

**Supplementary information for the paper ‘Design of
self-assembling mesoscopic Goldberg polyhedra’[†]**

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Table I: ϵ^{rep} values for the excluded volume interaction between the different sites of the rigid building blocks for an alternative parameterisation that also yields highly symmetric closed shells as global minima for M_nL_{2n} clusters.

site	A	B	C	D
A	-	10^5	1	10^5
B	10^5	10^5	1	10^5
C	1	1	-	10^5
D	10^5	10^5	10^5	10^5

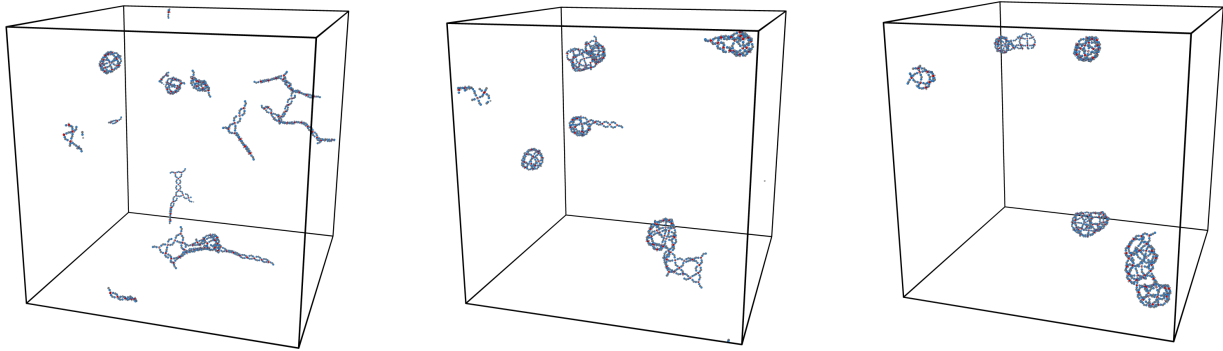


Figure S1: Snapshots along a trajectory with $kT = 0.01$ (150 M and 300 L particles), featuring long chains and head-tail structures as intermediates.

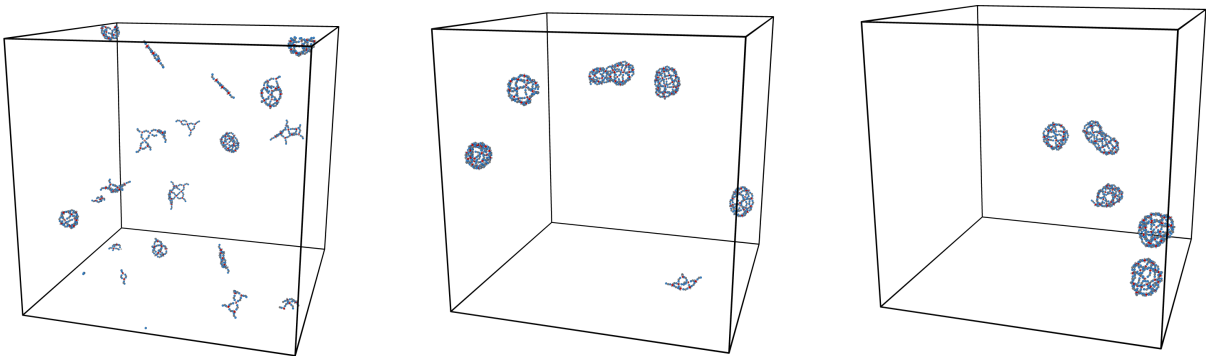


Figure S2: Snapshots along a trajectory with $kT = 0.02$ (150 M and 300 L particles).

Supplementary Movie 1: Change of the potential energy surface shown in Figure 1 as the ‘ligand’ particle is rotated in-plane around a vertical axis centered on site D.

