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Quantifying the brush structure and assembly of mixed brush nanoparticles in solution JASON KOSKI, AMALIE FRISCHKNECHT, Sandia National Labs — The arrangement of nanoparticles in a polymer melt or solution is critical to the resulting material properties. A common strategy to control the distribution of nanoparticles is to graft polymer chains onto the surface of the nanoparticles. An emerging strategy to further control the arrangement of nanoparticles is to graft polymer chains of different types and/or different lengths onto the surface of the nanoparticle, though this considerably increases the parameter space needed to describe the system. Theoretical models that are capable of predicting the assembly of nanoparticles in a melt or solution are thus desirable to guide experiments. In this talk, I will describe a recently developed non-equilibrium method that is appealing in its ability to tractably account for fluctuations and that can directly relate to experiments. To showcase the utility of this method, I apply it to mixed brush grafted nanoparticles in solution where fluctuations are prominent. Specifically, I investigate the role of experimentally relevant parameters on the structure of the brush and the corresponding effects on the assembly of the nanoparticles in solution. These results can be directly linked to experiments to help narrow the relevant parameter space for optimizing these materials.

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