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Equilibrium and Beyond Equilibrium Properties of Polyelectrolytes - Ewald-Like Approach for Fluctuating Hydrodynamic and Electrostatic Interactions JUAN P. HERNANDEZ-ORTIZ, Department of Materials, Universidad Nacional de Colombia, Sede Medellin, MICHAEL D. GRAHAM, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — A method is proposed for self consistent simulations of the equilibrium and beyond equlibrium structures and transport properties of polyelectrolytes in solution. The method incorporates solution of the Nernst-Planck diffusion equation for ions and counter-ions within the solvent, and simultaneous description of fluctuating hydrodynamic interactions by means of a Green's function formalism. The proposed approach generalizes our $O(N)$ general geometry Ewald-like method to simultaneous treatment of hydrodynamics and electrostatics. With this method, we examine the transport properties of polyelectrolytes solutions at rest and in various flow fields, and we make direct comparisons to results from explicit ion Brownian dynamics simulations and experimental observations.

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