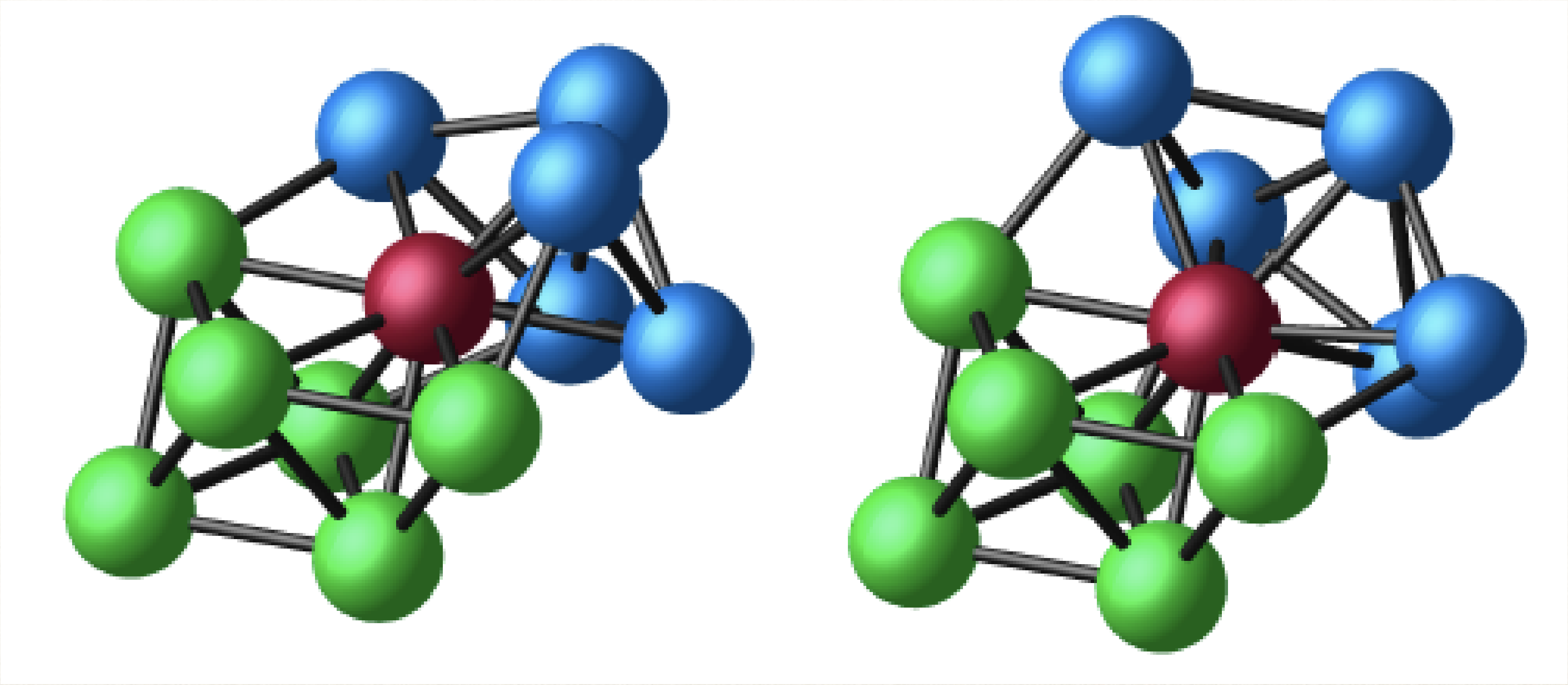


# of contacts ~ 2N when N large

Clusters with the same adjacency matrix

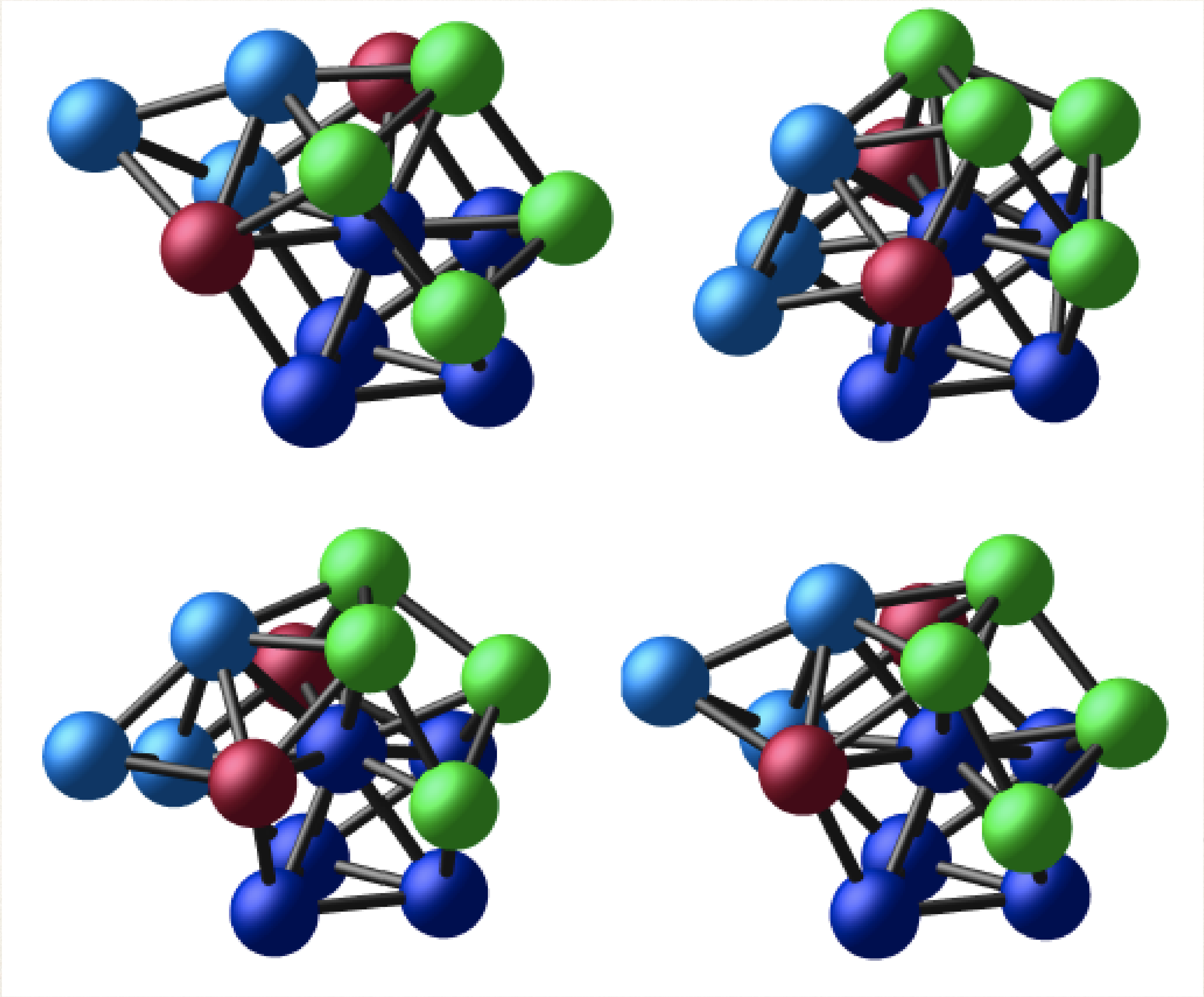


N=11

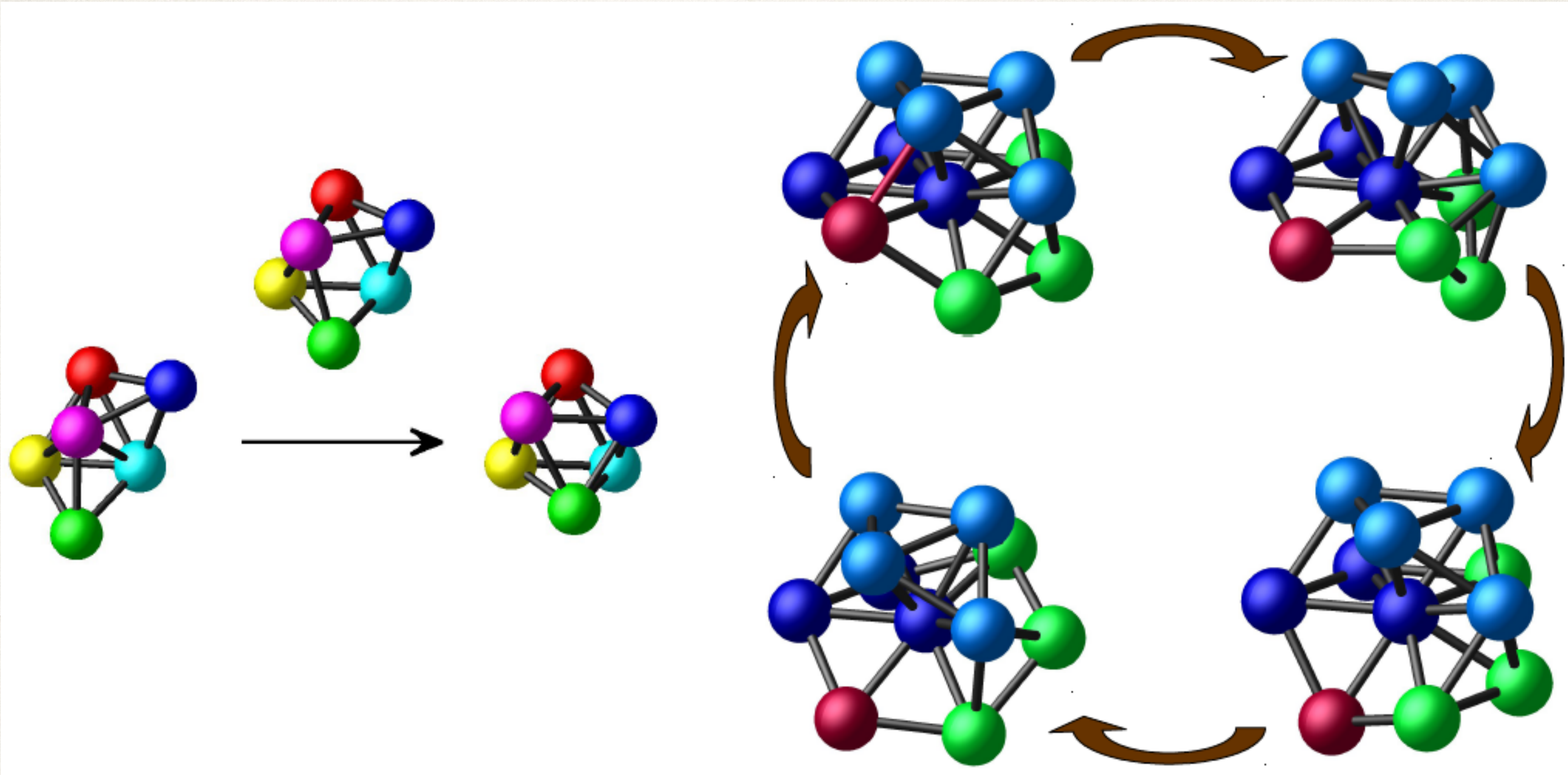


N=12

4 clusters with the same adjacency matrix (N=14)



Circular transition paths

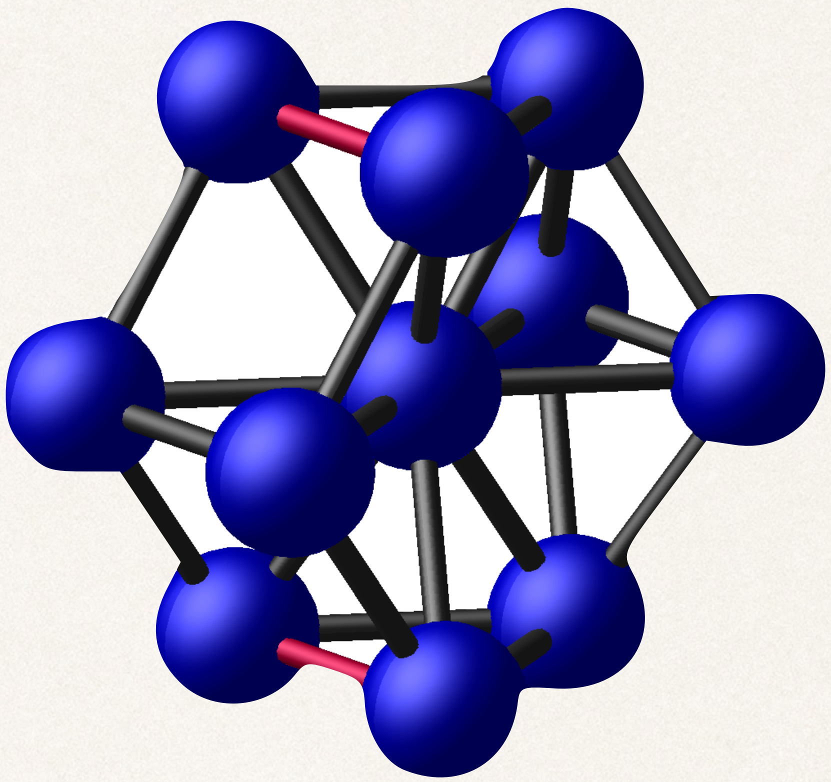


> 18,000 circular paths when N=13!

—> are there floppy local minima too? If so, how would we find them?

