

Supporting information for
“Co-assembly of Cellulose Nanocrystals and Gold Nanorods: Insights from Molecular
Dynamics Modelling”

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SUPPLEMENTARY FIGURES

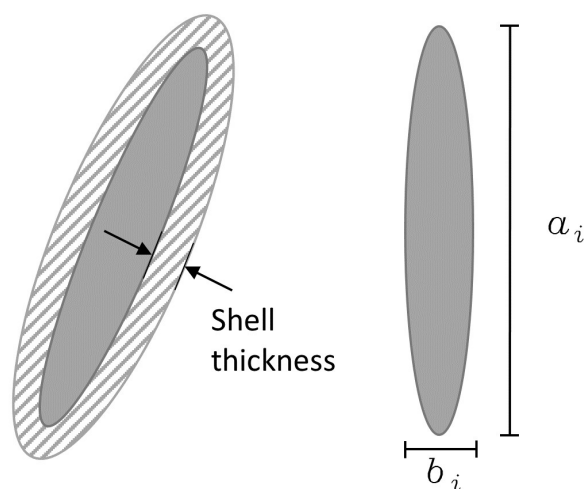


Fig. S1. Core-Shell contact model. The solid grey-shaded ellipse represents a CNC particle, and the dashed area represents the shell thickness, such that ellipses are assumed to be in mutual contact when a grey region intersects the dashed shell

TABLE I. Well depth parameters for side-side and tip-tip interactions between CNCs and AuNRs.

	ϵ (kJ/mol)
CNC side-side	55.48
CNC tip-tip	4.75
AuNR side-side	45.21
AuNR tip-tip	4.33

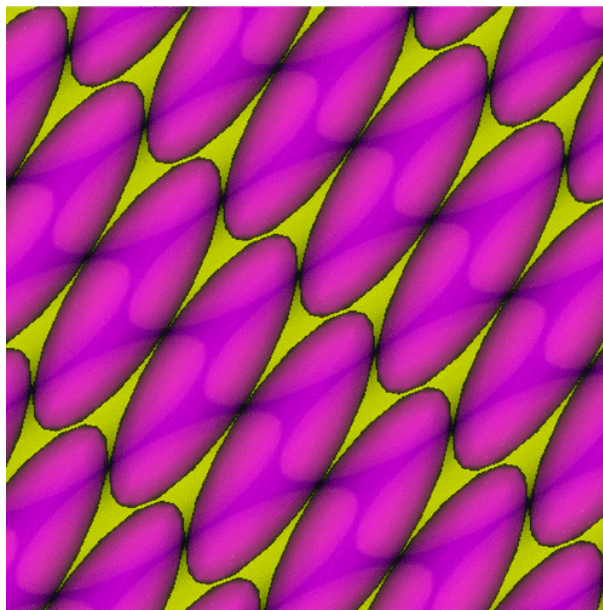


Fig. S2. The layers of the densest known packing of ellipsoids with maximal aspect ratio of 3[1].

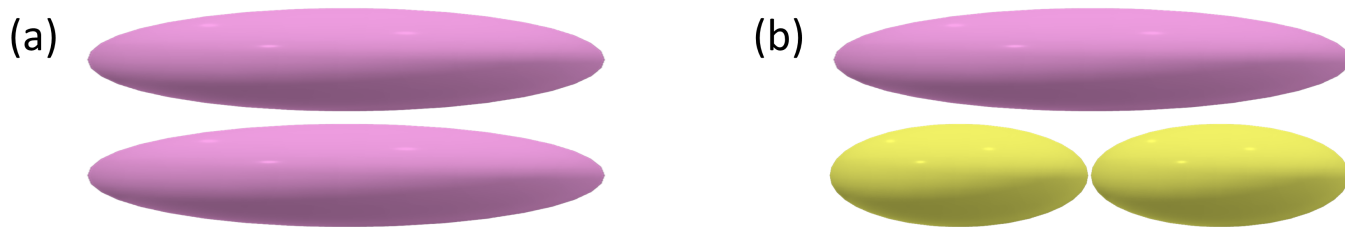


Fig. S3. Packing in homogeneous (a) and heterogeneous (b) systems. The ratio of long axis of two particles is 2:1. In a homogeneous system (a), each particle contribute same value of 1 to kissing number; in heterogeneous system (b), the short particle only contribute 0.5 to the kissing number value of long particle, whereas the long particle contribute 2 to that of the short ellipsoid.

