A minimal model for self-assembling hollow shells and 2D quasicrystals from colloidal building blocks

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Provitam Foundation

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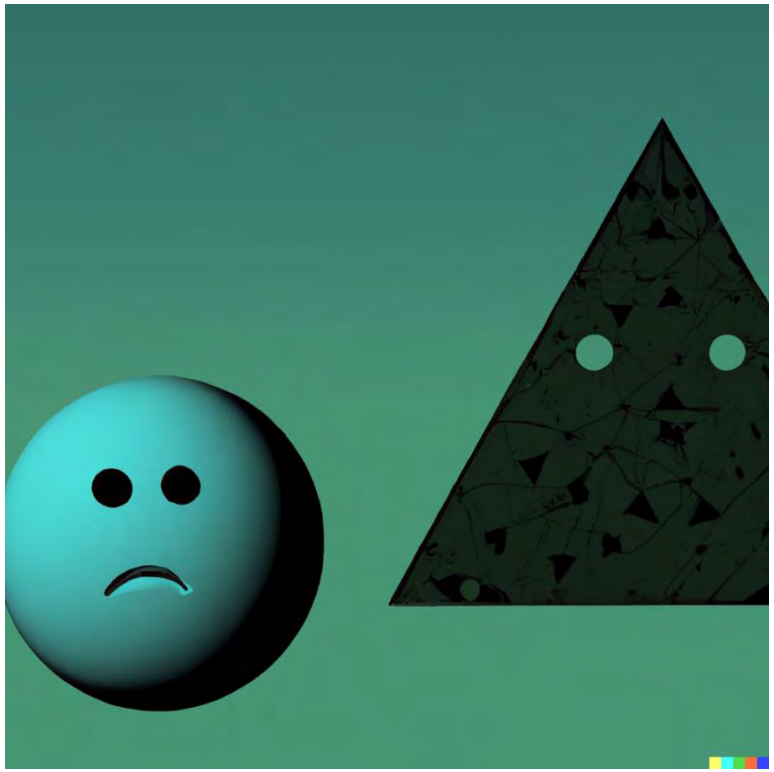
RESEARCH AND OTHER MEDICAL ACTIVITIES

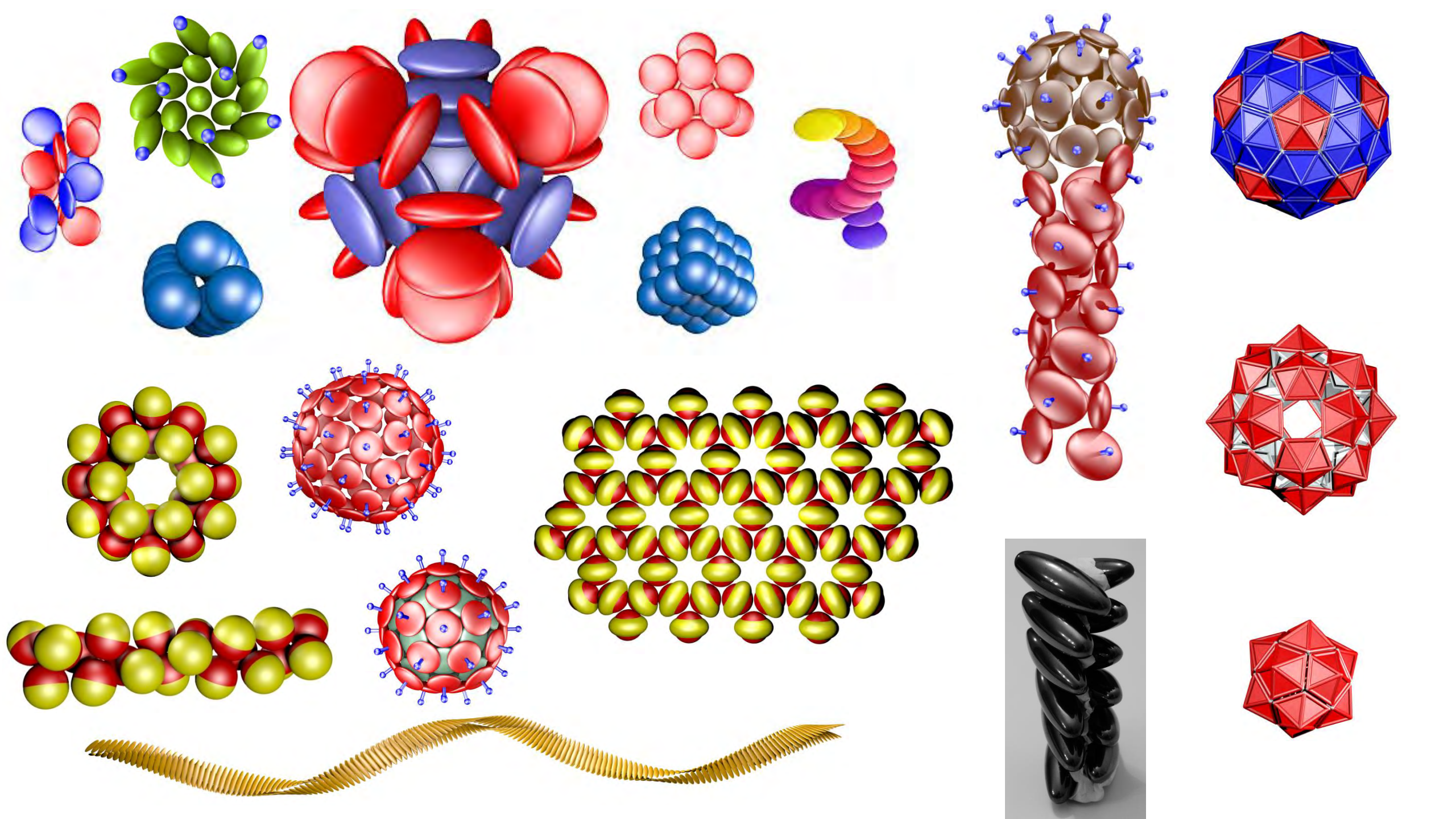
How do we define shape on the mesoscopic length scale?

- Interactions and shape “go together like a horse and carriage ... You can’t have one, you can’t have none, you can’t have one without the other”(Sinatra)

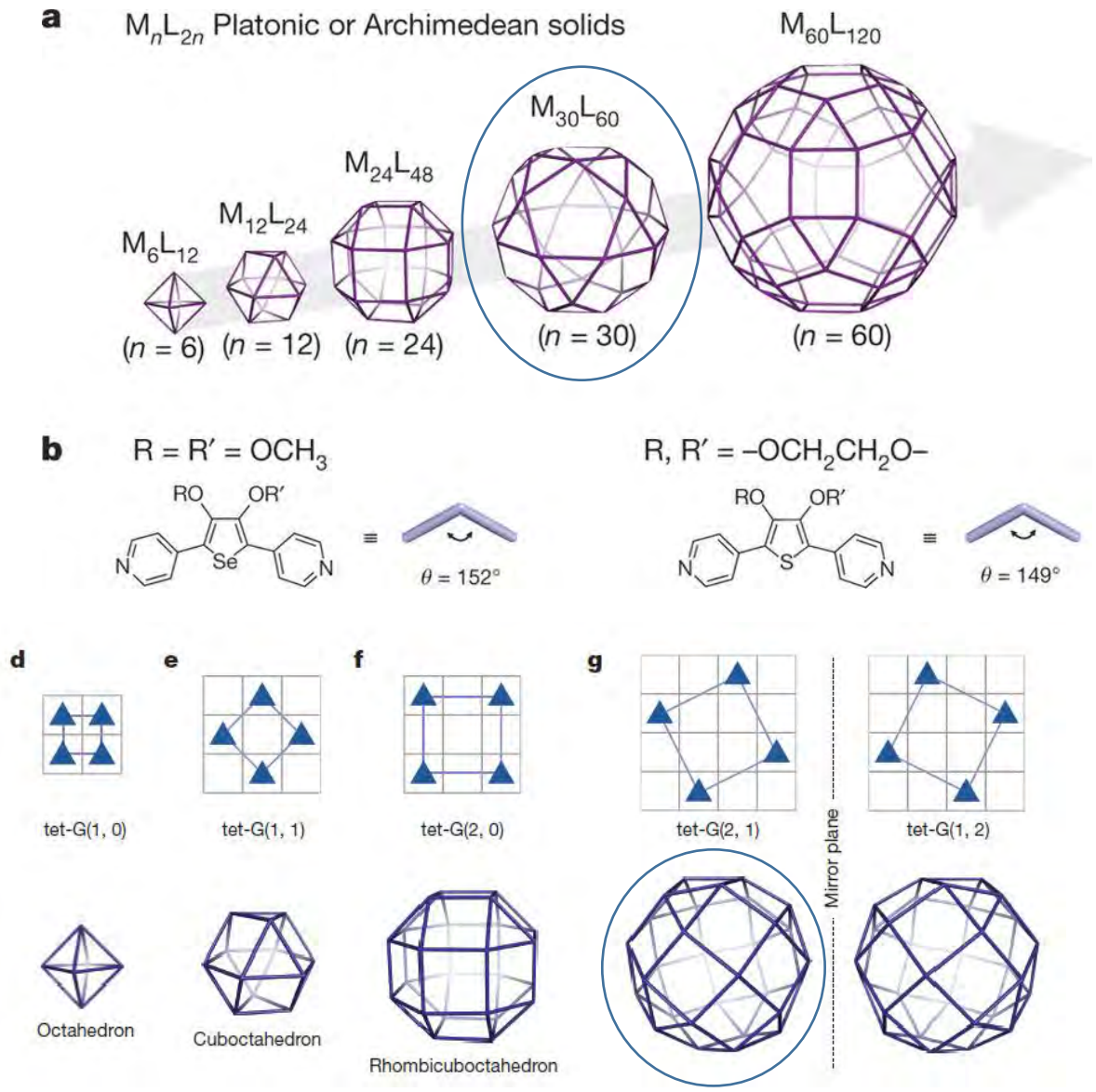
- We are interested in what can we encode in terms of emergent behaviour in simple building blocks