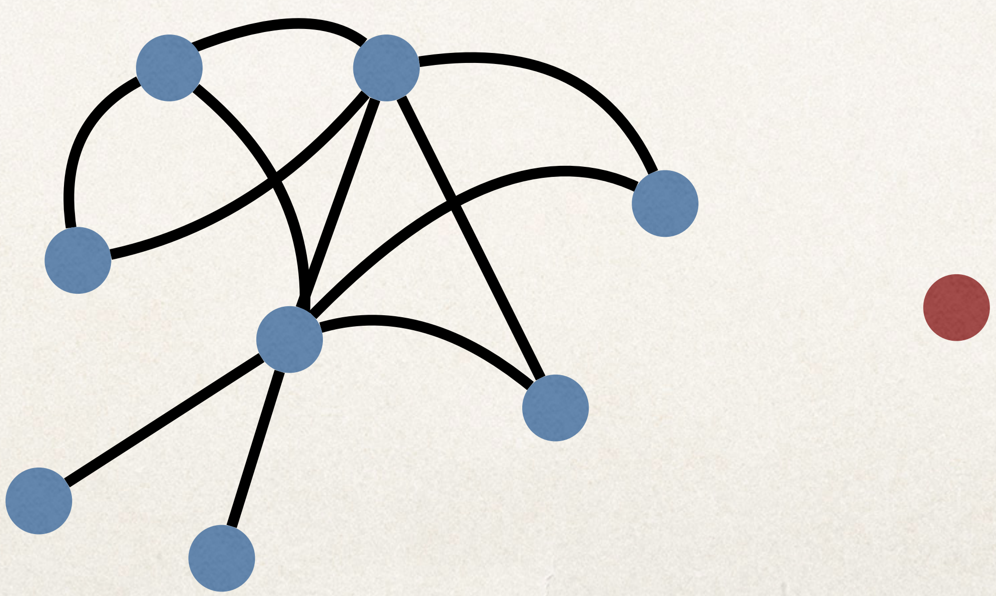
Does the algorithm find everything?

No……… here's an example:



N=11
hypostatic
3N-7 contacts
hcp fragment

Cluster landscape looks like:



Question:
Is the landscape ever connected (by 1 dof motions), under additional assumptions?
e.g. clusters are regular, isostatic, have random diameters, ….

Statistical Mechanics

What is the probability of a cluster $x \in \mathbb{R}^{3N}$ in the sticky-sphere (short-ranged interaction) limit?