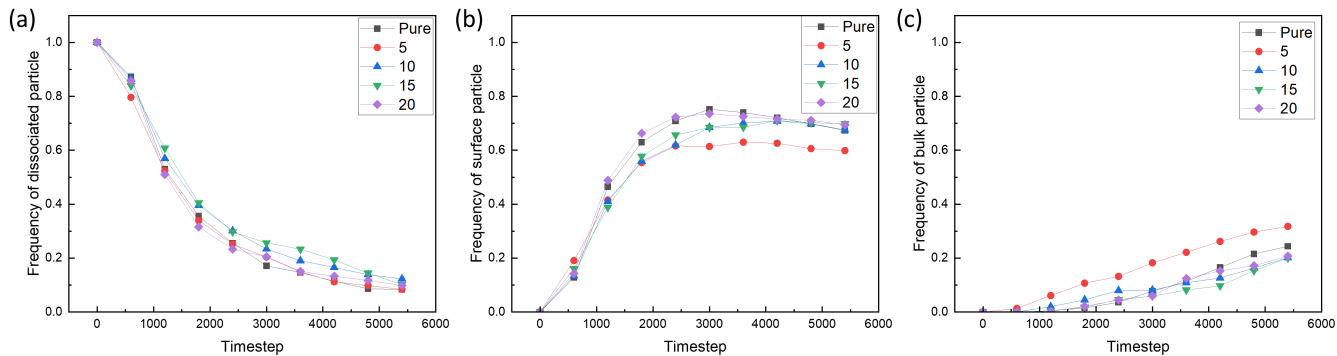


Fig. S4. Projction representation of dissociated, surface and bulk particles. Each group shows a same trend during self-assembly.

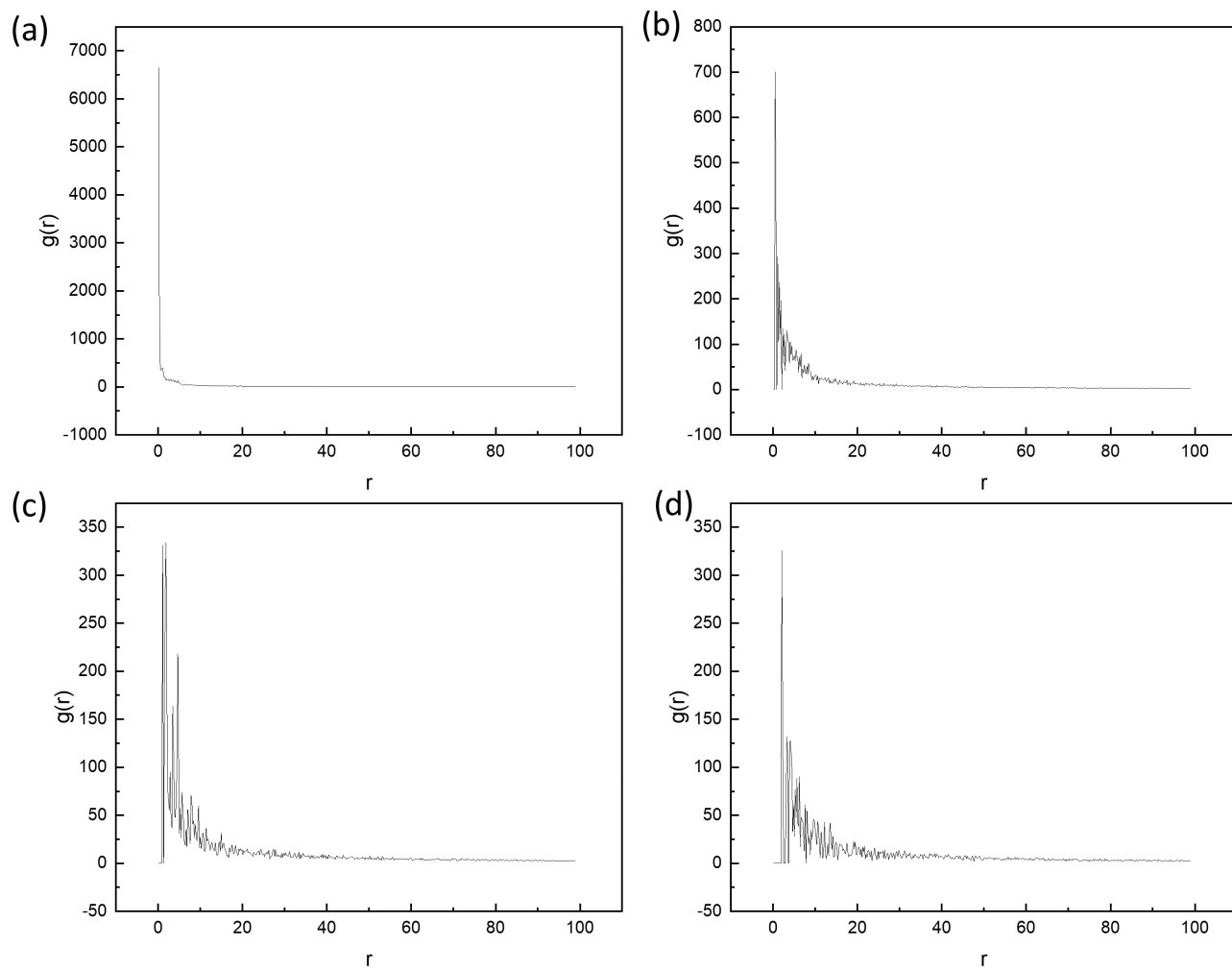


Fig. S5. Radial distribution function for AuNRs with AR of 2.5, 5, 7.5 and 10.

REFERENCES

- [1] A. Donev, F. H. Stillinger, P. Chaikin, and S. Torquato, Physical review letters **92**, 255506 (2004).