Supplementary Information

S1: Potential energy functions used to describe inter and intramolecular interactions:

Stretching potential:

$$V_{Stretching} = \frac{1}{2} k_r (r_{ij} - r_0)^2$$

Bending potential:

$$V_{Bending} = \frac{1}{2} k_\theta (\theta_{ijk} - \theta_0)^2$$

Torsion potential:

$$V_{Torsion} = a_0 + a_1 \cos(\varphi_{ijkl}) + a_2 \cos^2(\varphi_{ijkl}) + a_3 \cos^3(\varphi_{ijkl}) + a_4 \cos^4(\varphi_{ijkl}) + a_5 \cos^5(\varphi_{ijkl})$$

Lennard-Jones potential:

$$V_{LJ} = 4\varepsilon \left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right)$$

S2: Diagram of a nanoparticle contained in a sphere with radius rb, and containing a sphere with radius ra