M. H.-C., S. Gortler, M.P.Brenner, PNAS (2013)
Y. Kallus, M. H.-C., Phys. Rev. E (2017)

Probability(cluster x) ∝ Partition function Z_x

$$Z_x = \int_{N(x)} e^{-\beta V(x')} dx'$$

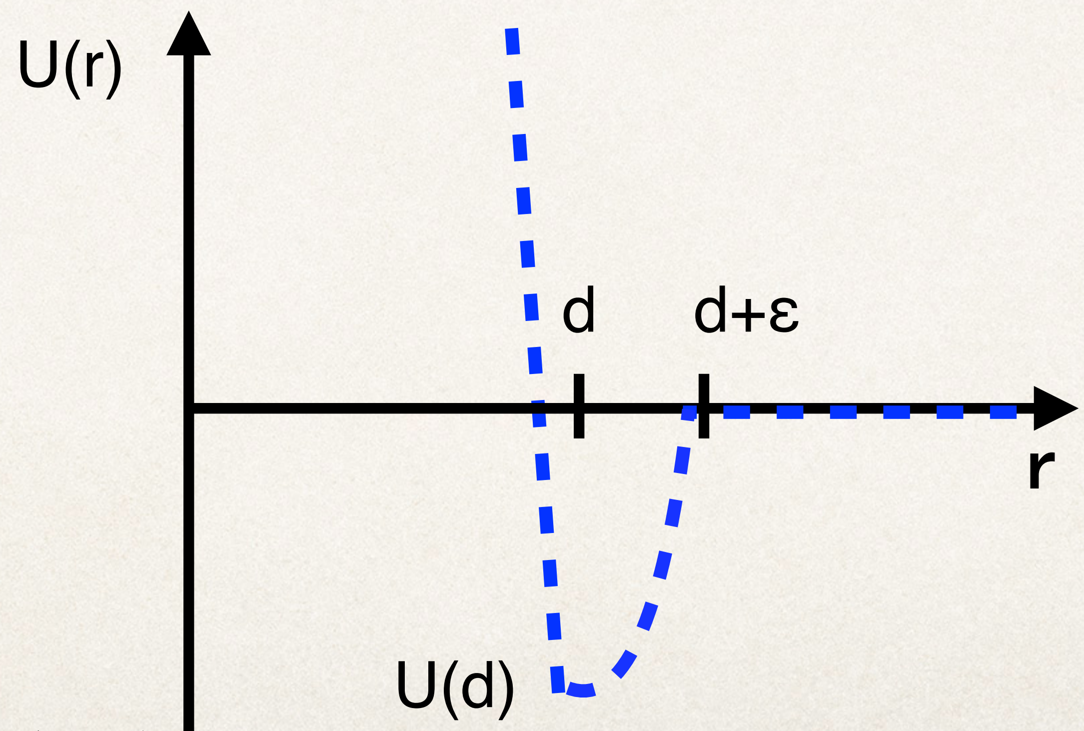
- V(x) = energy of configuration x,
- $\beta = 1/k_B T$ = inverse temperature
- N(x) = neighbourhood of x, including translations, rotations, permutations, and bonds with lengths ∊ (d - ε, d + ε)

$V(x) = \sum_{i \neq j} U(|x_i - x_j|)$

energy of a pair = $U(|x_i - x_j|)$
x_i=center of i^{th} sphere,
$x=(x_1,x_2,\ldots,x_N)$

Sticky-sphere limit:

- Range ε « d
- Depth U(d) » 1



M. H.-C., S. Gortler, M.P. Brenner, PNAS (2013)
Y. Kallus, M. H.-C., Phys. Rev. E (2017)

"Geometry" of the calculation

B = # of bonds

Asymptotically as ε —> 0:

$$Z_x \sim e^{-\beta B U(d)} \int_{\{-\epsilon \leq y_k(x) \leq \epsilon\}_{k=1}^{B}} dx$$

constraints ``fattened'' by ε

$y_k(x) = |x_{i_k} - x_{j_k}| - 1$ = excess bond distance between spheres i_k, j_k

$\{x : y_k(x) = 0\}$ is hypersurface where sphere i_k touches sphere j_k

Z_x ≈ Exp(U(d)*# of contacts) * Volume(constraint intersection region)

$\rightarrow \infty$ "energy"

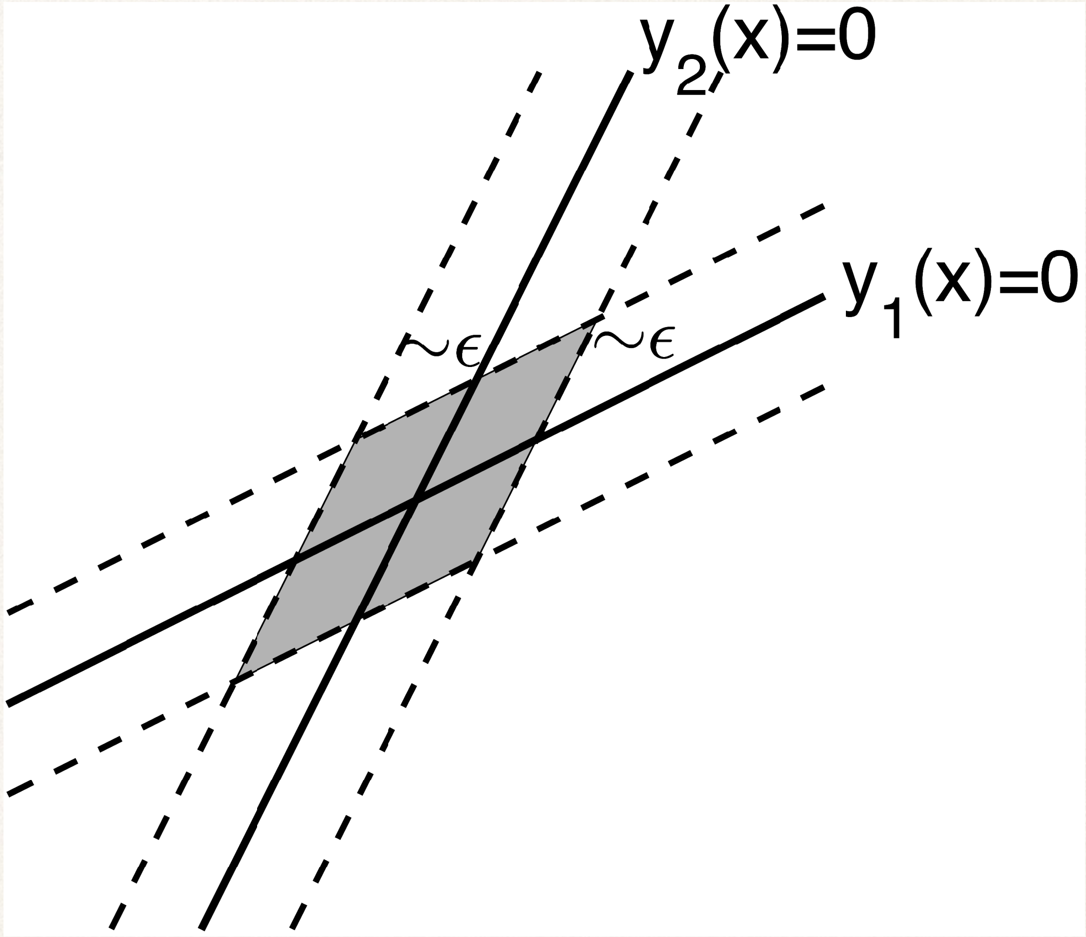
$\rightarrow 0$ "entropy"

Example (regular)

$x \in R^2$

$y_1(x) = v_1 \cdot x$

$y_2(x) = v_2 \cdot x$



$$\text{Vol} = 4 \, | \, v_1 \times v_2 \, |^{-1} \, \varepsilon^2$$

"Regular" constraints should have volumes that scale as

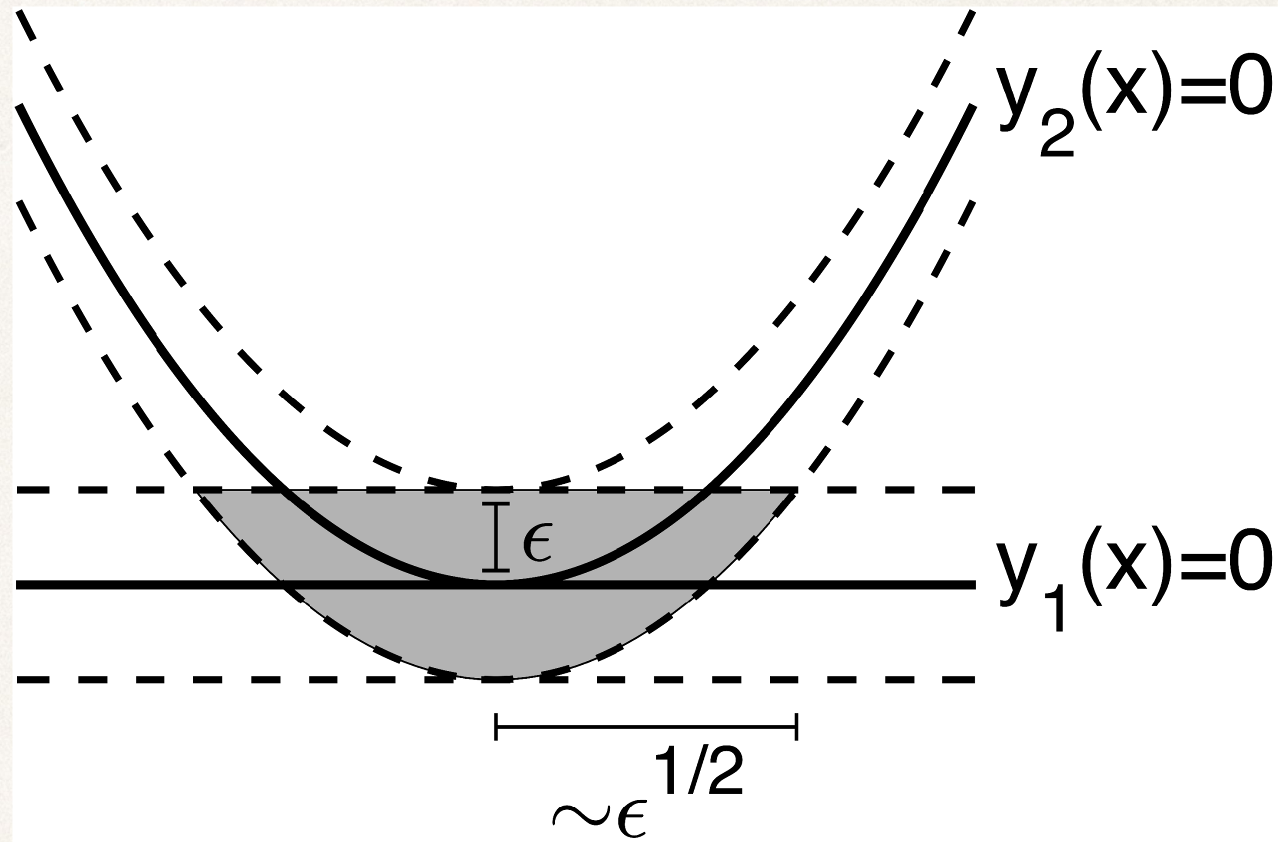
$\varepsilon^{\text{dimension of intersection set}}$

