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Effective interactions between pH-responsive particles JOS ZWANIKKEN, RASTKO SKNEPNEK, MONICA OLVERA DE LA CRUZ, Northwestern University — The DLVO potential is commonly used to describe the pair interactions between charged macroions in solution. It neglects effects due to responsive surface groups, by which the charge and surface entropy can fluctuate. Here, within the framework of density functional theory, we calculate the pair potential between reactive macromolecules. We compare with results found by molecular dynamics simulations of the restricted primitive model, including a short ranged binding potential between the ions and the macroions. Thereby, we extend DLVO-theory significantly, and even find conditions for a like-charge attraction and opposite-charge repulsion.

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