Supplementary Movie 2: Highly cooperative low-energy single transition state rear-

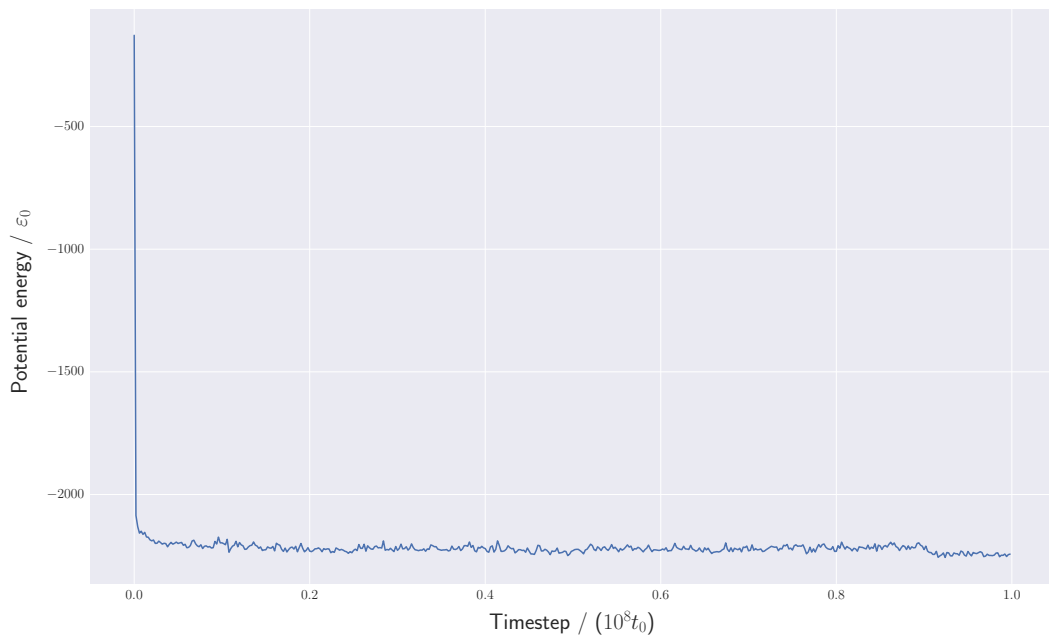
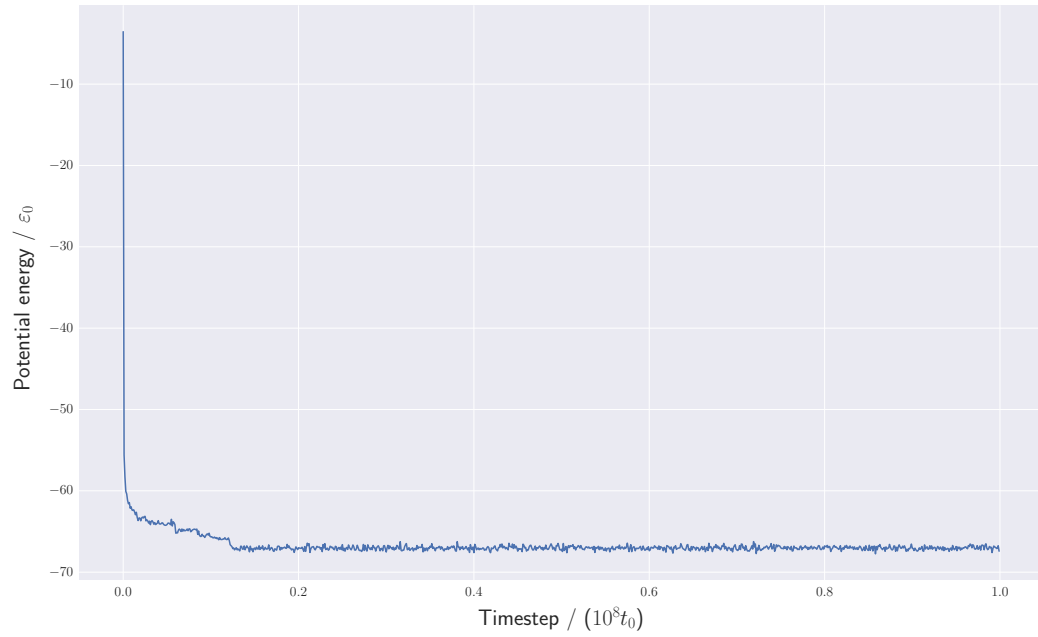


Figure S3: Energy profiles along trajectories for 12 M and 24 L particles ($kT = 0.02$, top), and 30 M and 60 L particles ($kT = 0.32$, bottom).

