Simulations of concentrated solutions of monoclonal antibodies and sticky cylindrical particles using open-source software

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The advantages of using simulation to analyze and interpret small angle scattering data are exemplified in recent work on the solution structure of coarse-grained models of monoclonal antibodies (mAbs) under concentrated conditions, and on the clustering of cylindrical colloids with short-range attractions. For the first example, rational strategies need to be developed to avoid physical instabilities in mAb formulations such as aggregation and increased viscosity. In the second example, cylindrical particles are promising materials for applications of fillers in nanocomposite materials and additives to control rheological properties of colloidal suspensions. In both examples, we performed flat histogram Monte Carlo simulations of these systems with specialized algorithms using the Free Energy and Advanced Sampling Simulation Toolkit (FEASST). FEASST is freely available at https://pages.nist.gov/feasst. We highlight the effect of intra-domain flexibility of the mAbs on the small angle scattering data. We also show how scattering data for cylindrical particles was used to collapse the attractive-driven gel boundary over a range of aspect ratios.