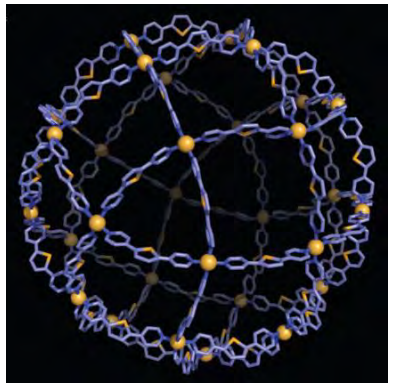
Dall-E (prompt: a sad triangular particle figure looking at an interaction between two spherical particles)



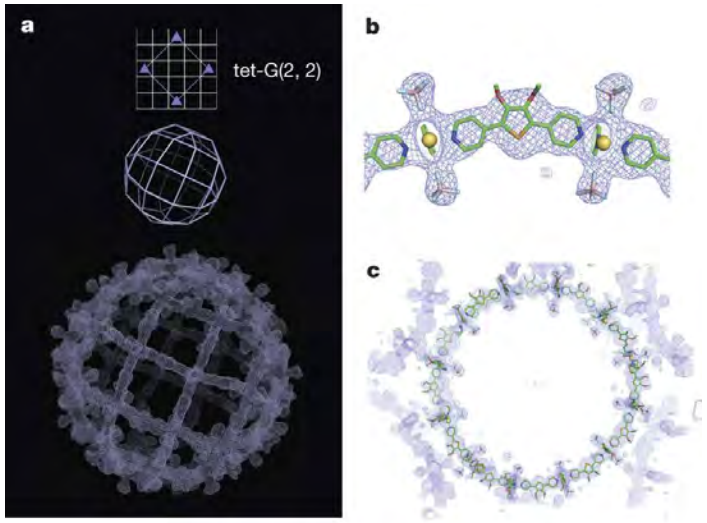
Molecular Goldberg cages

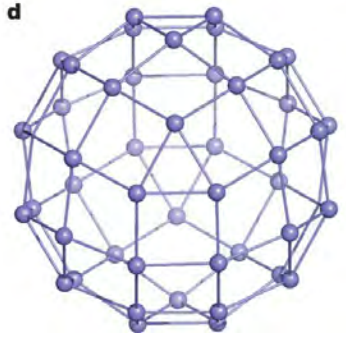


Fujita et al., Nature 540, 563-566 (2016)



30





48

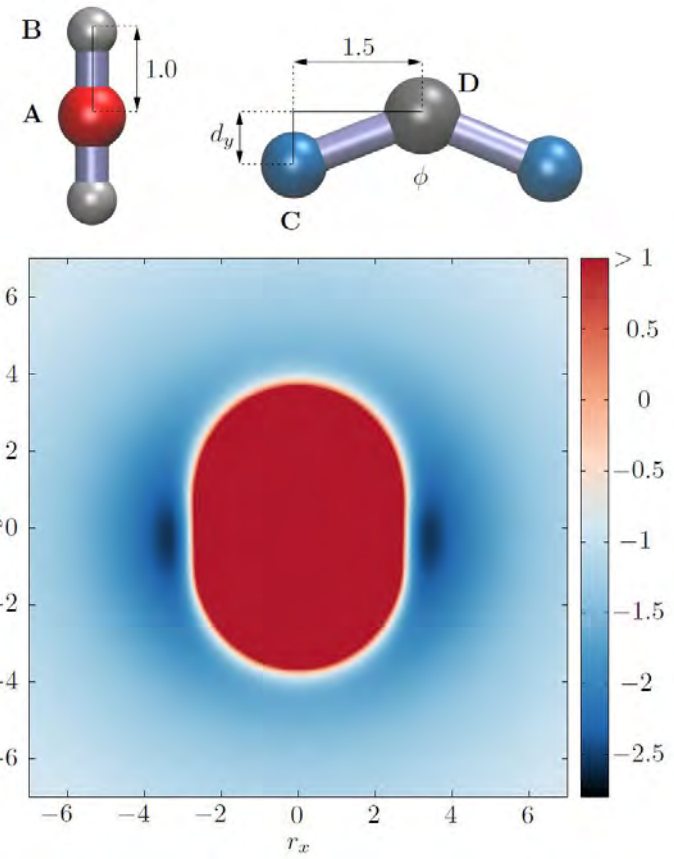
the largest molecular cage to date

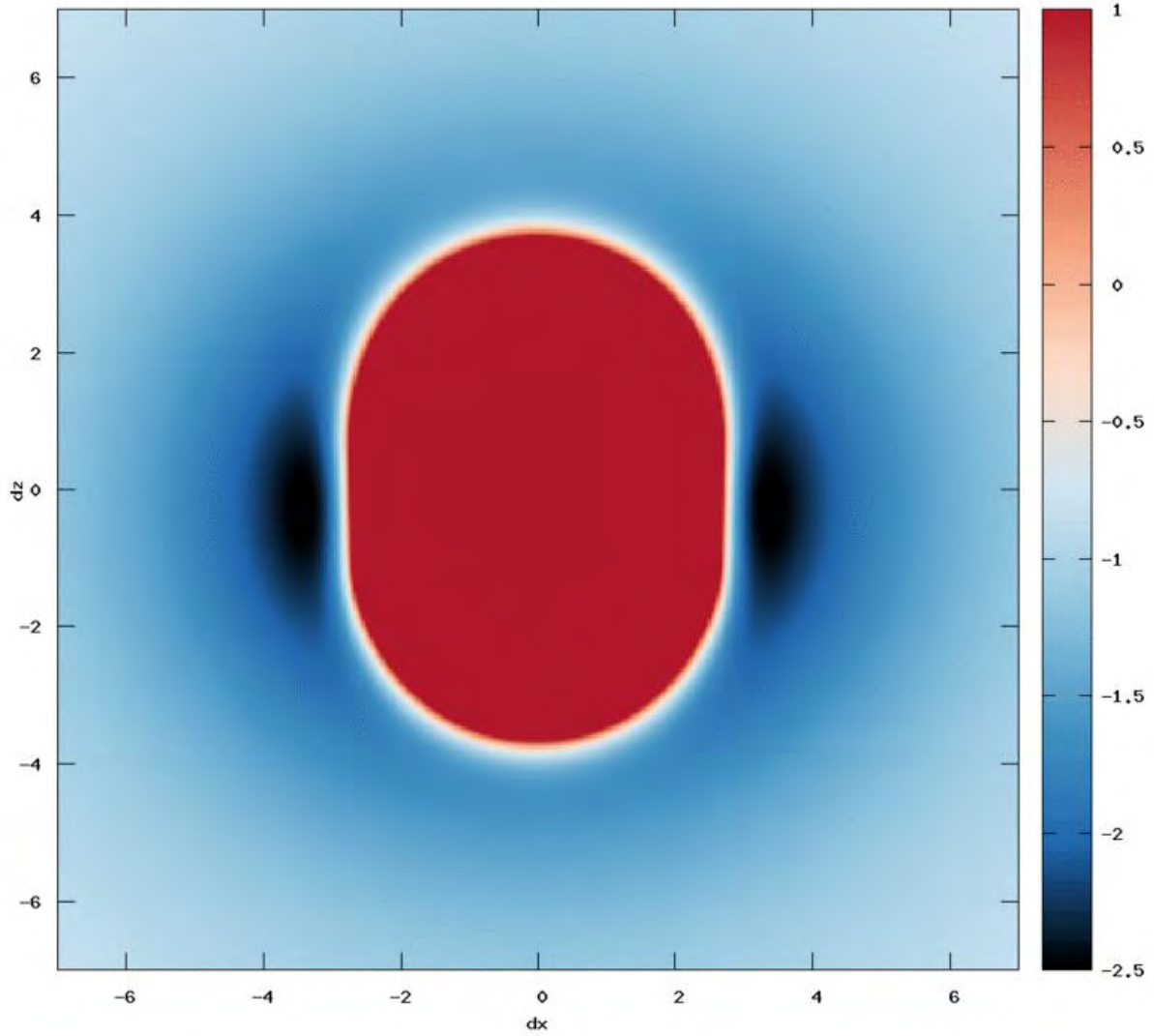
Hollow shells

- What are the minimal conditions to replicate self-assembly into hollow shells in a binary system?
- Particle shape depends on the anisotropy of interactions with its neighbours – it is not an absolute value
- Interaction is fairly long range, compared to particle size