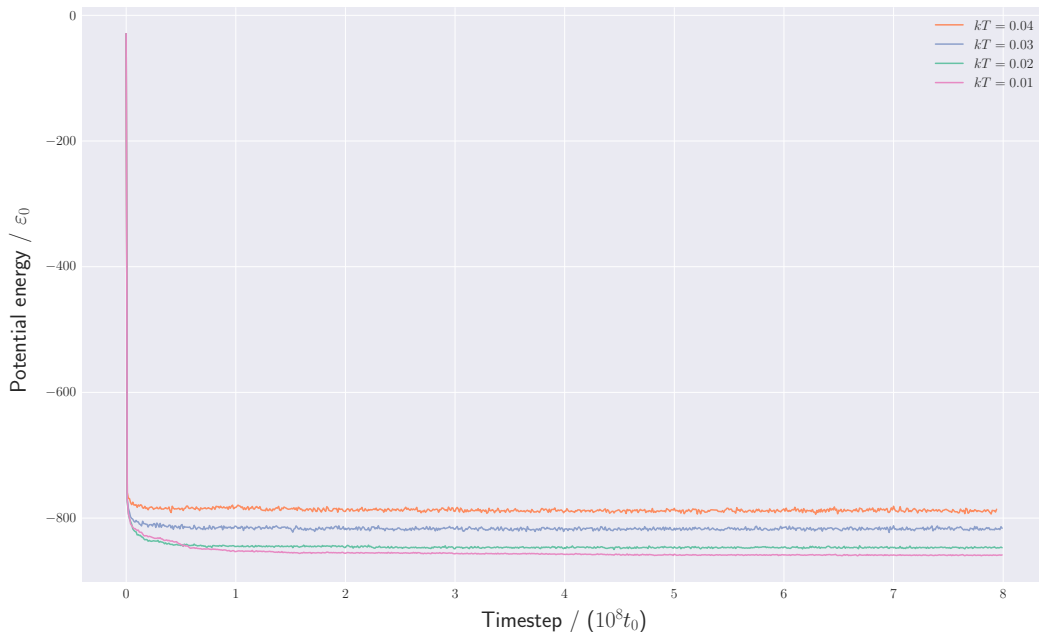


Figure S4: Energy profiles along trajectories for 150 M and 300 L particles at different temperatures.

rangement between a pseudorhombicuboctahedral structure and the rhombicuboctahedral global minimum (right panel of Figure 3).

Supplementary Movie 3: Lowest energy pathway for interconversion between the tetravalent Goldberg global minimum and the icosahedral structure shown in Figure 2b.

Supplementary Movie 4: Smoothed molecular dynamics trajectory for $M_{30}L_{60}$, showing the final steps of assembly into an icosahedral structure. This file can be downloaded from <https://szilard.ro/files/goldberg/supmovie4.avi>.

trajectories.zip: MD trajectories and their corresponding input and log files for 150 M and 300 L particles under four different temperatures ($kT=0.01, 0.02, 0.03, 0.04$), assembly of a cuboctahedral $M_{12}L_{24}$ shell, assembly of an icosahedral $M_{30}L_{60}$ shell. This file can be downloaded from <https://szilard.ro/files/goldberg/trajectories.zip>. The scripts needed to run these simulations can be downloaded from <https://github.com/horvathi94/hoomd-lab>.

