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Fachbereich Physik, Universität Stuttgart
Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme

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Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart-Vaihingen

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Coarse-grained membrane models for hydrodynamic, dielectric and hydration effects

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Abstract

Based on fully atomistic simulations of interacting bilayer membranes in water, we discuss how to construct continuum coarse-grained models that capture dielectric, hydrodynamic, and hydration effects. For this, we use novel MD simulation techniques that allow to efficiently determine the interaction pressure and the polarization fluctuations at constant water chemical potential. Coarse-grained models must reflect certain key observations: i) The dielectric and the viscosity response functions are tensorial, inhomogeneous functions of space. ii) The hydration repulsion is caused by a mixture of water polarization effects and the desorption of interfacial water, both effects must be included in coarse-grained modeling.