Supplementary information for the manuscript 'Design of a Kagome lattice from soft anisotropic particles'

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I.   RATIONALE BEHIND CHOOSING BUILDING BLOCK PARAMETERS

Given that experimental Kagome lattices from triblock Janus particles are stabilized by entropy, we have investigated in this paper the theoretical possibility of creating *energetically* stabilized Kagome lattices. In order to achieve this, we need longer range attractive interactions than the van der Waals interactions arising between the hydrophobic patches of colloidal building blocks. Instead of using an explicit range parameter, we decided to decrease the default interaction range of PY spheres (corresponding to isotropic Lennard-Jones interaction for a sphere with a radius of 0.5 length units). This is possible by changing two parameters in the PY potential: increasing the particle radius, and increasing isotropically the difference between the attractive and repulsive semiaxes. The latter also has an effect of increasing the well depth.

Additionally, the particle should be repulsive for side-by-side interactions. We used the simplest building block geometries that would give us a patch half opening angle close to 60° (the theoretical maximum allowing for only two bonds per patch for spherical particles confined into two dimensions, without considering additional effects such as equilibrium separation, interaction strength and anisotropy), in order to maintain the experimental patch geometry of the particle. We achieved this by adding to the building block an oblate, repulsive ellipsoid with an anisotropy ratio of 0.6, which disfavours side-by-side geometries.

We chose the longest semiaxis to correspond with our previous model for Janus building blocks (1.5 length units) [1]. The shorter semiaxis length became 0.9, and the radius for ellipsoid B was chosen to be the arithmetic mean of the two semiaxes of ellipsoid A. The patch half opening angle became 56° with these parameters.

II.   DETAILS OF THE SCALING FOR SEDIMENTATION FORCES

In order to scale the sedimentation forces experienced by a micrometre sized triblock Janus particle to the absolute units used in the paper, we need the following data:

1. apparent weight of the particle (m_{app}, arising from the density mismatch between that of the particle and water (assumed to be on the order of $0.1\,\mathrm{g/cm}^3$) and the particle volume ($1\,\mu\mathrm{m}$ diameter, $5.23 \cdot 10^{-13}\mathrm{cm}^3$);

2. scaling of the energies, assuming the interparticle interaction energy to be $10\,k_BT$ at

298 K. This quantity is $3.17\,\epsilon_0$ in our units. $k_B T = 4.11 \cdot 10^{-21}\,\mathrm{J} = 0.317\,\epsilon_0$.

3. scaling of the particle diameter: $1\,\mu\mathrm{m}$ corresponds to 2.4 length units. We took as a reference the diameter of the attractive sphere in our model.

The energy gradient due to sedimentation will be $\epsilon^{\mathrm{g}} = m_{\mathrm{app}} \cdot g$, where g is the gravitational constant $(9.81\,\mathrm{m/s^2})$. $\epsilon^{\mathrm{g}} = 5.13 \cdot 10^{-22}\,\mathrm{J}/\mu\mathrm{m}$. ϵ^{g} in reduced units will be therefore

$$\epsilon^{\mathrm{g}} = 5.13 \cdot 10^{-22}\,\mathrm{J}/\mu\mathrm{m} \cdot 0.317\,\epsilon_0/(4.11 \cdot 10^{-21}\,\mathrm{J}) \cdot 1\mu\mathrm{m}/(2.4\,\mathrm{l_0}) = 0.0165\,\epsilon_0/\mathrm{l_0}. \qquad (1)$$

It is important to note that sedimentation forces can vary greatly under different experimental settings, by varying the density of the solvent or the particles (e.g. using metallic coatings of different thickness, or that of the gravitational constant (microgravity or adding centrifugal forces). The value calculated here is therefore an order of magnitude estimate for general experimental settings on micrometre-sized particles in an aqueous solution.

III. SUPPLEMENTARY MOVIE 1 LEGEND

Movie for the fastest pathway between a linear chain and a Kagome structure for $N = 12$ particles, with no gravity effects considered.