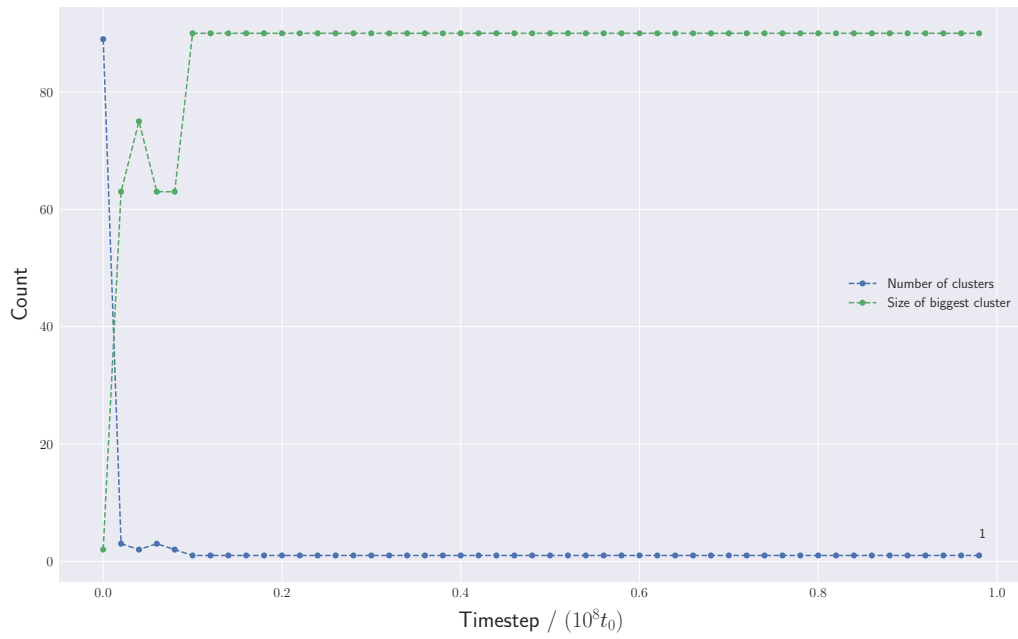
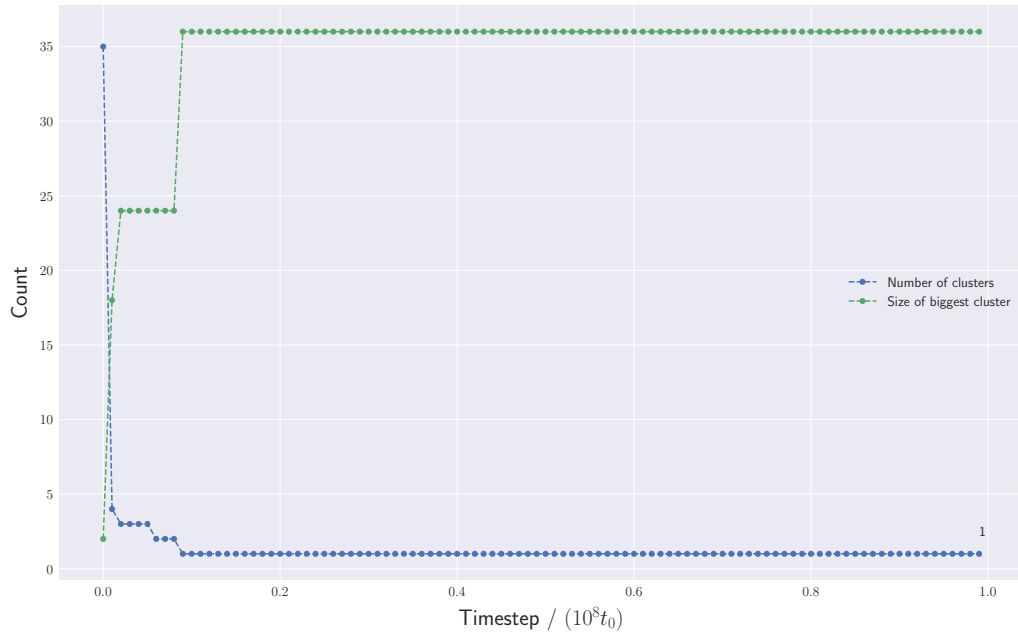


Figure S5: Size of the largest cluster and number of distinct clusters for $M_{12}L_{24}$ (top) and $M_{30}L_{60}$ (bottom), for the trajectories shown in Figure S3.