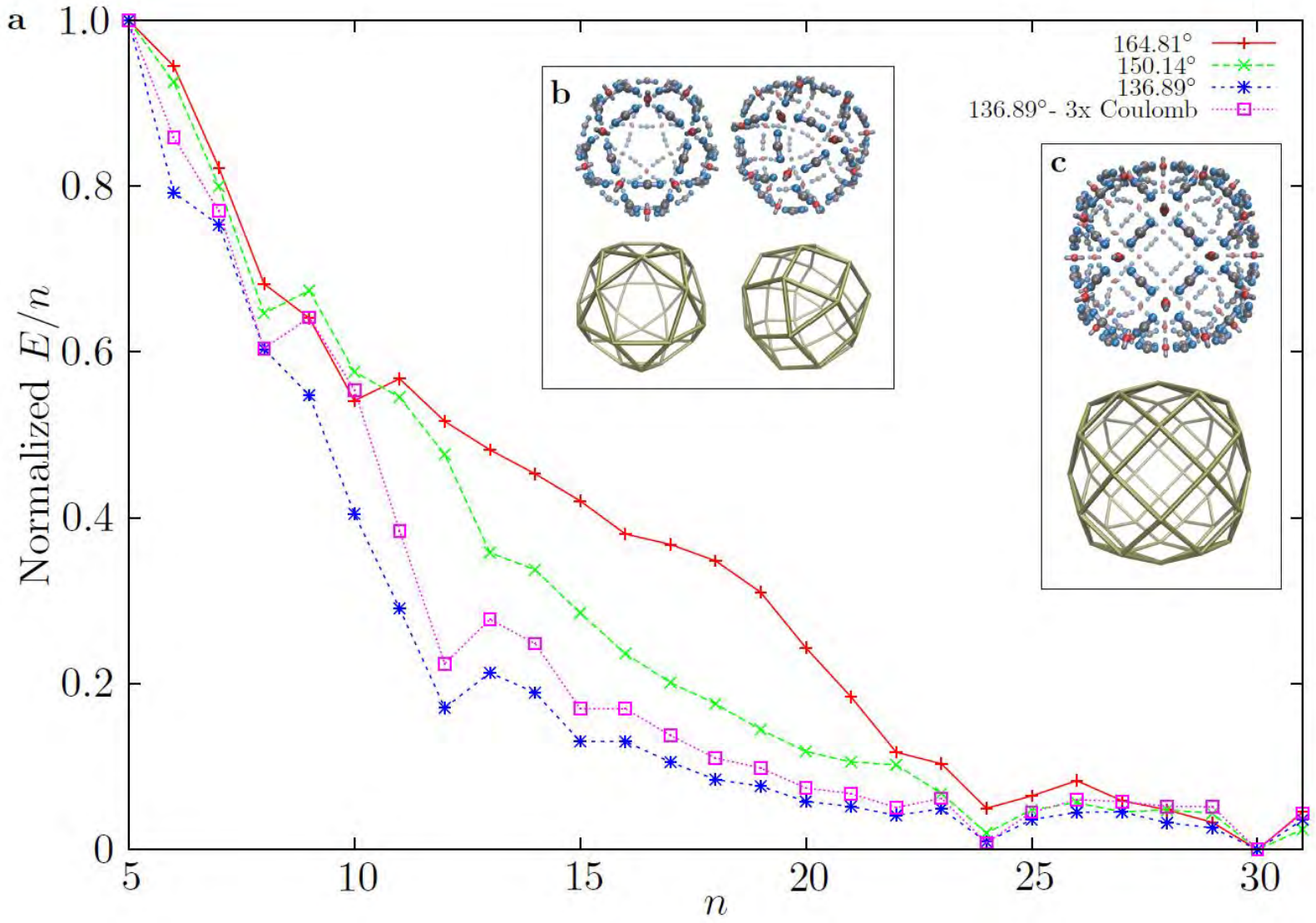
$$V = \sum_{i<j} \left(\frac{\varepsilon_{ij}^{\mathrm{rep}}}{r_{ij}^{12}} + \varepsilon^{\mathrm{Q}} \frac{q_i q_j}{r_{ij}} \right)$$