IV. SUPPLEMENTARY MOVIE 2 LEGEND

Fastest pathway from a low-energy kinetic trap to a Kagome structure and back, for $N = 26$ particles, with no gravity effects considered. The kinetic trap contains a five-membered ring, which introduces curvature in the lattice.

V. SUPPLEMENTARY MOVIE 3 LEGEND

Fastest pathway from a low-energy kinetic trap to a Kagome structure and back, for $N = 26$ particles, with the largest gravity effects considered. The repulsive plane is shown in grey. The five-membered and seven-membered rings cannot distort the planar geometry because of the gravity, and all rearrangements happen in plane.
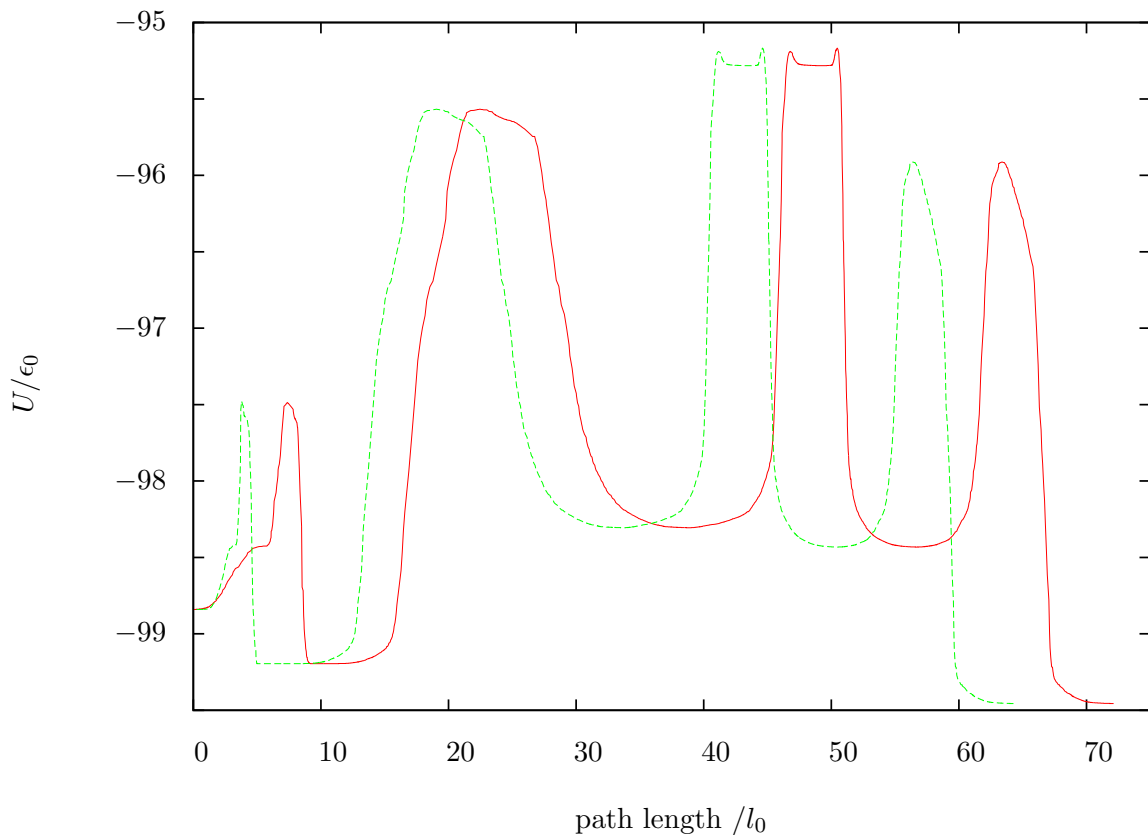
FIG. 1: Fastest pathway between a low-energy kinetic trap (containing a five-membered ring) and a Kagome structure for $N = 26$ building blocks, with no gravity effects considered. The highest energy minimum on the pathway contains a particle 'hovering' above the centre of a six-membered ring. Other minima along the pathway contain one tetrahedral motif, while the lowest energy minima are planar. See also Supplementary Movie 2. Green line: path length calculated with respect to the centre-of-mass displacements only; red line: path length calculated by including two additional sites along the z axis of the building block, displaced symmetrically by $1\,l_0$ from the origin.

