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Hydrodynamic interactions effects on the dipole-induced self-assembly of β -peptides and Brownian-induced polymer pore translocation

JUAN HERNANDEZ-ORTIZ, Departamento de Materiales, Universidad Nacional de Colombia, Sede Medellin, MICHAEL GRAHAM, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — A novel method that scales linearly with the number of particles is used to study Brownian-systems considering fluctuating hydrodynamic interactions. The method is demonstrated in the context of two applications: the dipole-induced self-assembly of β -peptides and the Brownian-motion-induced translocation of a polymer through a rectangular pore. The method includes the long-range interactions by the Green's function formalism. It allows the consideration of peptides at intermediate concentrations and the inclusion of the non-periodic domain of the translocation. The hydrodynamic interactions affect the dynamics of the peptides agglomeration and the mean-squared-displacement indicates significant changes in the long-time diffusion coefficient. The polymer translocation is studied using a transition path sampling based methodology. In particular it is used to calculate the translocation rate constant. Even for a single bead there are differences once hydrodynamics are included. These differences are due to the changes of mobility near walls and the change in polymer chain diffusion coefficient.

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