M **L**



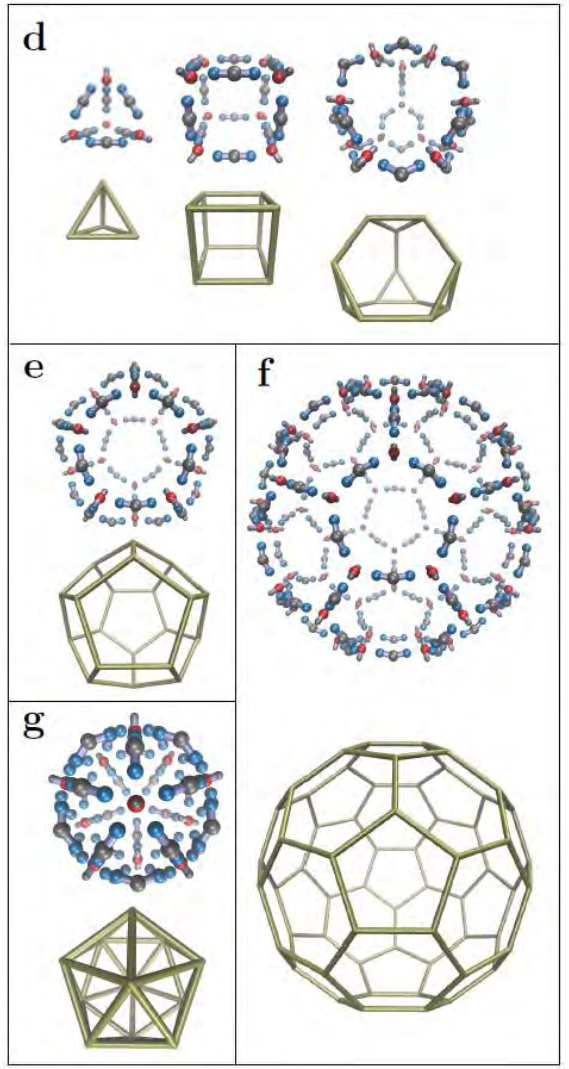


Global optimization

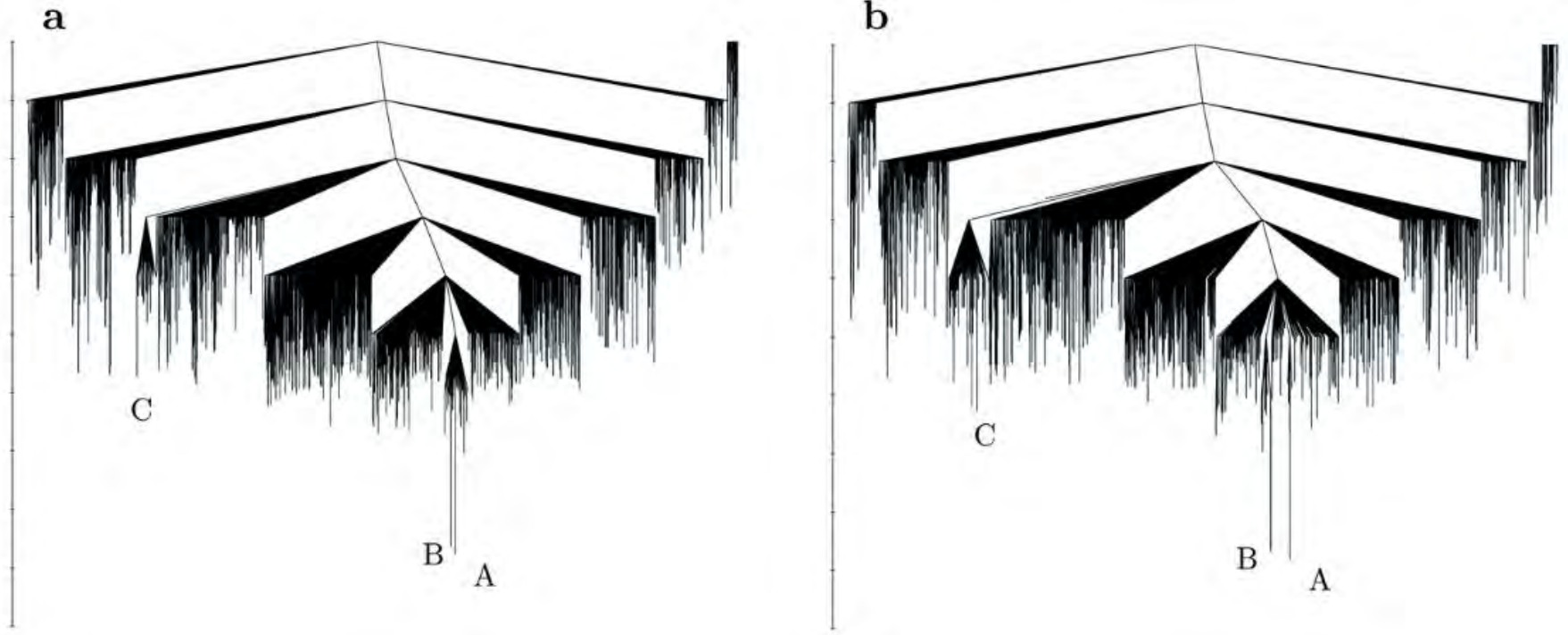


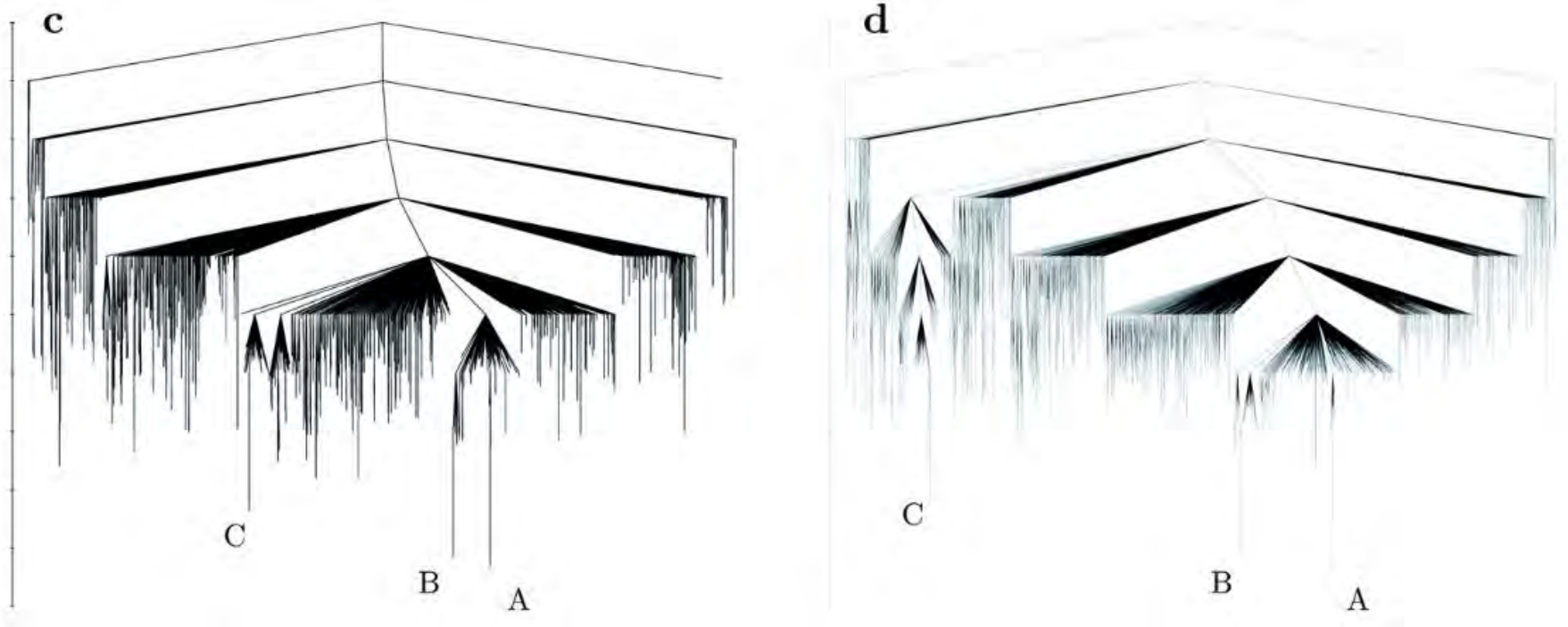
M_nL_{2n}

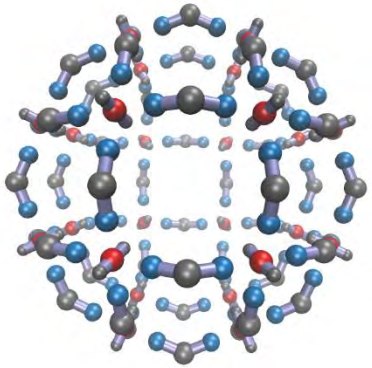
$M_{2x}L_{3x}$



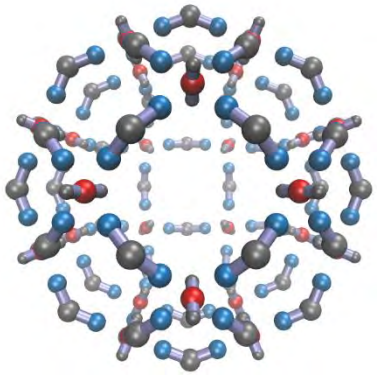
$M_{2x}L_{5x}$ $M_{2x}L_{3x}$





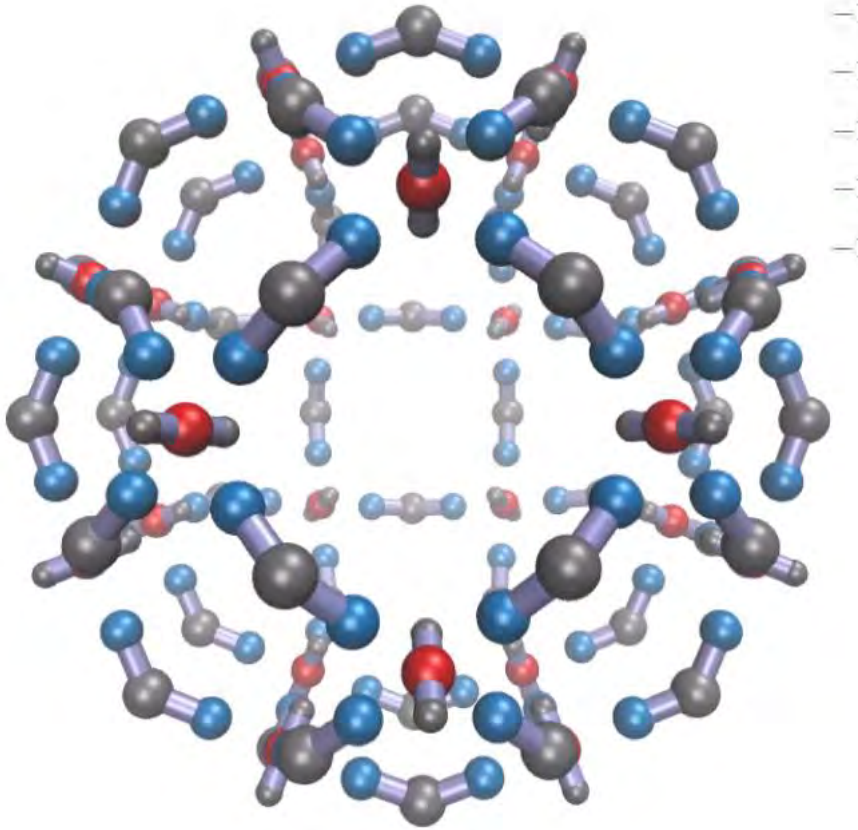


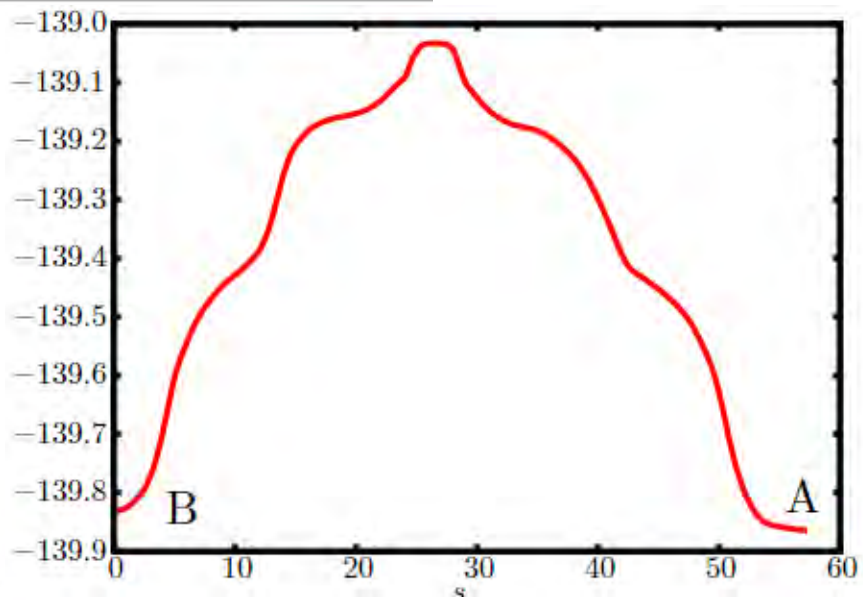