VI.   SUPPLEMENTARY FIGURES

[1] S. N. Fejer, D. Chakrabarti, H. Kusumaatmaja and D. J. Wales, *Nanoscale*, 2014, **6**, 9448–9456.
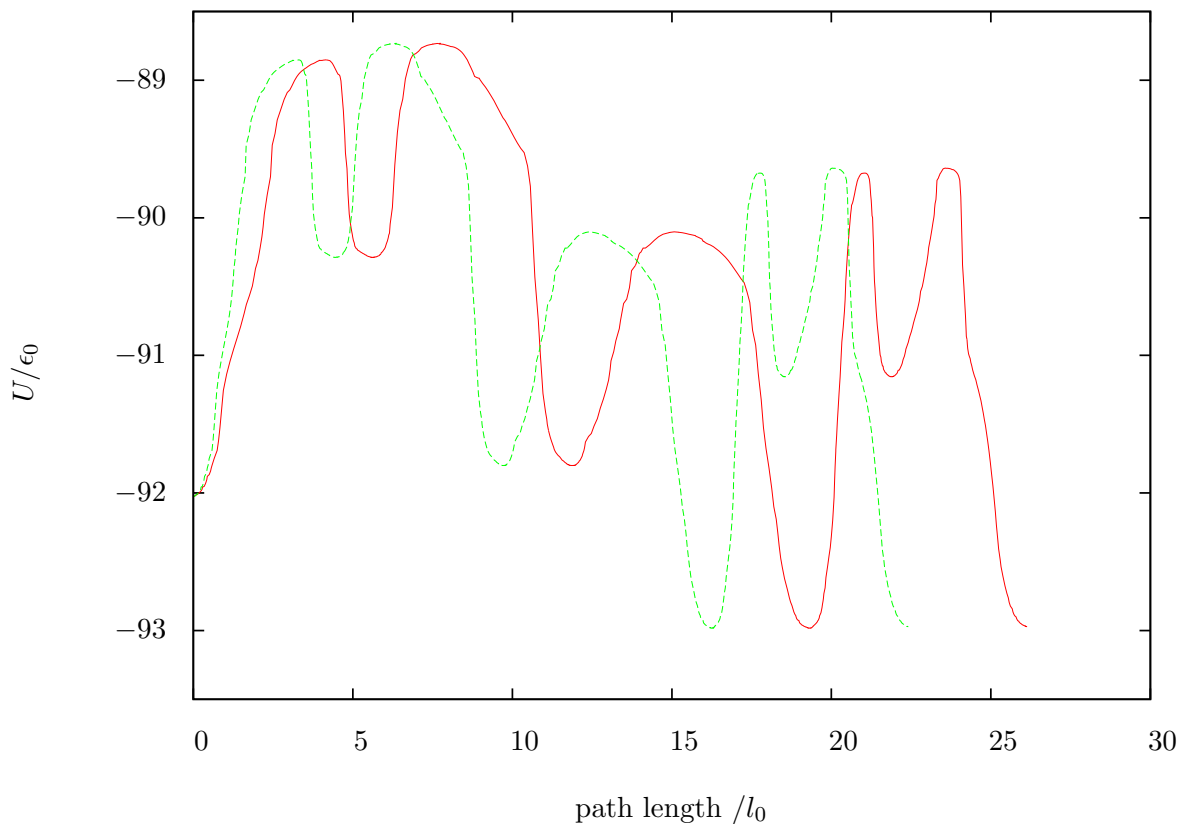
FIG. 2: Fastest pathway between a low-energy kinetic trap (containing a five-membered and seven-membered ring) and a Kagome structure for $N = 26$ building blocks, with the largest gravity effects considered. All rearrangements take place in the xy plane, so that every stationary point along the pathway is planar. See also Supplementary Movie 3. Green line: path length calculated with respect to the centre-of-mass displacements only; red line: path length calculated by including two additional sites along the z axis of the building block, displaced symmetrically by $1\,l_0$ from the origin.