## Supracolloidal reconfigurable polyhedra via hierarchical self-assembly

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## **Supplementary Results**

In Table S1, we present some geometric features for the set of *convex snub polyhedra*.<sup>1</sup> It is evident that the snub tetrahedron is the smallest in this series. We note here that the snub tetrahedron is an icosahedron for having twenty faces; however, we have preferred to use the name 'snub tetrahedron' when it is of tetrahedral symmetry as it is then informative of the symmetry of the structure it refers to.

Table S1: A comparison of the geometric features of convex snub polyhedra. Here V is the number of vertices, F is the number of faces and E denotes the number of edges.

Polyhedron	Symmetry	V	F	Е
Snub tetrahedron	Т	12	20	30
Snub cube	0	24	38	60
Snub dodecahedron	Ι	60	92	150

Table S2: A comparison of the anti-parallel arrangements of the dipoles in two neighbouring secondary building blocks of two low-lying minima for N = 12 charge-stabilised colloidal magnetic particles, where  $\theta = 0^{\circ}$ .  $\phi$  is the angle between the dipole vectors,  $R_{ij}$  is the distance between the centers of the spherical colloidal particles,  $r_{ij}$  is the distance between the point-dipoles and  $E_{ap}$  is the potential energy contribution arising from the two dipoles.

Minimum	$\phi$	$R_{ij}/\sigma$	$r_{ij}/\sigma$	$E_{ap}/\varepsilon_{ m Y}$
The bowl structure	172.8	1.02	0.8	-7.66
The spherical structure	164.8	1.05	0.86	-6.04

Table S3: A comparison of the anti-parallel arrangements of the dipoles in two neighbouring secondary building blocks of two low-lying minima for N = 12 charge-stabilised colloidal magnetic particles, where  $\theta = 10^{\circ}$ .  $\phi$  is the angle between the dipole vectors,  $R_{ij}$  is the distance between the centers of the spherical colloidal particles,  $r_{ij}$  is the distance between the point-dipoles and  $E_{ap}$  is the potential energy contribution arising from the two dipoles.

Minimum	φ	$R_{ij}/\sigma$	$r_{ij}/\sigma$	$E_{ap}/\epsilon_{ m Y}$
The spherical structure	166.3	1.07	0.94	-4.74
The bowl structure	174.7	1.05	0.92	-5.11



Figure S1: The triangular subunits formed as the secondary building blocks in the hierarchical self-assembly route to hollow spherical structures. (a) The triangular subunit for  $\theta = 0^{\circ}$ ; (b) the triangular subunit for  $\theta = 10^{\circ}$ .



Figure S2: The competing structures, characterised as the low-lying minima on the energy landscape, for N = 12 charge-stabilised magnetic colloids. Representative examples of the anti-parallel arrangement of the dipoles in neighbouring secondary building blocks are clearly shown here and the dipoles concerned are highlighted in yellow. (a) The ground state structure for  $\theta = 0^{\circ}$ ; (b) the ground state structure for  $\theta = 10^{\circ}$ . Here  $\theta$  defines the angle between the direction of the dipole and the radial shift.



Figure S3: The two structures characterised as the low lying minima on the energy landscape for N = 15 charge-stabilised colloidal magnetic particles, where  $\theta = 10^{\circ}$ . (a) The ground state structure, which consisted of the snub tetrahedron plus an additional triangular subunit; (b) the bowl structure, a low lying minimum, with an emergent five-fold rotational symmetry.

## Movies

- Movie 1: The dominant pathway characterised for the self-assembly into the tubular anti-prismatic ground state structure for N = 16 charge-stabilised magnetic colloidal particles where  $\theta = 90^{\circ}$  and  $\alpha = 0.3$ , starting from a high-energy, relatively disordered local minimum. The secondary building blocks are colour-coded distinctly as they are formed for visual aid.
- Movie 2: The dominant pathway characterised for the self-assembly into the ground state structure, topologically equivalent to the snub tetrahedron, for N = 12 charge-stabilised magnetic colloidal particles where  $\theta = 10^{\circ}$  and  $\alpha = 0.6$ , starting from a high-energy, relatively disordered local minimum. The secondary building blocks are colour-coded distinctly as they are formed for visual aid.

## References

[1] P. R. Cromwell, Polyhedra, Cambridge University Press, Cambridge, 1997.