Example (singular)

$x \in R^2$

$y_1(x) = x_2$

$y_2(x) = (x_1)^2 - x_2$



$Y_1 = y_1 / \varepsilon$

$Y_2 = y_2 / \varepsilon^{1/2}$

$$\frac{\partial Y}{\partial x} = 2\epsilon^{-3/2}\sqrt{Y_1 + Y_2}$$

$$\text{Vol} = \epsilon^{3/2} \iint\limits_{\substack{1 \leq Y_1 \leq 1 \\ 1 \leq Y_2 \leq 1 \\ Y_1 + Y_2 \geq 0}} \frac{1}{2\sqrt{Y_1 + Y_2}} dY_1 dY_2 = \epsilon^{3/2} \cdot O(1)$$

blows up as (Y_1, Y_2)—>(0,0), but in an integrable way

$$\frac{\text{Vol(Example 2)}}{\text{Vol(Example 1)}} \sim \frac{1}{\epsilon^{1/2}} \qquad \nearrow \infty \quad \text{as } \epsilon \to 0$$

—> Equilibrium probability of singular clusters should dominate that of regular clusters (with the same number of contacts), in the sticky-sphere limit.

Physically, they have more *entropy*.

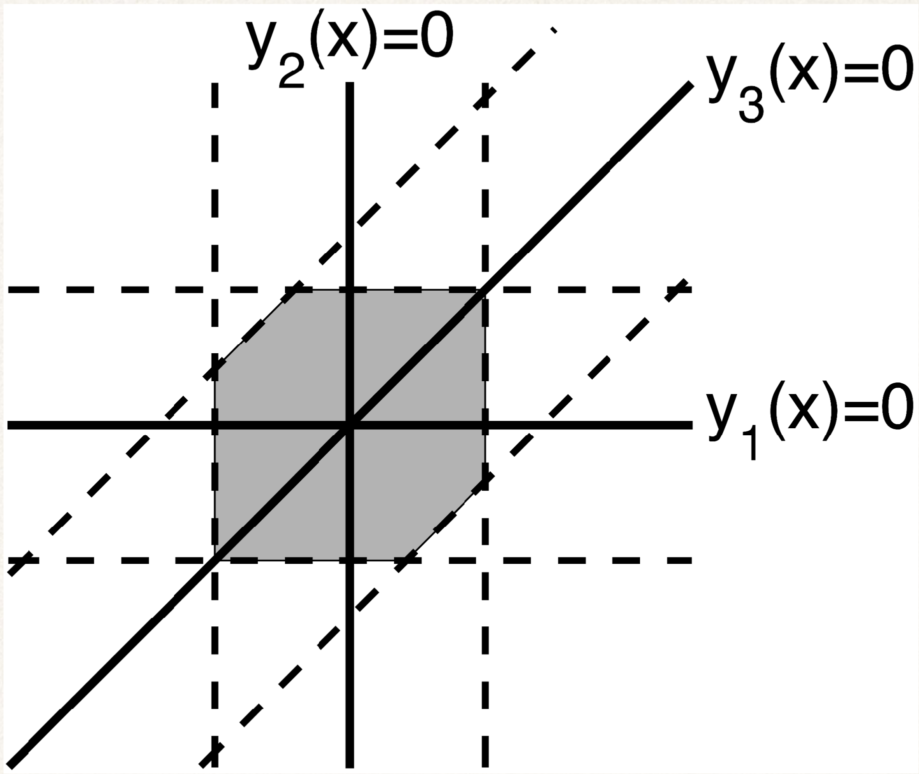
Example (hyperstatic)

$x \in R^2$

$y_1(x) = v_1 \cdot x$

$y_2(x) = v_2 \cdot x$

$y_3(x) = v_3 \cdot x$



Vol $\propto$ ε^2

$$Z_x \propto e^{-3\beta U(d)} \epsilon^2$$

$$\frac{Z_x(\text{hyperstatic example})}{Z_x(\text{regular example})} \propto e^{-\beta U(d)} \to \infty \quad \text{as } U(d) \to -\infty$$

—> Free energy of hyperstatic clusters should dominate that of regular clusters, in the sticky-sphere limit.
Physically, they have lower *energy*.

Who wins: singular clusters or hyperstatic clusters?

General case

How does the free energy of singular clusters scale with ε?

Algebraic geometry:

$$\mathrm{Vol} \sim \epsilon^q (\log \epsilon)^k, \qquad q \in \mathbb{Q}, \quad k \in \mathbb{Z}$$

q,k related to the algebraic nature of the singularity, i.e. what it looks like once it is "resolved"

IGUSA INTEGRALS AND VOLUME ASYMPTOTICS
IN ANALYTIC AND ADELIC GEOMETRY

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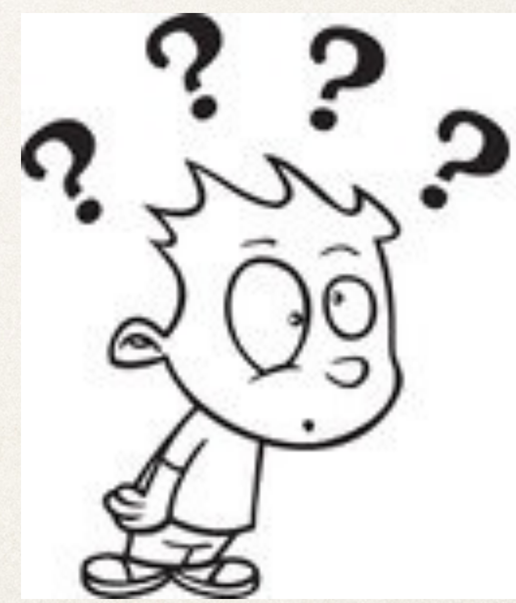
We establish asymptotic formulas for volumes of height balls in analytic varieties over local fields and in adelic points of algebraic varieties over number fields, relating the Mellin transforms of height functions to Igusa integrals and to global geometric invariants of the underlying variety. In the adelic setting, this involves the construction of general Tamagawa measures.

Keywords: Heights; Poisson formula; Manin's conjecture; Tamagawa measure.