A
rhombicuboctahedron



B
pseudorhombicuboctahedron

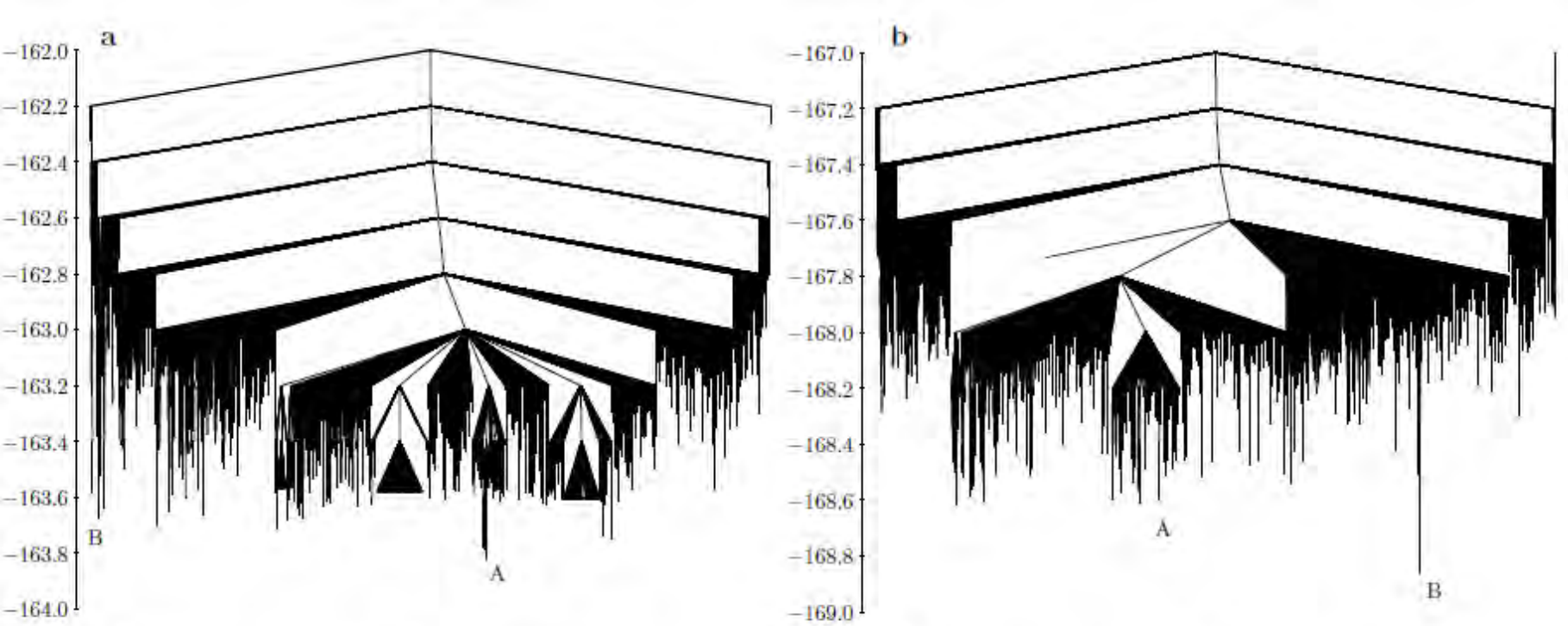
$M_{24}L_{48}$

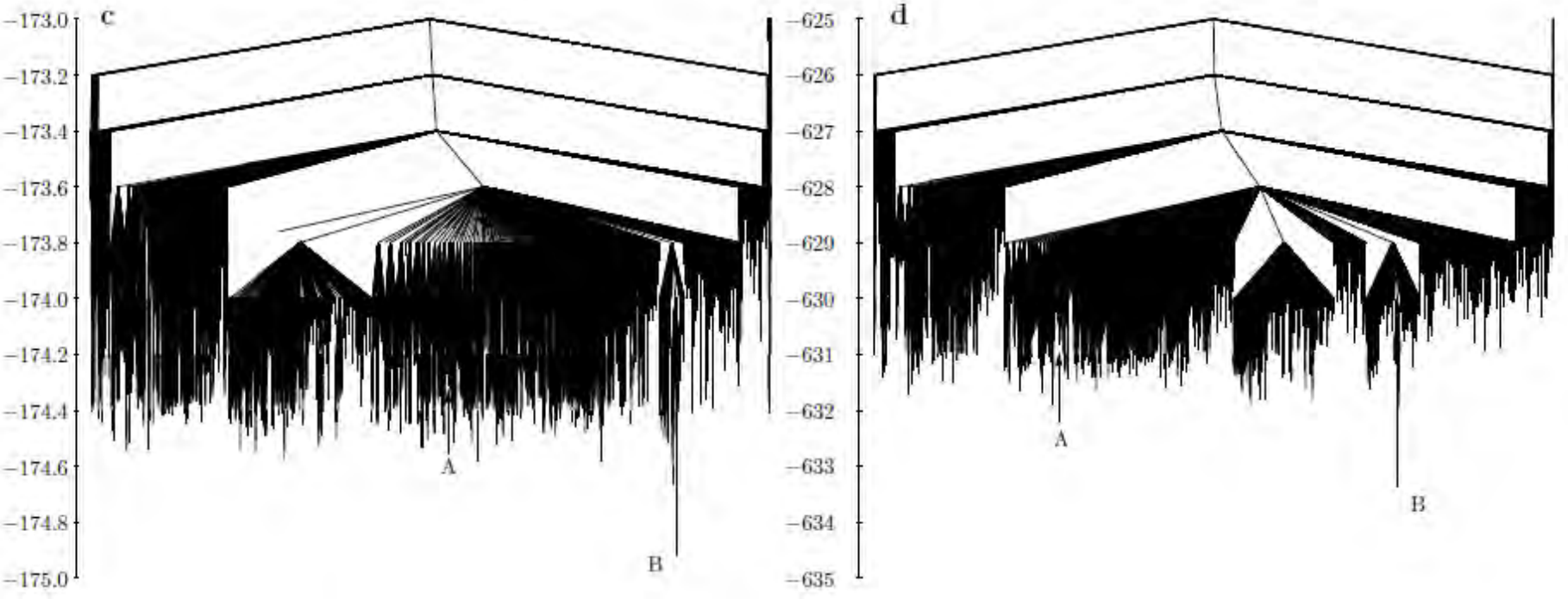


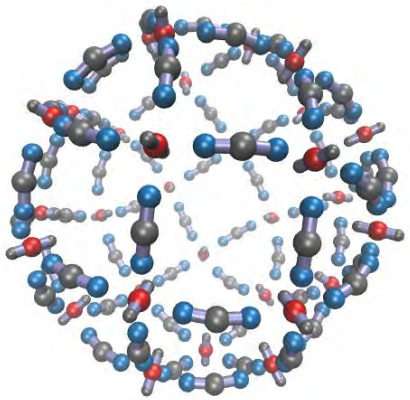


pseudorhombicuboctahedral to rhombicuboctahedral transition

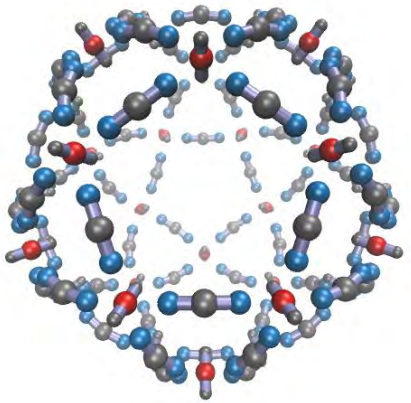
highly cooperative
single transition state rearrangement





