Phase diagram of hard board like colloids from computer simulations

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Supplementary Information FILE

S1. Phase diagram of hard spheroplatelets with pairs (w^*, l^*) in which simulations have been performed

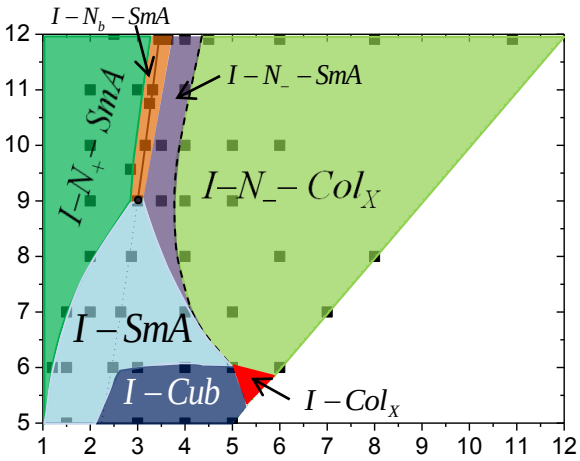

Fig. S1. The phase diagram of hard spheroplatelets (see main manuscript for details). The black squares on the diagram indicate the molecular geometries (w^*, l^*) for which the actual simulations were performed.

S2. Representative Equations of State (EOS)

We present characteristic pressure (p^*) versus packing fraction (η) equations of state for various $\left(w^*,l^*\right)$ pairs. More specifically, for the following enantiotropic phase sequences: (a) $I-N_{-}-Col_X$, (b) $I-N_{-}-SmA$ (c) $I-SmA$, and (d) $I-N_b-SmA$(see Fig. S2).

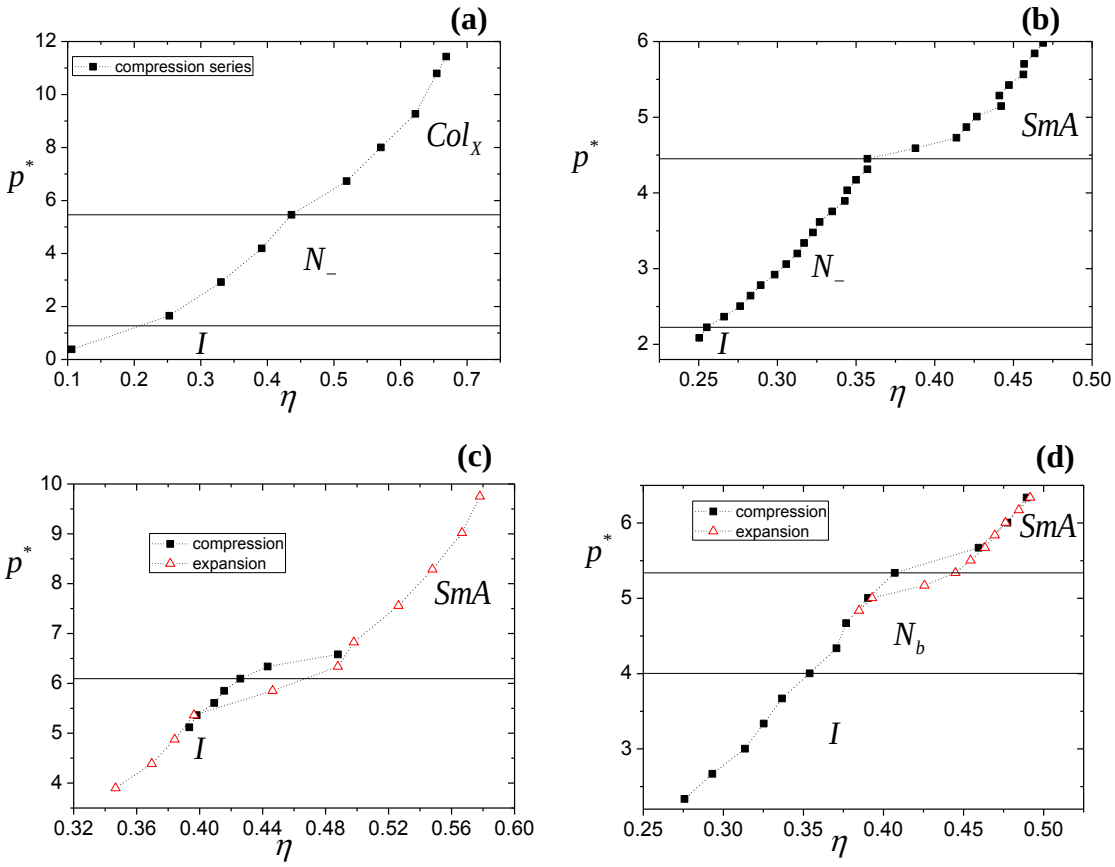

Fig. S2. Equations of state for systems consisting of SP particles (a) $\left(w^*,l^*\right)=\left(11,12\right)$, (b) $\left(w^*,l^*\right)=\left(4,12\right)$, (c) $\left(w^*,l^*\right)=\left(3,9\right)$ and (d) $\left(w^*,l^*\right)=\left(\sqrt{11},11\right)$. The solid symbols correspond to EOS calculated from compression runs from well equilibrated low-density isotropic states and the open symbols are EOS obtained by expansion from close packed states. The density jump accompanying the $N-I$ phase transition is rather small in comparison with the corresponding jump along the $N-Sm$ and $I-Sm$ phase transitions.