AMS Subject Classification: 11G50 (11G35, 14G05)



Our approach

$$Z_x = \int_{N(x)} e^{-\beta V(x')} dx'$$

- Taylor-expand the potential V(x) = $\sum_{i \neq j} U(|x_i - x_j|)$

$$\begin{aligned}
\partial_1\partial_2\partial_3 V &= \sum_{\langle i,j\rangle} U_0'''(\partial_1 r \partial_2 r \partial_3 r) + U_0''(\partial_{13} r \partial_2 r + \partial_{23} r \partial_1 r + \partial_{12} r \partial_3 r) \\
\partial_1\partial_2\partial_3\partial_4 V &= \sum_{\langle i,j\rangle} U_0''''(\partial_1 r \partial_2 r \partial_3 r \partial_4 r) \\
&+ U_0'''(\partial_{14} r \partial_2 r \partial_3 r + \partial_{13} r \partial_2 r \partial_4 r + \partial_{12} r \partial_3 r \partial_4 r + \partial_{24} r \partial_1 r \partial_3 r + \partial_{23} r \partial_1 r \partial_4 r + \partial_{34} r \partial_1 r \partial_1 r) \\
&+ U_0''(\partial_{123} r \partial_4 r + \partial_{124} r \partial_2 r + \partial_{234} r \partial_1 r + \partial_{12} r \partial_{34} r + \partial_{13} r \partial_{24} r + \partial_{14} r \partial_{24} r)
\end{aligned}$$

- Evaluate integral using Laplace asymptotics

- Asymptotically the same scaling as square-well potential:
  log(Z_{square}) ~ log(Z_x)   as ε→0, U(d)→∞   (Kallus & H.-C., Phys Rev E (2017))

Partition function for second-order rigid cluster

$$Z_x = (\text{const}) \cdot \ \gamma^{\Delta B} \alpha^{d_X} \ z_x$$

where the geometrical part is

$$z_x = (\text{const}) \cdot \ \frac{\sqrt{I(x)}}{\sigma} \prod_{\lambda_i \neq 0} \lambda_i^{-1/2}(x) \int_X e^{-Q(\tilde{\mathbf{x}})} d\tilde{\mathbf{x}}$$

parameters are

$$\begin{aligned} \gamma &= e^{-\beta U(d)} \\ &\approx \exp(\text{depth}) \\ \alpha &= (U''(d)\beta d^2)^{1/4} \\ &\approx \text{width}^{-1/2} \end{aligned}$$

Only TWO parameters needed!

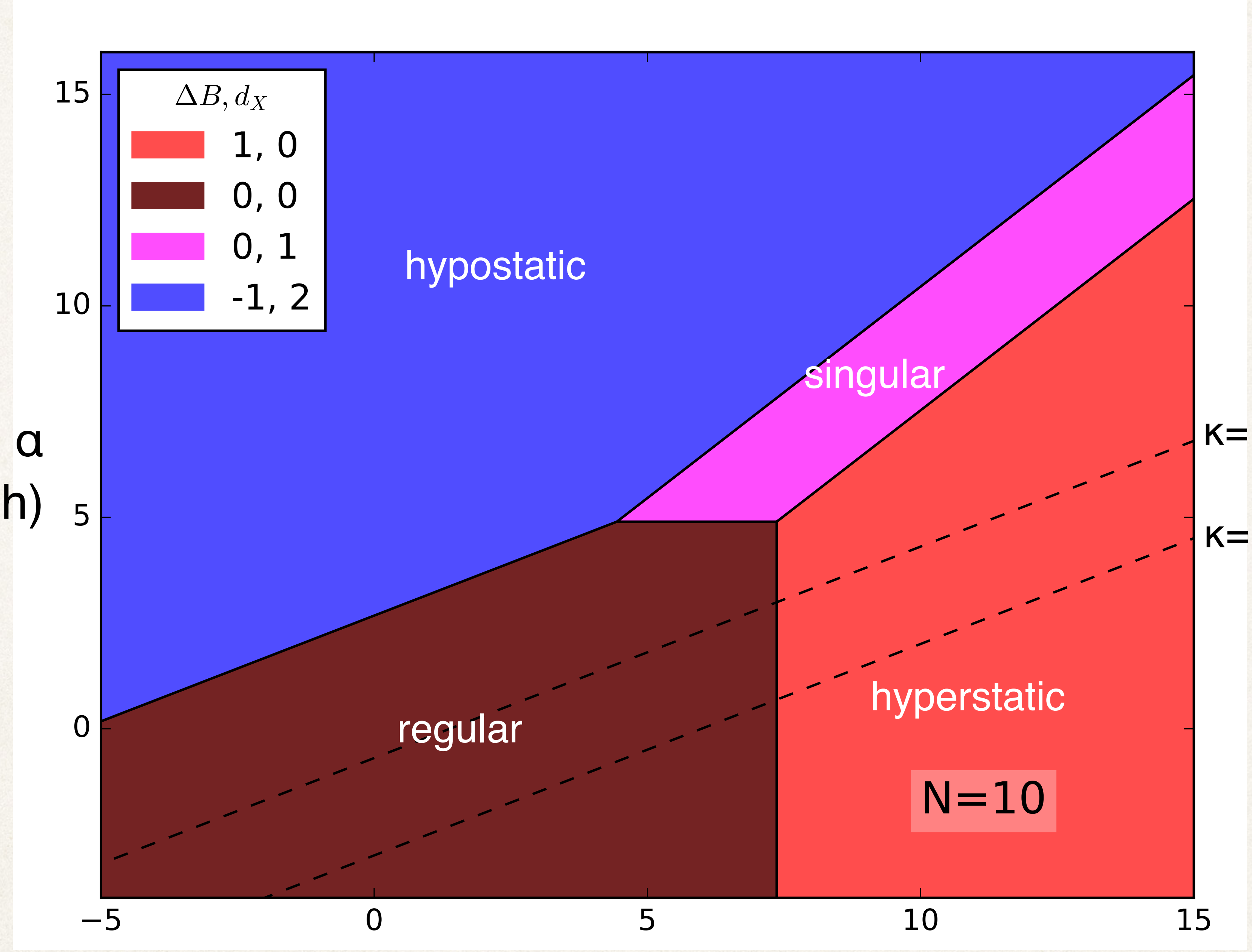
geometry-dependent variables are

$$\begin{aligned} \Delta B &= B - (3N - 6) \\ &= \text{\# of bonds beyond isostatic} \\ d_X &= \text{\# of singular directions} \\ I(x) &= \text{determinant of moment of inertia tensor} \\ \sigma &= \text{symmetry number} \\ \lambda_i(x) &= \text{eigenvalues of Hessian } \nabla\nabla V = R(x)R^T(x) \\ Q(\mathbf{x}) &= \text{quartic function on subspace of} \\ &\quad\ \text{singular directions} \end{aligned}$$

Y. Kallus and M. H.-C., Phys. Rev. E (2017).

Comparing hyperstatic & singular clusters

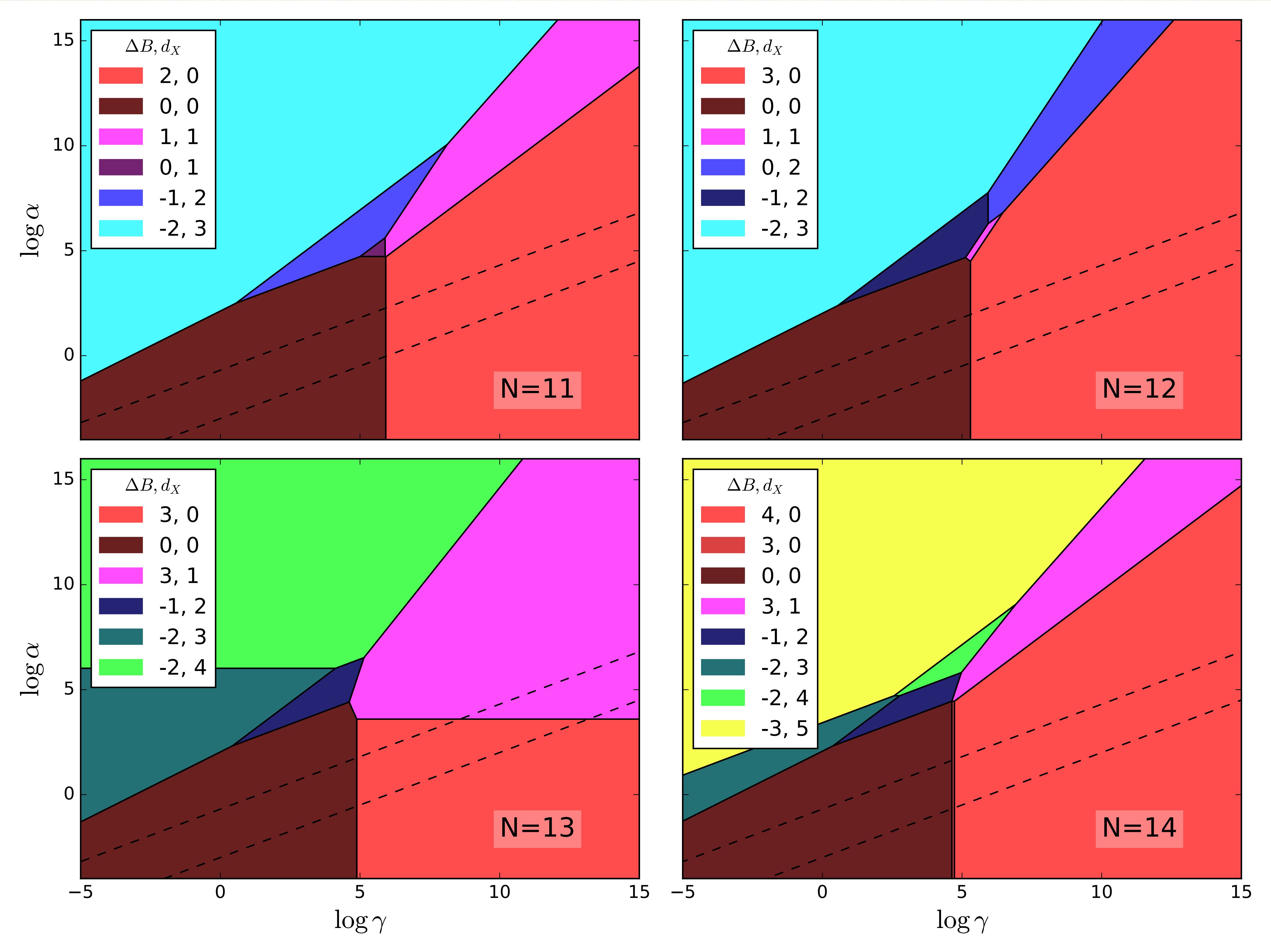
N = 10



log α
-½log(width)

