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**Modeling Anisotropic Self-Assembly of Isotropic Objects: from Hairy Nanoparticles to Methylcellulose Fibrils**[1]

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Spontaneous symmetry breaking and formation of anisotropic structures from apparently isotropic building blocks is an exciting and not fully understood topic. I will discuss two examples of such self-assembly. The first example is related to the assembly of "hairy" nanoparticles in homopolymer matrices[1]. The particles can assemble into long strings (they can also form other morphologies, as well) even though the shape of each particle and the distribution of ligands on the particle surface is spherically symmetric. Using the approach developed by Thompson, Ginzburg, Matsen, and Balazs[2], we show that presence of other particles can re-distribute the ligands and effectively "polarize" the particle-particle interaction, giving rise to the formation of 1d particle strings[3]. In the second example, we consider aqueous solutions of methylcellulose (MC) polymers. It has been shown recently[4] that at high temperature, the polymers form high-aspect ratio "fibrils" with diameter ˜15 nm and length in the hundreds on nanometers. Using coarse-grained Molecular Dynamics (CG-MD), we propose that the "fibrils" are result of one-dimensional self-assembly of single molecule "rings". Each MC polymer chain is forced into a ring because of the balance between internal chain rigidity (favoring more expanded configuration) and unfavorable polymer-water interactions (favoring more collapsed conformation). We also develop a theory predicting rheology and phase behavior of aqueous MC, and validate it against experimental data[5]. Both examples show that anisotropic self-assembly can show up in unexpected places, and various theoretical tools are needed to successfully model it. 1. P. Akcora et al., Nature Mater. 8, 354 (2009). 2. R. Thompson, V. Ginzburg, M. Matsen, and A. Balazs, Science 292, 2469 (2001). 3. V. Ginzburg, Macromolecules 46, 9898 (2013). 4. S. Arvidson et al., Macromolecules 46, 300 (2013). 5. V. Ginzburg, R. Sammler, W. Huang, and R. Larson, submitted for publication.

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