Novel route to colloidal photonic crystals via complex building blocks

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A considerable amount of research in the colloidal science community deals with the design and the fabrication of crystalline phases to be employed as photonic crystals, structures which have a rather broad applicability spectrum, ranging from optical fibers and displays, to (bio-)sensing and bio-medical engineering, and finally to energy storage and security [1-2]. Here, we suggest a novel route to the fabrication of colloidal Laves phases – the precursors of photonic crystals – from a binary mixture of hard spheres and hard tetrahedral clusters. By using Monte Carlo simulations and free energy calculations we compute the phase diagram of such a mixture of colloidal building blocks, and focus on the stability of the Laves phase structure. We stress that the studied mixture is well within current experimental capabilities [3-4]. We present the phase diagram of the system in the reduced pressure – composition representation. Our findings show a relatively large fluid-crystal coexistence region which is potentially accessible by experiments, uncovering a new path in the self-assembly scenario. To facilitate a comparison with experimental results, we additionally compute the phase diagram in the packing fraction of tetramers – packing fraction of spheres representation, and identify the region where the fluid is in coexistence with the Laves crystal.

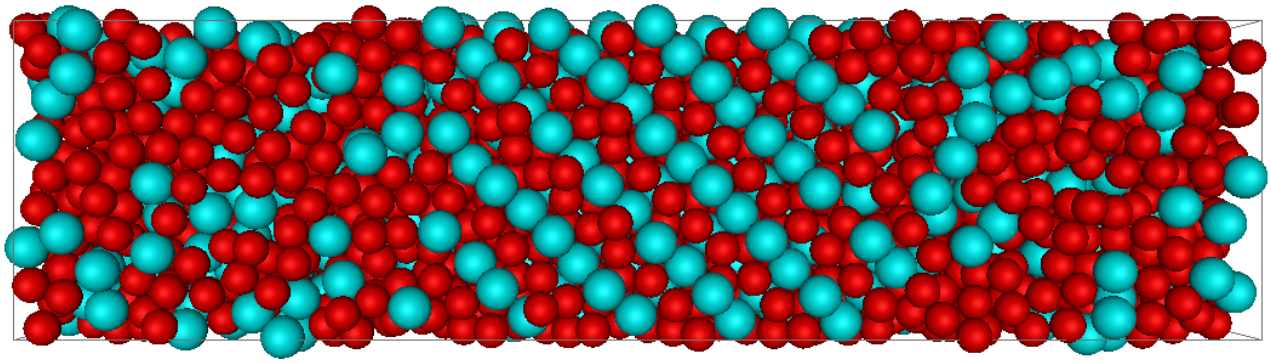

Figure 1 Final configuration obtained from a direct coexistence simulation of the Laves crystal of hard tetramers and hard spheres and the fluid phase.

[1] A. Stein, B. E. Wilson and S. G. Rudisill, *Chem. Soc. Rev.*, 2013, **42**, 2763.
[2] G. von Freymann *et al.*, *Chem. Soc. Rev*, 2013, **42**, 2528.
[3] V. N. Manoharan, M. T. Elsesser and D. J. Pine, *Science*, 2003, **301**, 483.
[4] C. Young-Sang *et al.*, *Chemistry of Materials*, 2005, **17**, 5006.