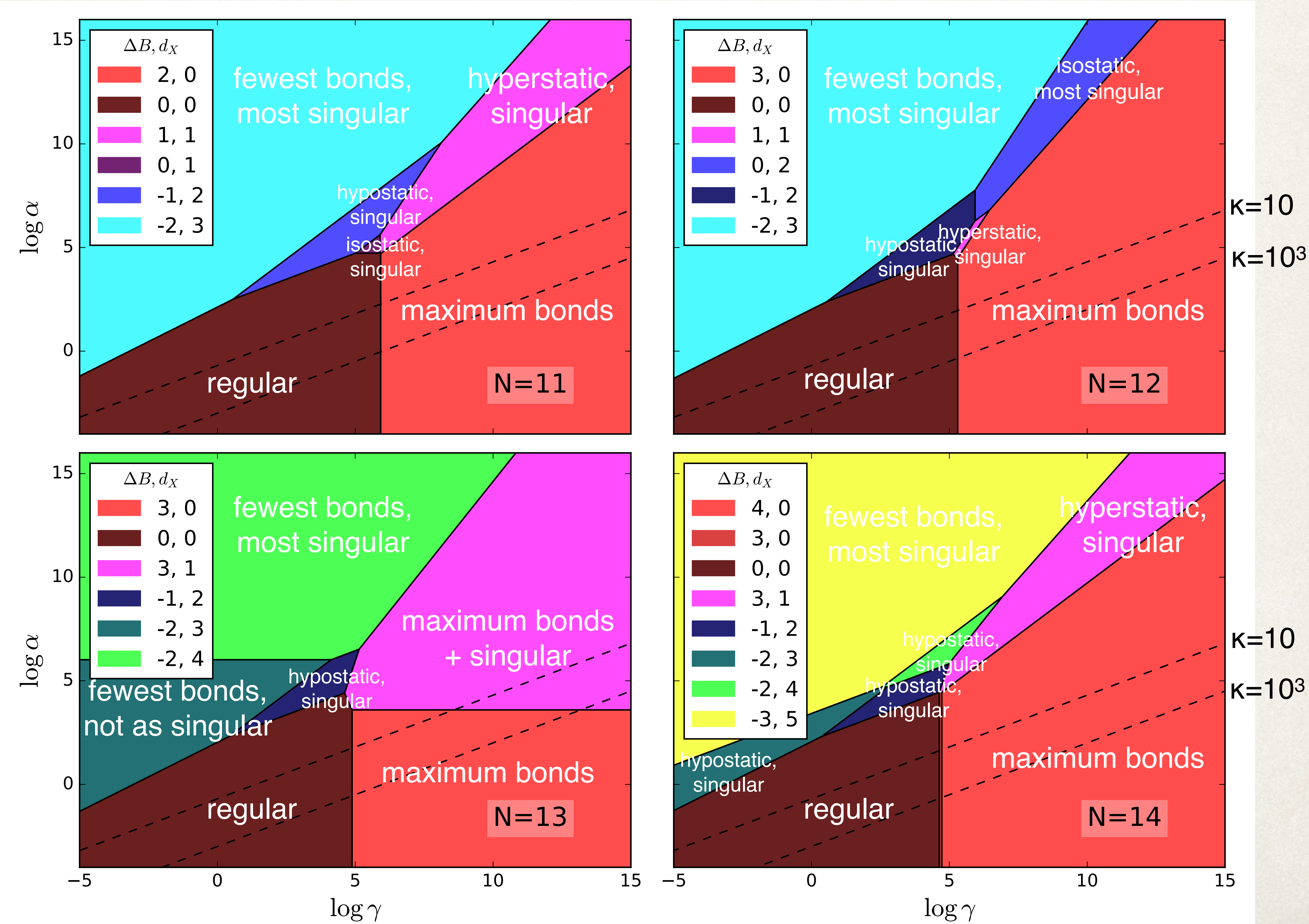
log γ
(depth)

N = 11-14

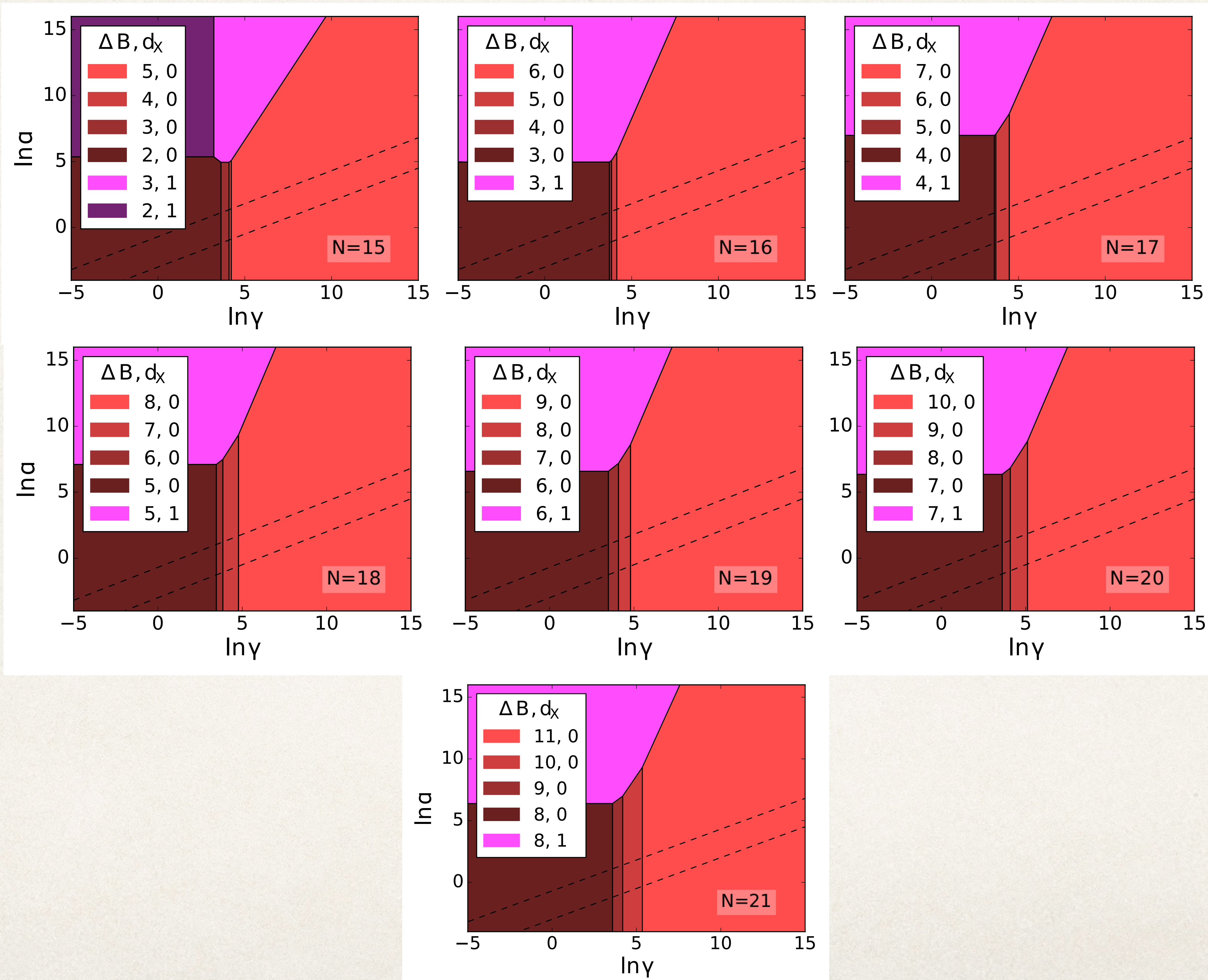


$\Delta B, d_X$
2, 0
0, 0
1, 1
0, 1
-1, 2
-2, 3
N=11
$\Delta B, d_X$
3, 0
0, 0
1, 1
0, 2
-1, 2
-2, 3
N=12
$\Delta B, d_X$
3, 0
0, 0
3, 1
-1, 2
-2, 3
-2, 4
N=13
$\Delta B, d_X$
4, 0
3, 0
0, 0
3, 1
-1, 2
-2, 3
-2, 4
-3, 5
N=14
$\log \alpha$
$\log \gamma$
15
10
5
0
−5