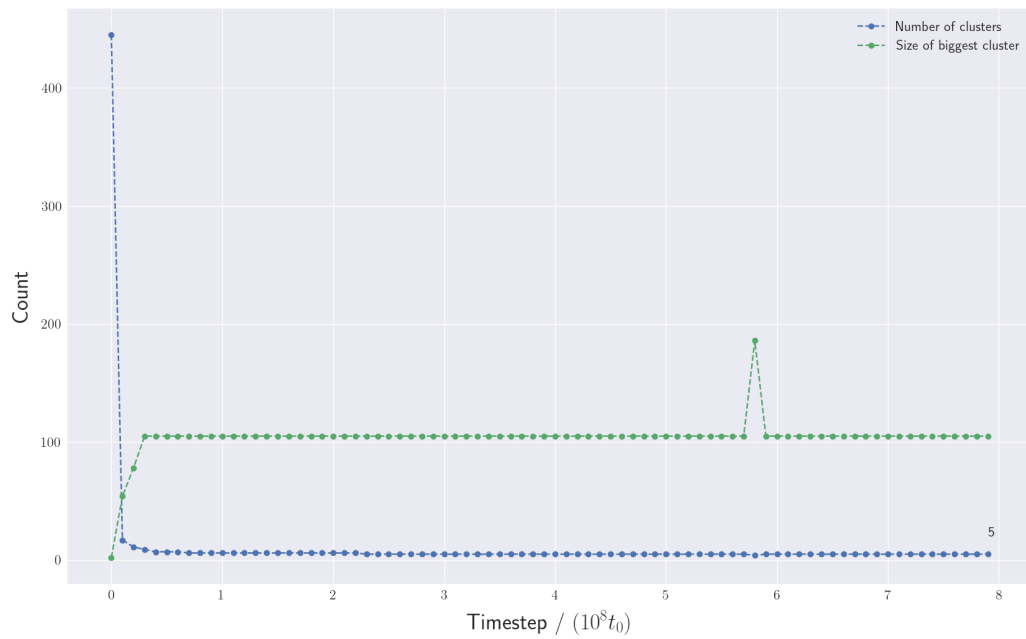
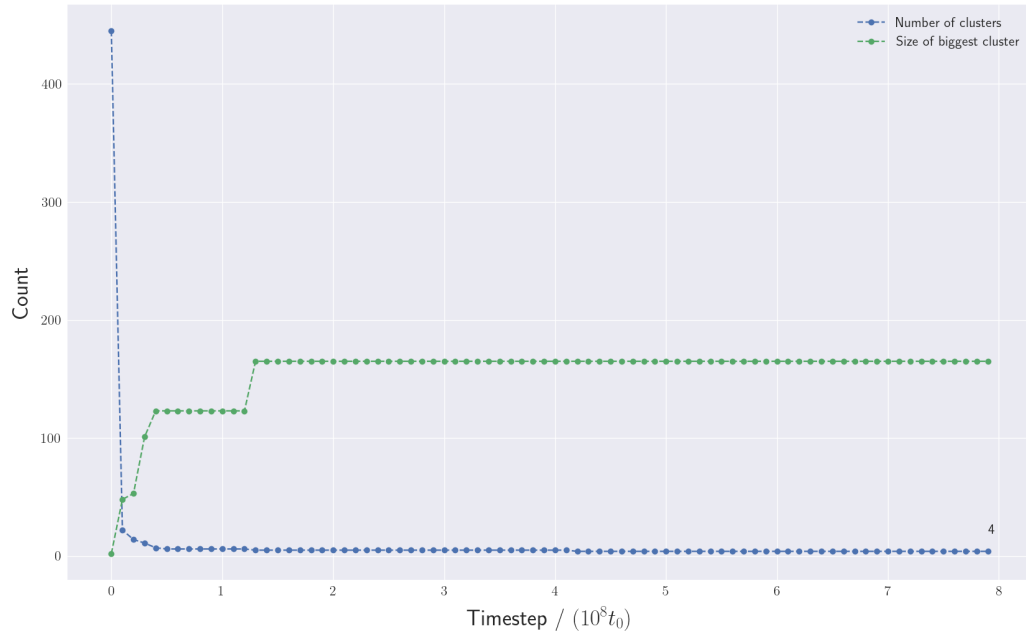


Figure S6: Size of the largest cluster and number of distinct clusters for $M_{150}L_{300}$ at $kT = 0.01$ (top) and $kT = 0.02$ (bottom), for the trajectories shown in Figure S4.

