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Brownian dynamics simulations of amelogenin microribbons formation[1] WEI LI, ANTHONY PEREZ LOPEZ, YA LIU, Lehigh University, AMIT CHAKRABARTI, Kansas State University, JAMES GUNTON, Lehigh University — Recent advances in chemical particle synthesis have emphasized the fundamental role of surface colloidal heterogeneities and their detailed chemical composition, which is particularly significant for an important subclass of colloidal systems, namely, proteins. Recently, the process of self-assembly of amelogenin monomers with a hydrophobic/hydrophilic bipolar nature into ordered ribbon structures has been studied experimentally. In this work, we study this dynamical process by means of a Brownian dynamic simulation of a simple model which represents the bipolar character of the globular amelogenin molecule and the hydrophilic C-terminal tail. We monitor the kinetics of self-assembly through a study of the structure factor. We also calculate the phase diagram of the model using Gibbs ensemble Monte Carlo simulation and thermodynamic perturbation theory.

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