N = 11-14


$\Delta B, d_X$
2, 0
0, 0
1, 1
0, 1
-1, 2
-2, 3
fewest bonds, most singular
hyperstatic, singular
hypostatic, singular
isostatic, singular
maximum bonds
regular
N=11
$\Delta B, d_X$
3, 0
0, 0
1, 1
0, 2
-1, 2
-2, 3
fewest bonds, most singular
isostatic, most singular
hypostatic, singular
hyperstatic, singular
maximum bonds
regular
N=12
κ=10
κ=10³
$\Delta B, d_X$
3, 0
0, 0
3, 1
-1, 2
-2, 3
-2, 4
fewest bonds, most singular
maximum bonds + singular
fewest bonds, not as singular
hypostatic, singular
maximum bonds
regular
N=13
$\Delta B, d_X$
4, 0
3, 0
0, 0
3, 1
-1, 2
-2, 3
-2, 4
-3, 5
fewest bonds, most singular
hyperstatic, singular
hypostatic, singular
hypostatic, singular
hypostatic, singular
maximum bonds
regular
N=14
κ=10
κ=10³
$\log \alpha$
$\log \gamma$

N=15-21



ΔB, d_X
5, 0
4, 0
3, 0
2, 0
3, 1
2, 1
N=15
ΔB, d_X
6, 0
5, 0
4, 0
3, 0
3, 1
N=16
ΔB, d_X
7, 0
6, 0
5, 0
4, 0
4, 1
N=17
ΔB, d_X
8, 0
7, 0
6, 0
5, 0
5, 1
N=18
ΔB, d_X
9, 0
8, 0
7, 0
6, 0
6, 1
N=19
ΔB, d_X
10, 0
9, 0
8, 0
7, 0
7, 1
N=20
ΔB, d_X
11, 0
10, 0
9, 0
8, 0
8, 1
N=21
lnα
lnγ

… back to frustration ….

- Symmetry (or lack thereof) doesn't seem to be particularly important
- Competition is between

  energy (of extra bonds),   and *"singular" entropy* (of 0-frequency modes):

energy   entropy

$$Z_x = (\text{const}) \cdot \; \gamma^{\Delta B} \alpha^{d_X} \; z_x$$

and *combinatorial entropy* (total number of states)

(also global entropy term — neglected here)

- For *identical spheres*, energy beats "singular entropy":
  Max-bond, crystalline states win for N ≥ 10, strong enough bonds

  —> Sticky spheres do not appear to be frustrated!

- **Question:** Are there systems where "singular entropy" dominates?
  (non-identical spheres, ellipsoids, …?)

Thanks to: Steven Gortler, Yoav Kallus, John Ryan, Louis Theran, **US DOE, NSF-FRG, Sloan**

Collaborators

Louis Theran,
St. Andrew's University

Yoav Kallus, Cornell/
Susquehanna International
Group

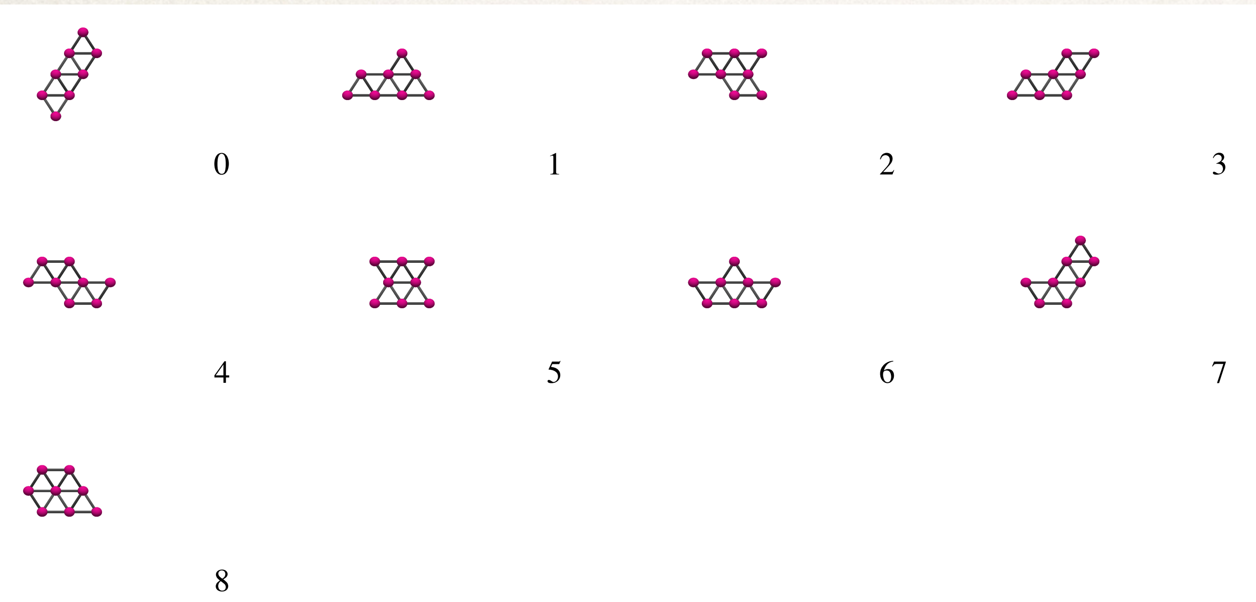
Steven Gortler,
Harvard University

John Ryan, Cornell/Google

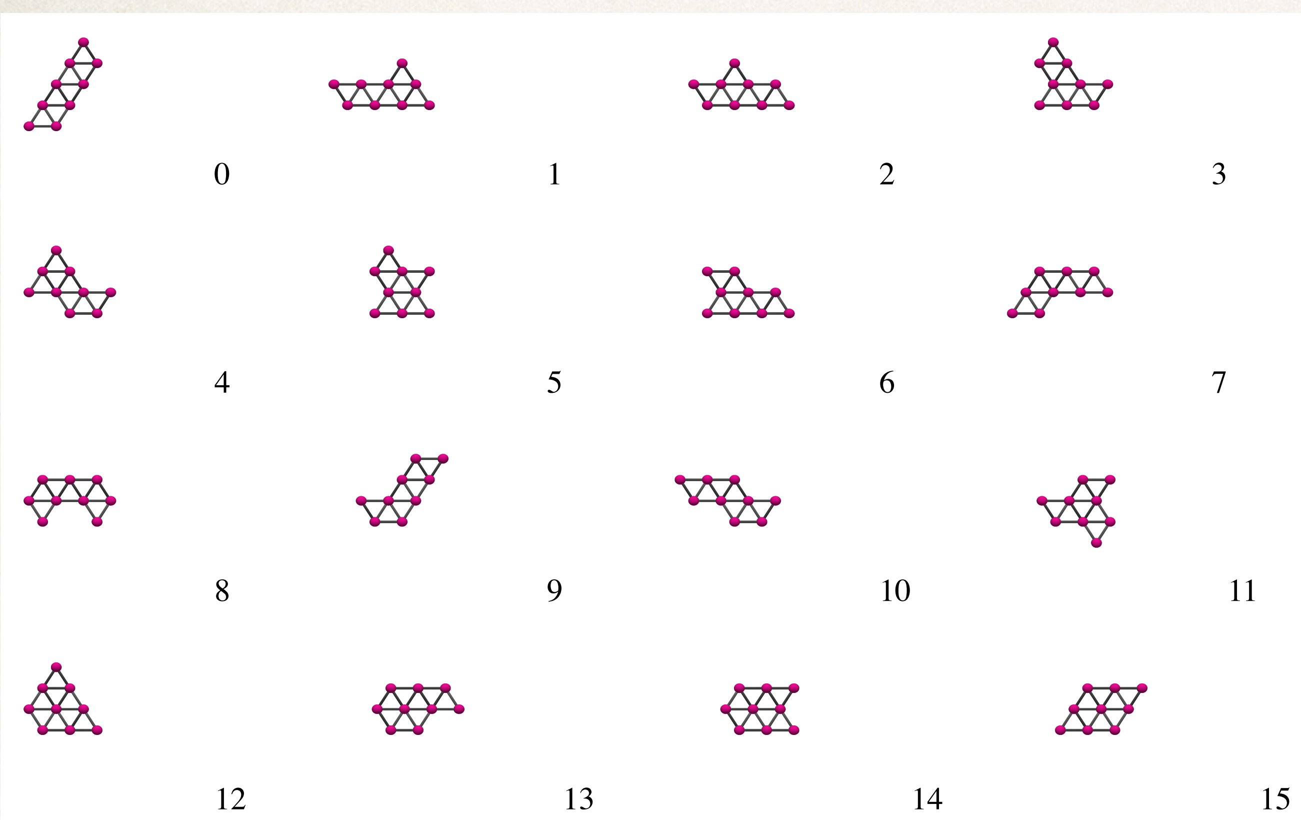
US Dept of Energy, NSF, Sloan Foundation

