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Dielectric many-body effects in arrays of charged cylindrical macromolecules DANIEL W SINKOVITS, University of Illinois at Urbana–Champaign, KIPTON BARROS, Los Alamos National Laboratory, JURE DOBNIKAR, University of Cambridge and Jožef Stefan Institute (IJS), MATEJ KANDUČ, Technische Universität München and IJS, ALI NAJI, Institute for Research in Fundamental Sciences (IPM), RUDOLF PODGORNIK, IJS and University of Ljubljana, ERIK LUIJTEN, Northwestern University — Nonuniform dielectric constants are a ubiquitous aspect of condensed-matter systems, but nevertheless widely ignored in simulations. Analytical work suggests that the polarization effects resulting from these inhomogeneities can produce many-body interactions that qualitatively alter the behavior of systems driven by electrostatic interactions, but such work relies on approximations. Recently, we have developed an algorithm that computes the fluctuating polarization charge at the interface between dielectric materials during a molecular dynamics simulation, without approximation. Here, we apply this approach to investigate arrays of charged cylindrical macromolecules in the presence of explicit counterions. We study the dielectric many-body effects as a function of separation, dielectric constant variation, and counterion valency. Our findings have implications for the aggregation of polyelectrolytes such as F-actin or DNA.

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