S3. Cubatic phase for two representative (w^*, l^*) molecular geometries.

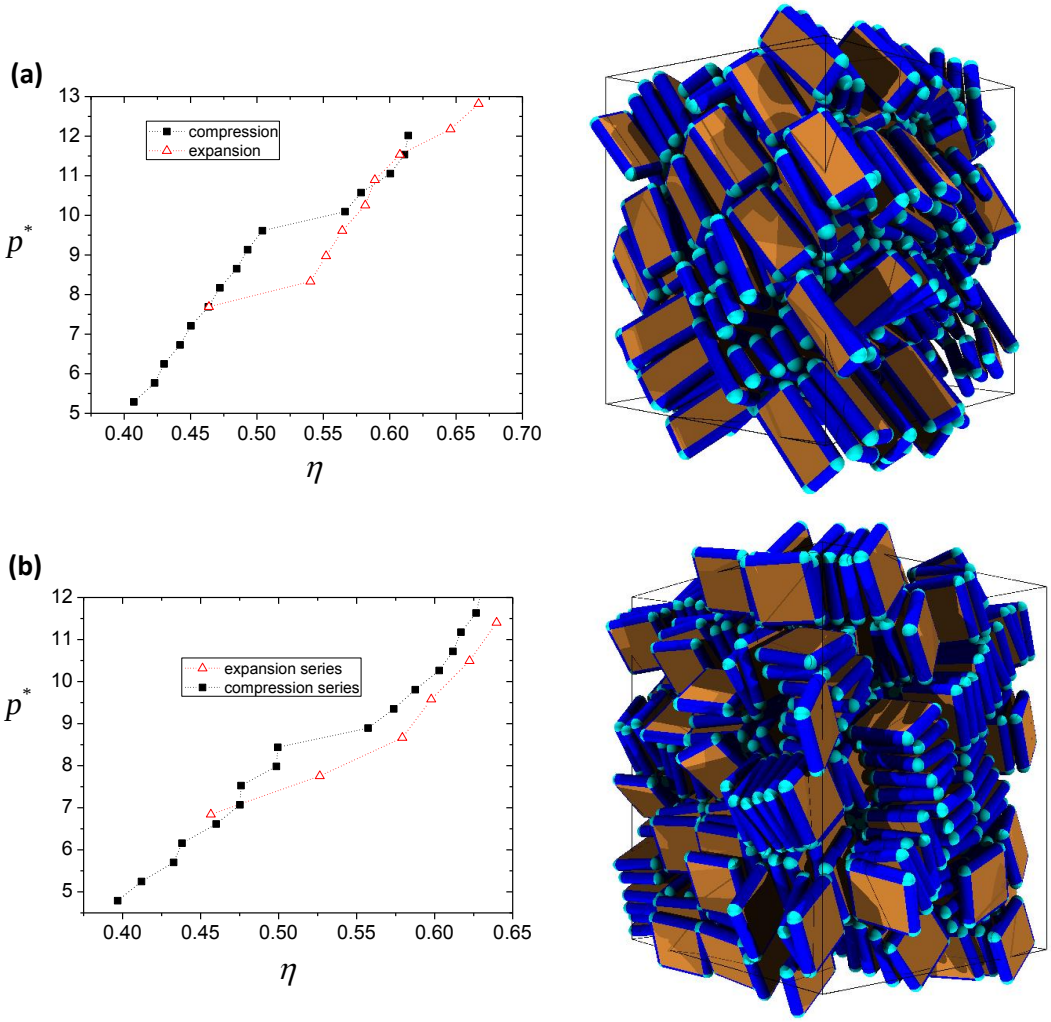

Fig. S3. Equations of state (pressure vs packing fraction) and representative snapshots of cubatic phases for systems consisting of SP particles with (a) $(w^*, l^*) = (3,6)$ and (b) $(w^*, l^*) = (5,5)$. The solid and open symbols correspond to compression and expansion runs respectively. The snapshot in (a) corresponds to $p^* = 11.54$ and indicates the formation of well defined stacks of particles forming short biaxial columns or Smectic-like clusters, while in (b) the particles form short uniaxial columns. In both cases the nematic-like orientational correlations diminish after a few molecular lengths.

Note that the relative stability of the cubatic phases with respect to SmA and/or the Columnar phase is still an open issue. For a detailed discussion see refs[1-3].

REFERENCES

[1] M. Marechal, A. Patti, M. Dennison, and M. Dijkstra. Frustration of the Isotropic-Columnar Phase Transition of Colloidal Hard Platelets by a Transient Cubatic Phase *Phys. Rev. Lett.*, 2012, 108, 206101.

[2] M. R. Wilson, P. D. Duncan, M. Dennison and A. J. Masters. Molecular dynamics simulation studies of platelets with square cross-sectional area: formation of a stable cubatic phase. *Soft Matter*, 2012, 8, 3348-3356.

[3] P. D. Duncan, A. J. Masters, and M. R. Wilson. Thermodynamic stability of the cubatic phase of hard cut spheres evaluated by expanded ensemble simulations. *Phys. Rev.* E 2011, **84**, 011702.