Two-dimensional rigid clusters

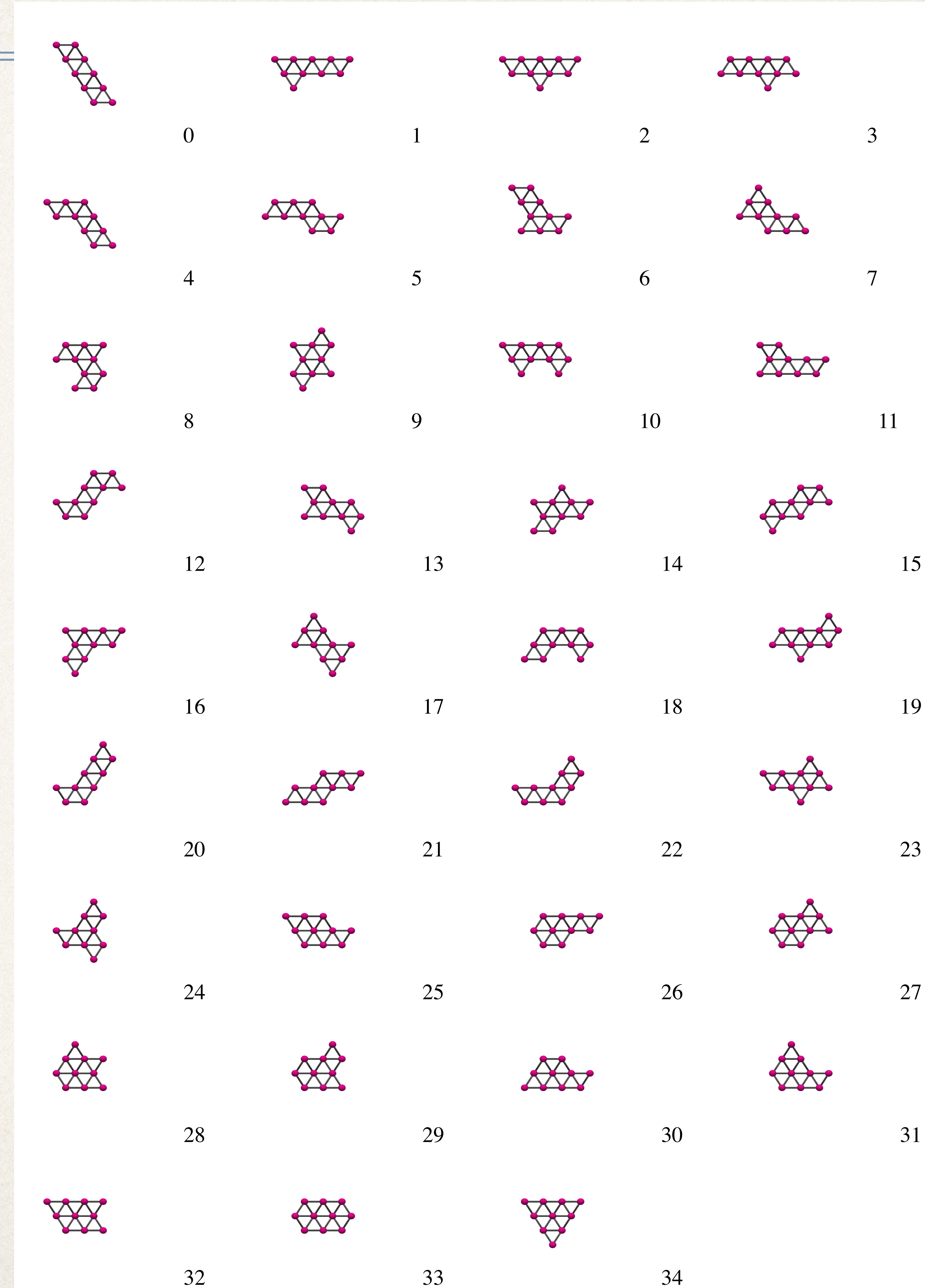
N=8



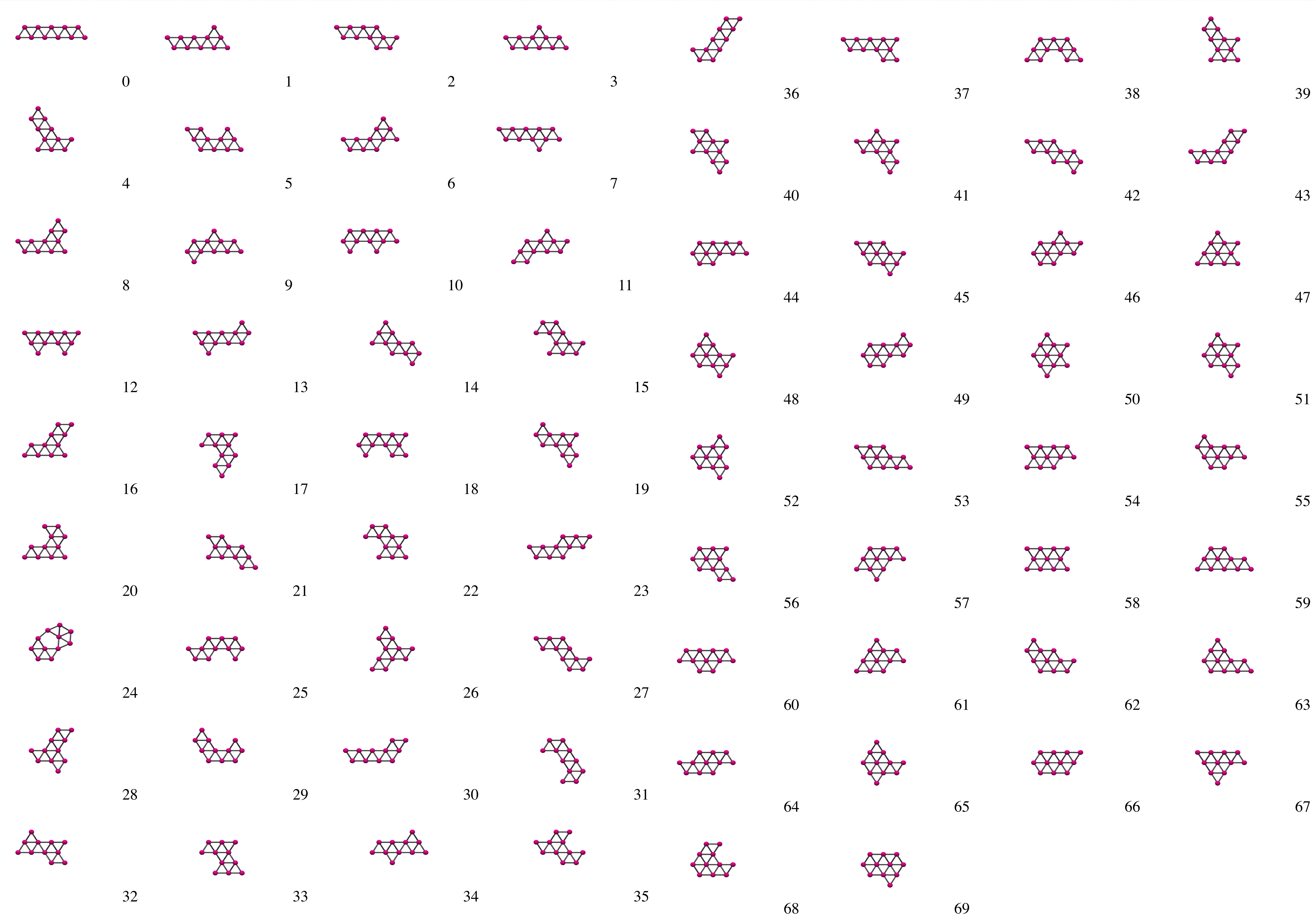
N=9



N=10



N=11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