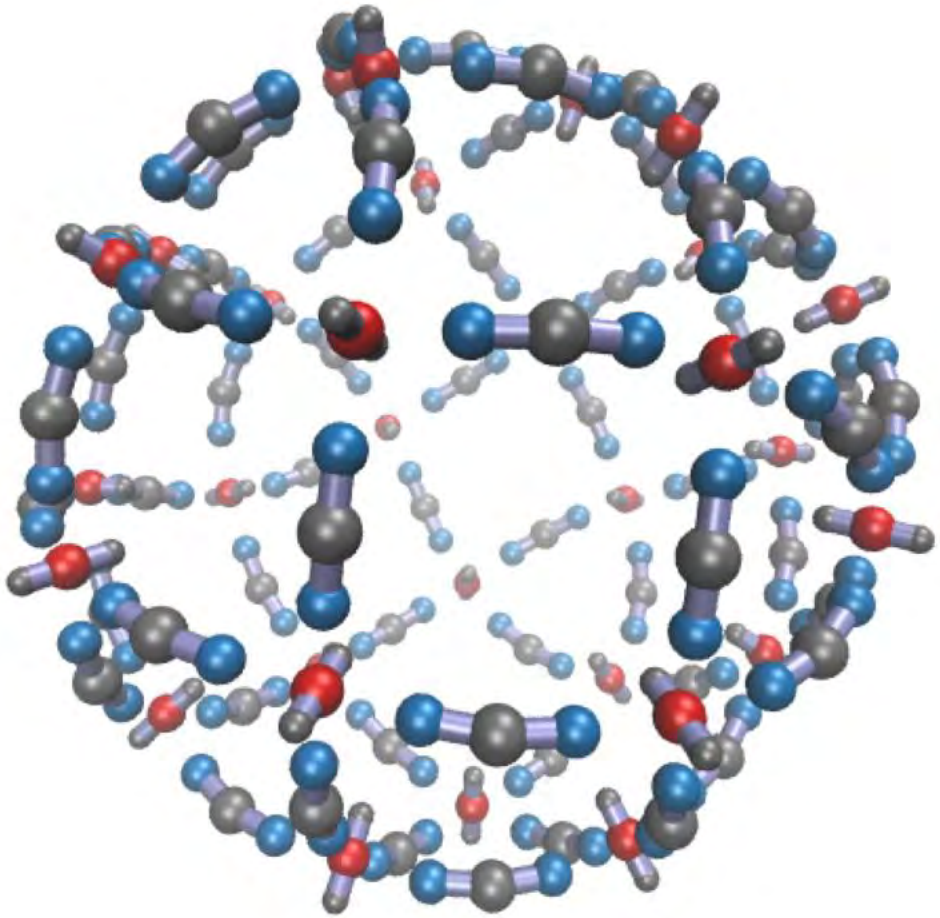


A
chiral tetravalent Goldberg



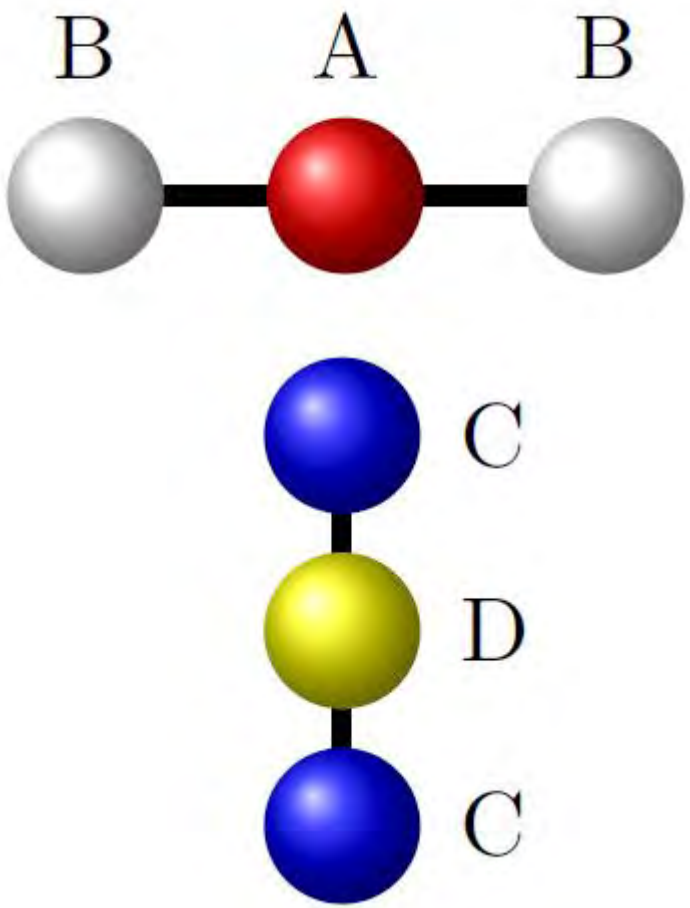
B
dodecahedral

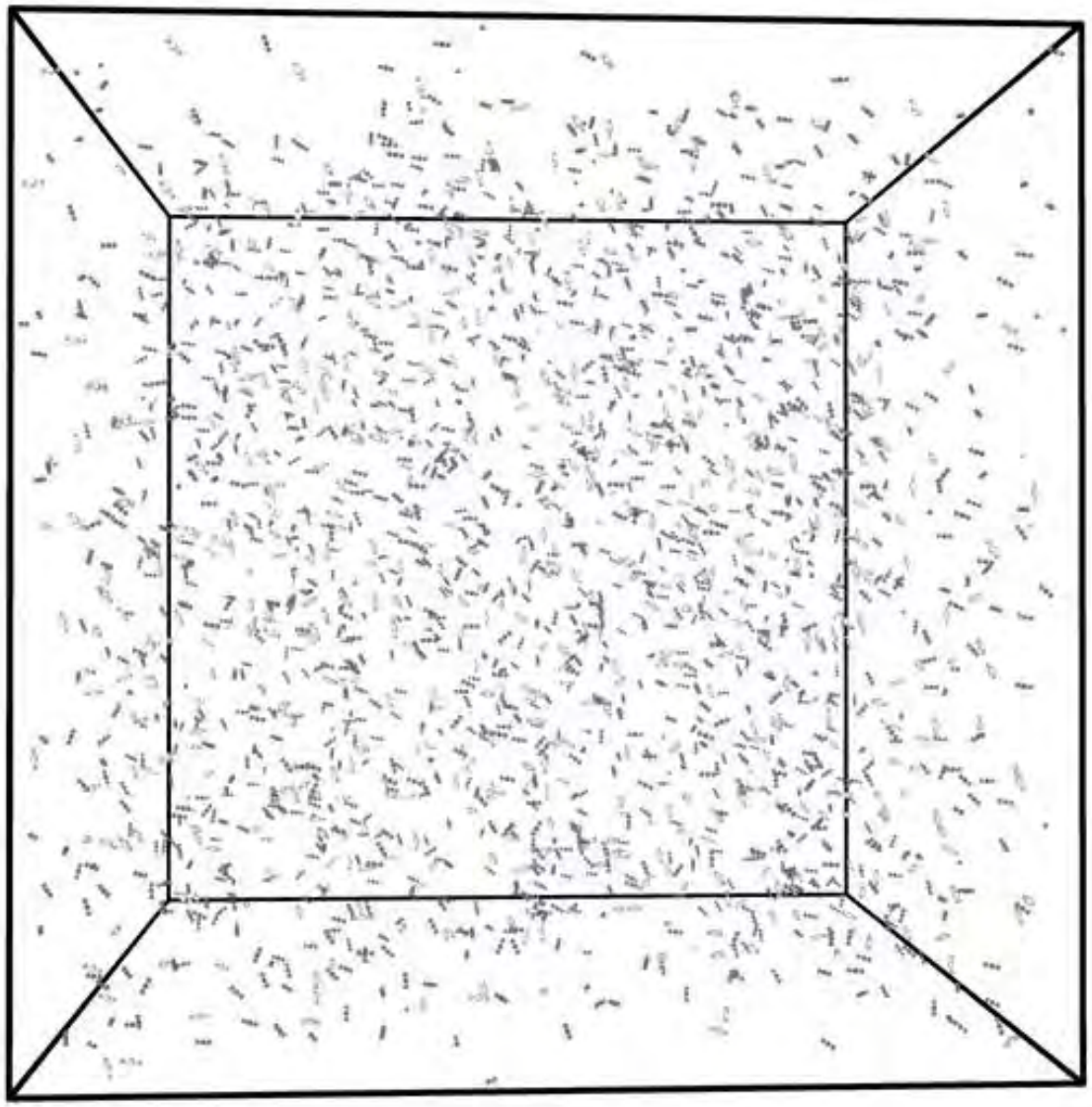
$M_{30}L_{60}$

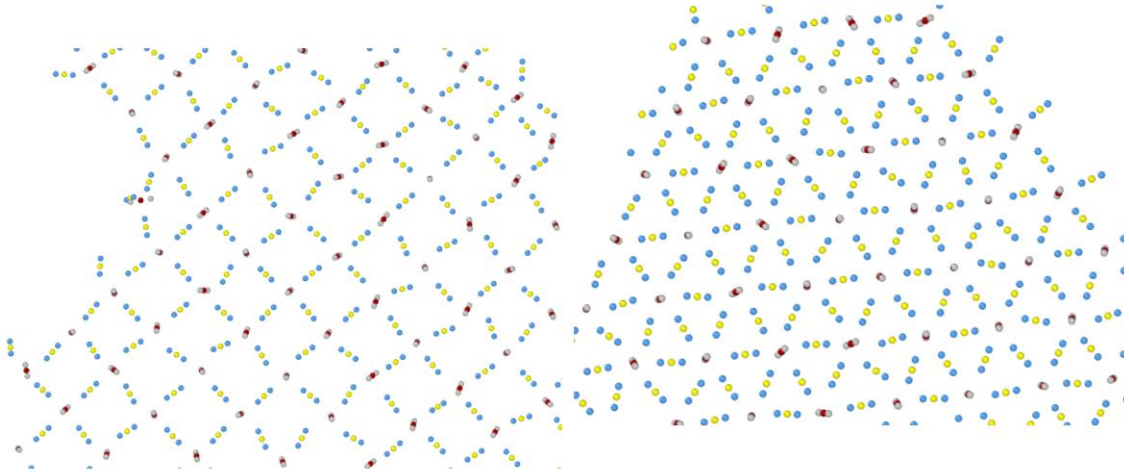


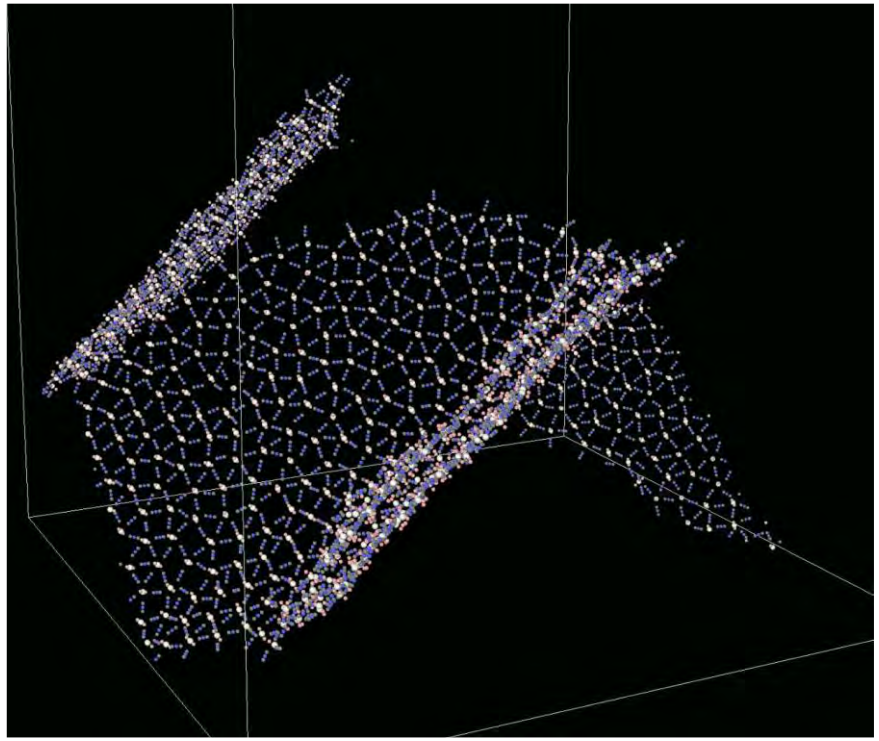
2D quasicrystalline approximants

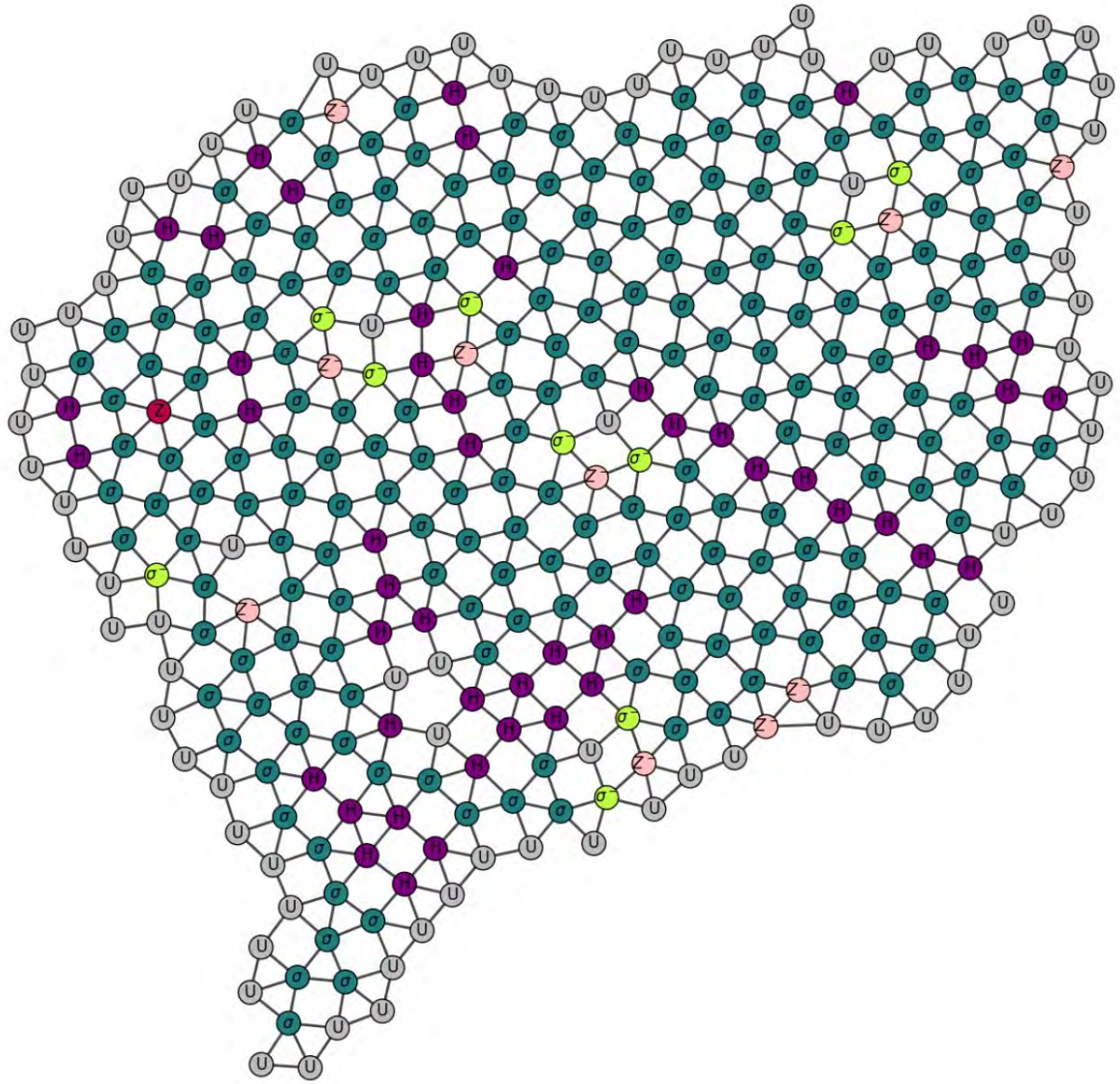
- linear building blocks
- two competing forces: planar vs fivefold coordination



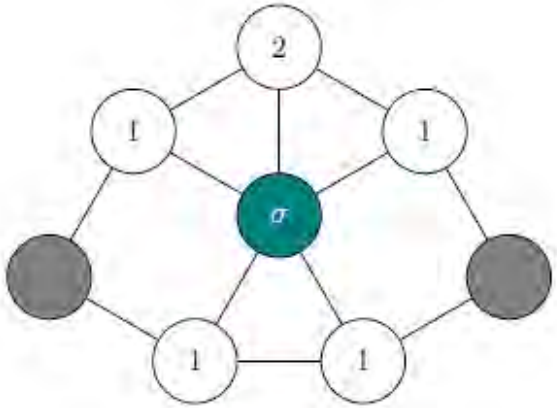