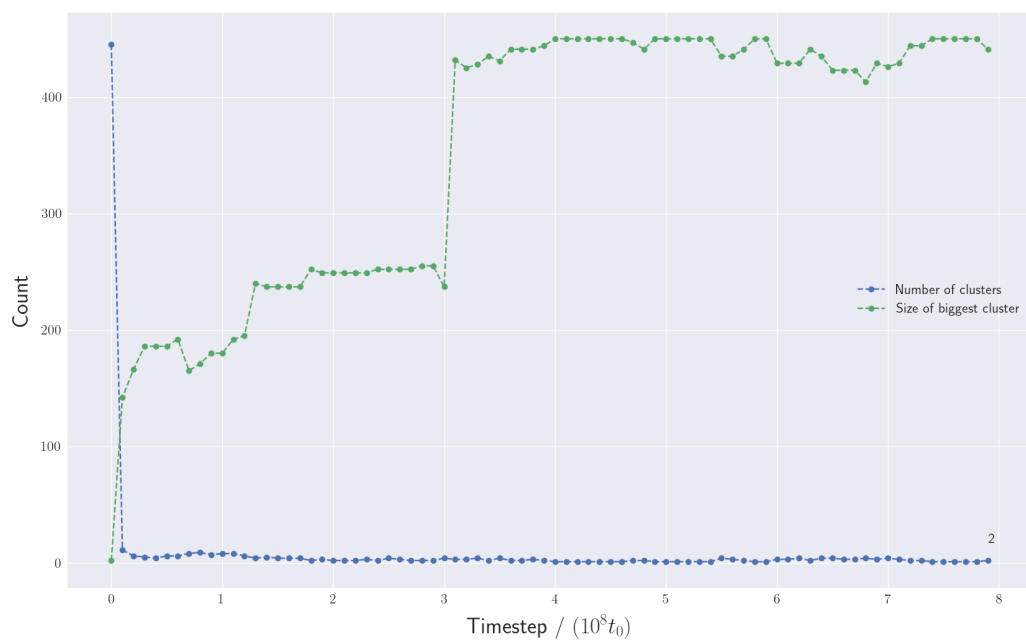
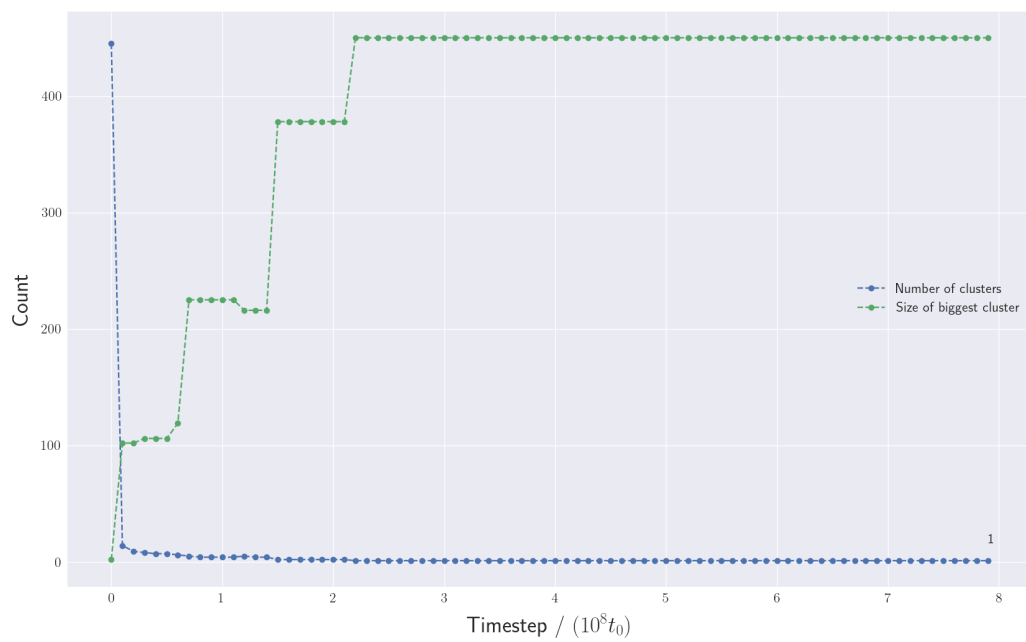


Figure S7: Size of the largest cluster and number of distinct clusters for $M_{150}L_{300}$ at $kT = 0.03$ (top) and $kT = 0.04$ (bottom), for the trajectories shown in Figure S4.