

Aggregation and self-assembly of decorated nanoparticles by coarse-grained molecular dynamics simulations

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We consider a range of generic models for the nanoparticles decorated by ligands with the liquid crystalline groups, including the case of photosensitive mesogens.

In a melt, such nanoparticles are found to self-assemble predominantly into a glass-like polydomain lamellar morphology. For the case of chromophoric liquid crystalline groups (e.g. azobenzene), application of illumination with a suitable wavelength leads to cyclic trans-cis-trans photoisomerisation events. These aid effective transformation of a disordered or a polydomain glass-like state into a monodomain lamellar morphology. A range of properties such as: molecular asphericity, nematic and smectic order parameters, as well as clustering characteristics are analysed in a course of this photo-induced self-assembly [1].

In a solution under poor solvent conditions, nanoparticles aggregate into a nanogel network, due to strong liquid crystalline interactions between their ligands. The dynamics of network formation, as well as the final structure of the network, are found to depend strongly on a decoration pattern of nanoparticles. The cases of polar, planar patchy-like and uniform equatorial, as well as icosahedral patterns are considered. Network characteristics such as: the size and the dimensions of a largest subnetwork, average rank and local clustering coefficient, alongside with the effective elastic constant for the network are evaluated and discussed [2].

1. J.M. Ilnytskyi, A. Slyusarchuk, M. Saphiannikova, Photocontrollable Self-Assembly of Azobenzene-Decorated Nanoparticles in Bulk: Computer Simulation Study, *Macromolecules* **49** (23), 9272–9282 (2016).
2. J.M. Ilnytskyi, A. Slyusarchuk, S. Sokołowski, Gelation of patchy ligand shell nanoparticles decorated by liquid-crystalline ligands: computer simulation study, *Soft Matter* **14**, 3799–3810 (2018).