Supporting Information

Title: Bistable self-assembly in homogeneous colloidal systems for flexible modular architectures

Gabi Steinbach*, Dennis Nissen, Manfred Albrecht, Ekaterina Novak, Pedro A. Sanchez, Sofia S. Kantorovich, Sibylle Gemming, and Artur Erbe

Movie:

Field-induced transformation between staggered and compact three-particle cluster. External field pulses with field intensity of 1.2mT and duration of 1ms are applied. The playback speed of the movie is accelerated by two with respect to the recording time.

Analytic expressions for the energies of three 3sd-particles

For a linear chain of three particles (meaning, that all three particle centers are on the y-axis,

so $\varphi = \psi = 0$ and equal to the polar angle of the third particle central dipole), we obtain the

distance between the dipoles belonging to the nearest neighboring particles in the chain

$$r^{ch-nn}_{ij} = 1 + s_i^2 + s_j^2 - 2s_i s_j Z_{ij}^{ch} - 2[s_i \cos(\beta i) - s_j \cos(\beta j)],$$

where $Z_{ij}^{ch} = \cos(\beta(i-j)).$

The distance between the dipoles in the next nearest neighboring (side particles) particles can

be obtained as:

$$r^{ch-sp}_{ij} = 4 + s_i^2 + s_j^2 - 2s_i s_j Z_{ij}^{ch} - 4[s_i \cos{(\beta i)} - s_j \cos{(\beta j)}].$$

Finally, the dipolar interaction in the linear chain of three particles has the form:

$$U_{total}^{ch} = 2\sum_{i,j=-1}^{1} m_i m_j \left(\frac{Z_{ij}^{ch}}{\left(r^{ch} - nn\right)^{\frac{3}{2}}} - 3\frac{\left[\cos\left(\beta i\right) + s_j Z_{ij}^{ch} - s_i\right] \left[\cos\left(\beta j\right) - s_i Z_{ij}^{ch} + s_j\right]}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} \right\} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} = 2\sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} = 2\sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} = 2\sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} = 2\sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} = 2\sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch} - nn\right)^{\frac{5}{2}}} + \sum_{i,j=-1}^{1} \frac{1}{\left(r^{ch}$$

For a staggered configuration, the energy will also depend on the stagger angle θ between the center-center distances of the side particles.

The distance between the dipoles in the nearest neighboring particles in a staggered chain can be written as:

$$r_{i(j)k}^{nn} = d^2 + s_j^2 + s_k^2 - 2s_k \left[d\cos\left(\beta k + (-)\frac{\theta}{2}\right) + s_{i(j)}Z_{i(j)k} \right] + 2ds_{i(j)}\sin\left(\alpha + (-)\beta i(j) + \frac{\theta}{2}\right) + \frac{1}{2} ds_{i(j)}\sin\left(\alpha + (-)\beta i(j) +$$

For the side particles, the distance between the dipoles is

$$r_{ij}^{sp} = 2d^{2} + s_{i}^{2} + s_{j}^{2} + 2s_{i}s_{j}Z_{ij} - 2d^{2}cos\theta + 4dsin\frac{\theta}{2}[s_{i}cos(\alpha + \beta i) + s_{j}cos(\alpha - \beta j)],$$

where $Z_{i(j)k} = sin(\alpha + (-)\beta(i(j) - k)), Z_{ij} = cos(2\alpha + \beta(i - j)).$

The energies are

$$\begin{split} U_{i(j)k}^{nn} &= m_{i(j)} m_k \Biggl\{ \frac{Z_{i(j)k}}{\left(r_{i(j)k}^{12}\right)^{\frac{3}{2}}} + (-)3 \frac{\left[s_k - d\cos\left(\beta k + (-)\frac{\theta}{2}\right) - s_{i(j)}Z_{i(j)k}\right] \left[s_{i(j)} + d\sin\left(\alpha + (-)\beta i(j) + \frac{\theta}{2}\right) - s_k Z_{i(j)k}\right]}{\left(r_{i(j)k}^{12}\right)^{\frac{5}{2}}} \Biggr\}, \\ U_{ij}^{sp} &= -m_i m_j \Biggl\{ \frac{Z_{ij}}{\left(r_{ij}^{13}\right)^{\frac{3}{2}}} + 3 \frac{\left[s_i + 2d\sin\frac{\theta}{2}\cos\frac{1}{100}(\alpha + \beta i) + s_j Z_{ij}\right] \left[s_j + 2d\sin\frac{\theta}{2}\cos\frac{1}{100}(\alpha - \beta i) - s_i Z_{ij}\right]}{\left(r_{ij}^{13}\right)^{\frac{5}{2}}} \Biggr\}, \\ U_{total}^{M} &= \sum_{i,j,k=-1}^{1} \left\{ U_{ik}^{12} + U_{ij}^{13} + U_{jk}^{23} \right\}. \end{split}$$

This energy has to be minimized with respect to α , for a given value of θ . The final candidate for the ground state is the ring, in which the central dipoles of three particles assume a triangular alignment. This energy depends on only one angle, characterizing the deviations of central moments from the sides of the triangle based on the dipoles' positions.

$$r_{ij}^{ring} = d^{2} + s_{i}^{2} + s_{j}^{2} - 2s_{i}s_{j}Z_{ij}^{ring} + 2d\left[s_{i}\sin\left(\frac{\pi}{6} + \varphi + \beta i\right) + s_{j}\cos\left(\varphi + \beta j\right)\right],$$

where $Z_{ij}^{ring} = -\sin\left(\frac{\pi}{6} + \beta(i-j)\right),$

$$U_{total}^{ring} = 3\sum_{i,j=-1}^{1} m_i m_j \left\{ \frac{Z_{ij}^{ring}}{\binom{3}{(r_{ij}^{ring})^{\frac{3}{2}}}} + 3\frac{\left[s_i - s_j Z_{ij}^{ring} + dsin\left(\frac{\pi}{6} + \varphi + \beta i\right)\right] \left[s_j - s_i Z_{ij}^{ring} + dcos\left(\varphi + \beta j\right)\right]}{\binom{5}{2}} \right\}.$$

The three candidates – the chain, the staggered chain and the ring – provide ground states or local energy minima depending on the parameters β , m_i , s_i for *i*=-1,0,1, as is shown in the main text.