Two-layered structures: the first layer acts as a template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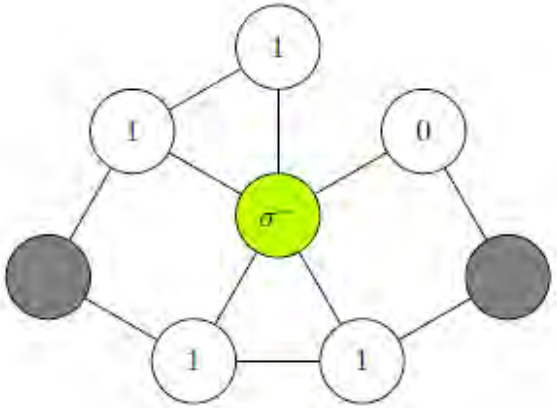
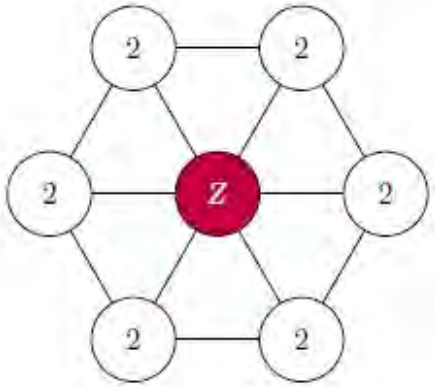
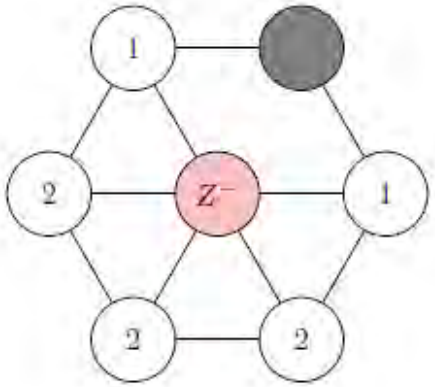
σ
1
1


1
1
0
σ^-
1
1


2
2
2
Z
2
2
2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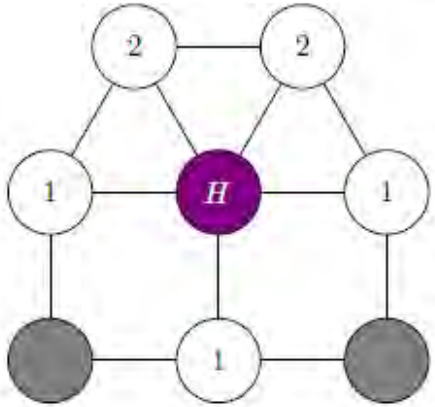
2
Z^-
1
2
2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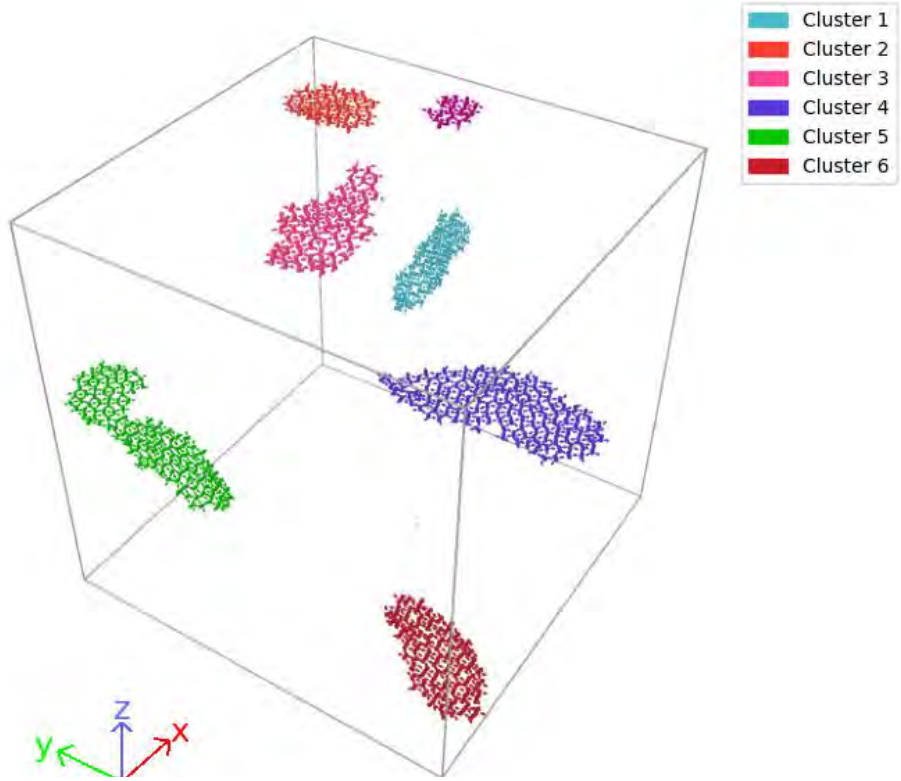
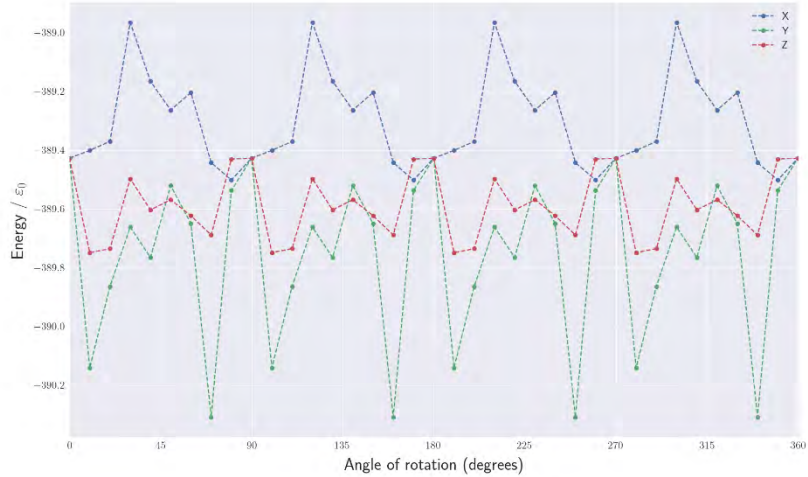
2
1
H
1
1


