

Accepted Manuscript

Suspensions of supracolloidal magnetic polymers: self-assembly properties from computer simulations

Novak E.V., Pyanzina E.S., Rozhkov D.A., Ronti M., Cerdà J.J., Sintes T., Sánchez P.A., Kantorovich S.S.



PII: S0167-7322(18)31361-8
DOI: doi:[10.1016/j.molliq.2018.08.145](https://doi.org/10.1016/j.molliq.2018.08.145)
Reference: MOLLIQ 9590
To appear in: *Journal of Molecular Liquids*
Received date: 15 March 2018
Revised date: 24 August 2018
Accepted date: 28 August 2018

Please cite this article as: Novak E.V., Pyanzina E.S., Rozhkov D.A., Ronti M., Cerdà J.J., Sintes T., Sánchez P.A., Kantorovich S.S. , Suspensions of supracolloidal magnetic polymers: self-assembly properties from computer simulations. Molliq (2018), doi:[10.1016/j.molliq.2018.08.145](https://doi.org/10.1016/j.molliq.2018.08.145)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Suspensions of supracolloidal magnetic polymers: self-assembly properties from computer simulations

Novak E.V.^a, Pyanzina E.S.^a, Rozhkov D.A.^b, Ronti M.^b, Cerdà J. J.^c, Sintès T.^d, Sánchez P.A.^{a,b}, Kantorovich S.S.^{a,b}

^aUral Federal University, Lenin Av. 51, Ekaterinburg, 620000, Russia

^bUniversity of Vienna, Sensengasse 8, 1090 Vienna, Austria

^cDepartament de Física, Universitat de les Illes Balears, E-07122, Palma de Mallorca, Spain

^dInstituto de Física Interdisciplinar y Sistemas complejos, IFISC (UIB-CSIC), E-07122, Palma de Mallorca, Spain

Abstract

We study self-assembly in suspensions of supracolloidal polymer-like structures made of crosslinked magnetic particles. Inspired by self-assembly motifs observed for dipolar hard spheres, we focus on four different topologies of the polymer-like structures: linear chains, rings, Y-shaped and X-shaped polymers. We show how the presence of the crosslinkers, the number of beads in the polymer and the magnetic interparticle interaction affect the structure of the suspension. It turns out that for the same set of parameters, the rings are the least active in assembling larger structures, whereas the system of Y- and especially X-like magnetic polymers tend to form very large loose aggregates.

Keywords: magnetic colloidal particles, self-assembly, crosslinked polymer-like structures, Langevin dynamics simulations

1. Introduction

Nowadays, the creation of smart materials relies on a multiscale design, from the nanoscale to macroscopic properties. The internal structure at the nano- and micro-levels determines the texture, elasticity, viscosity, taste and other macroscopic properties of soft materials. There are several techniques to change the properties of soft materials: by varying the pH balance, temperature, turning on and off the external fields. The essential condition to use a magnetic field as a control parameter is the presence of magnetically sensitive components in a soft material. There are several ways to incorporate such components into liquids and gels. The common thing for all the techniques is the size of the magnetic building blocks magnetic colloids in the range from a couple of nanometers to several microns. Magnetic colloids in liquid or elastic carriers, directed by applied magnetic fields, or under the action of intrinsic magnetic forces, exhibit hierarchical self-assembling and various structural-phase transitions, which, in turn, can lead to macroscopic changes of all soft material. The list of possible structures and phases is very large and is determined by the size, concentration, type and material of magnetic inclusions.

The oldest and, probably, the most understood example of magnetic soft matter is a ferrofluid [1], *i.e.* a system of surface-stabilised single-domain magnetic nanoparticles suspended in a magnetopassive carrier. Nanoparticles in this systems are known to self-assemble [2–6] and through clustering affect strongly viscous [7, 8], optical [9–11], magnetic [12, 13] and diffusion properties [14–16]. Even though the self-assembly of magnetic nanoparticles seems to be a promising tool to control the response of a ferrofluid, such structural transformations are very sensitive to noise created by temperature fluctuations [17],

particle polydispersity [18, 19] or particle asphericity [20, 21].

One of the avenues to avoid such a sensitivity of self-assembly is to predefine the structural motifs: to crosslink the magnetic particles in so-called magnetic filaments [22–27] or other polymer-like supracolloidal structures [28]. In this case, cluster sizes and shapes cannot be altered by temperature and such clusters will remain connected even under conditions for which self-assembly in a “regular ferrofluid” would have not taken place. However, the question arises: “will, and, in case, how, supracolloidal structures self-assemble?”

In the present computer simulation study, we investigate suspensions of supracolloidal magnetic polymer-like structures (SMP) of linear (LSMP), ring (RSMP), Y- (YSMP) and X-shapes (XSMP), since these structures are predominant at low temperatures in systems of dipolar fluids [12, 29, 30]. We vary the length of SMPs, that is the number of magnetic particles forming them; the concentration of SMPs in the suspension; and the strength of magnetic interparticle interactions. Additionally, we perform the analysis of a ferrofluid with non-crosslinked magnetic particles under the same set of conditions. In this way, we do not only elucidate the influence of crosslinkers on the hierarchical self-assembly, but can also envision the topology-driven structural transitions. We found that while RSMPs are inert and do not self-assemble, LSMPs under the same conditions can exhibit cluster formation, albeit not as strong as that found for YSMPs and XSMPs.

The structure of the manuscript is the following: firstly, in section 2, we discuss computational methods used to study SMPs; next, we present results on cluster-size distributions for various SMPs (section 3.1), analyse how the position of the magnetic bead in a SMP influences its ability to form a connection (section 3.2), and describe the topology of SMP clusters,

Download English Version:

<https://daneshyari.com/en/article/10141694>

Download Persian Version:

<https://daneshyari.com/article/10141694>

[Daneshyari.com](https://daneshyari.com)