Cluster 1
Cluster 2
Cluster 3
Cluster 4
Cluster 5
Cluster 6
z
y
x


X
Y
Z
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−389.2
−389.4
−389.6
−389.8
−390.0
−390.2
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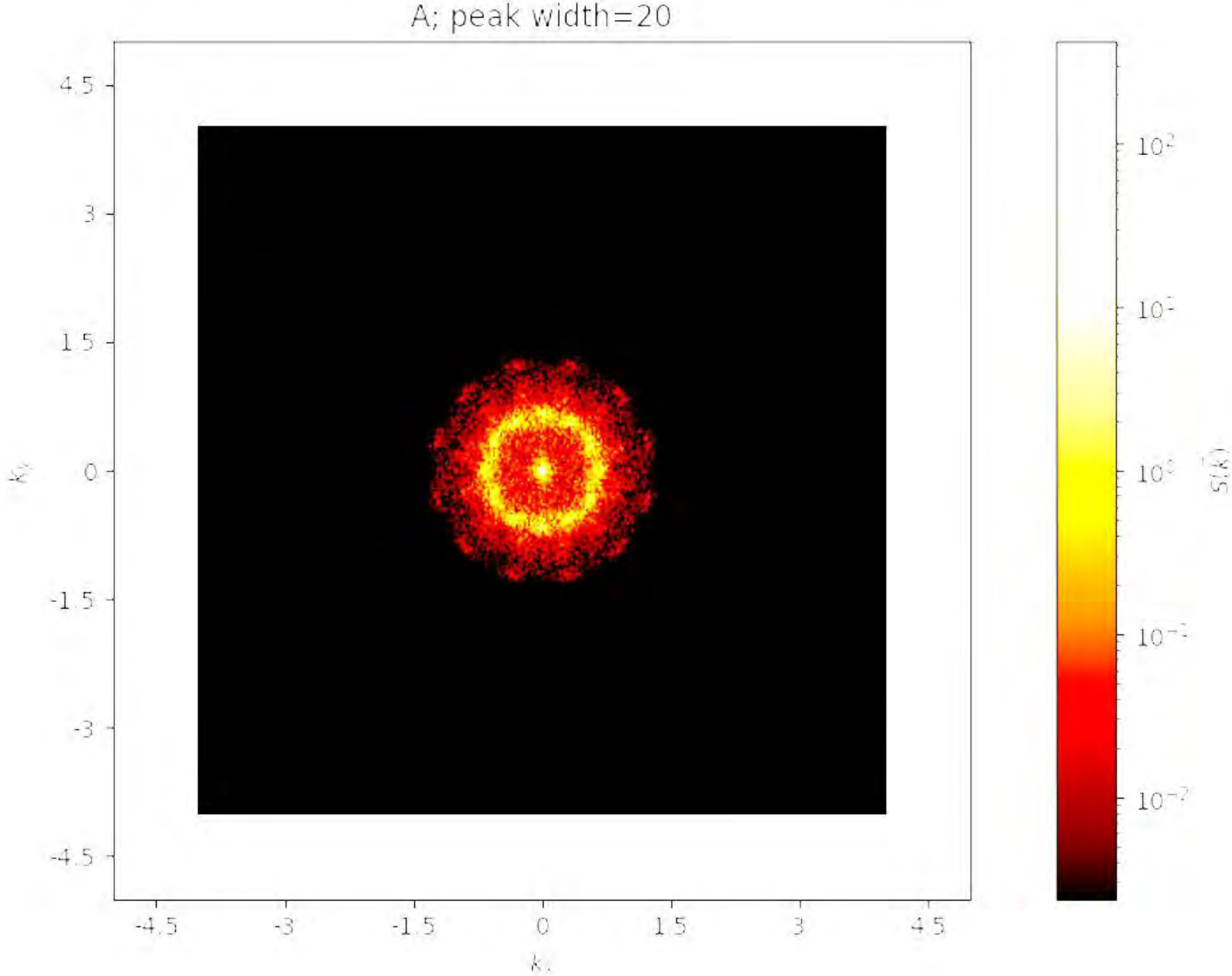
90
135
180
225
270
315
360
Angle of rotation (degrees)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-1.5
-3
-4.5
k_y
-4.5
-3
-1.5
0
1.5
3
4.5
k_x
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
$S(\vec{k})$

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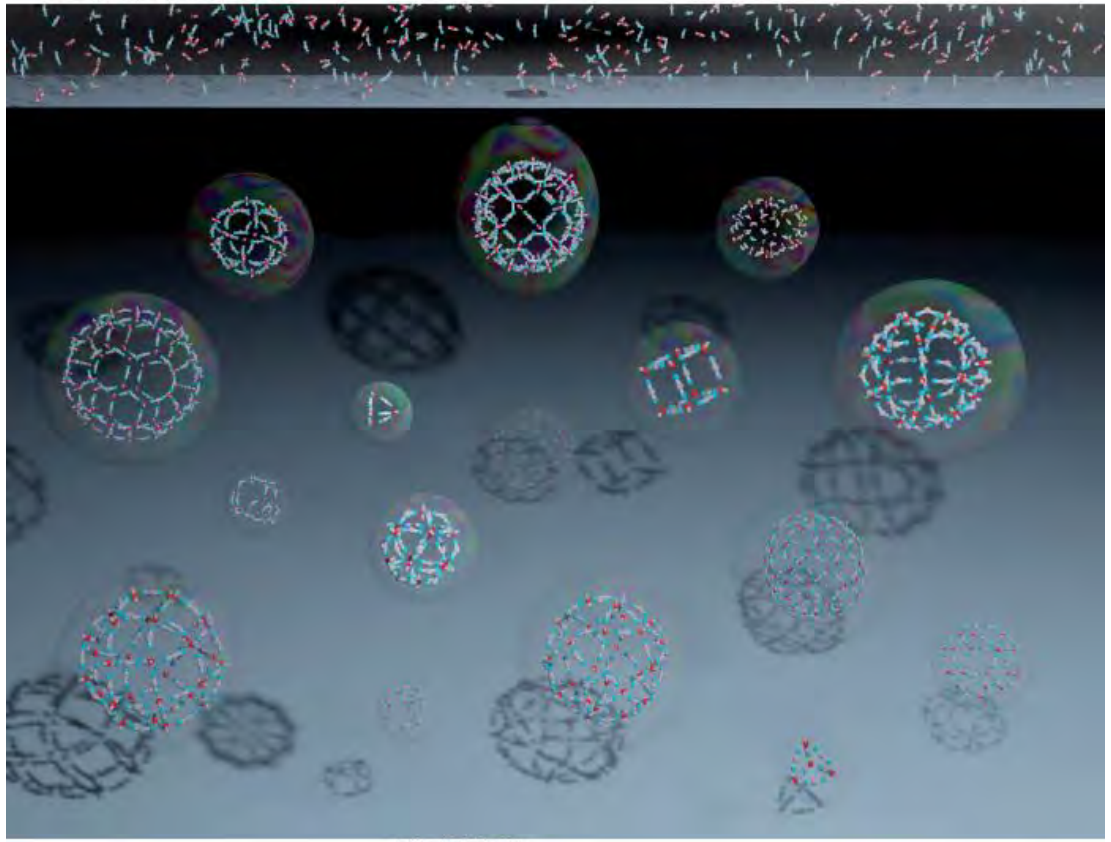

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ROYAL SOCIETY OF CHEMISTRY

PAPER
David J. Wales, Szilard N. Fejer *et al.*
Design of self-assembling mesoscopic Goldberg polyhedra

NCNST

I Horvath, DJ Wales, SN Fejer, Nanoscale Advances 4 (20), 4272-4278 (2022)