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Emergence of attraction in simulations of coarse-grained double stranded DNA SHAHZAD GHANBARIAN, JOERG ROTTLER, University of British Colombia — DNA condensation induced by multivalent counterions is believed to play an important role in DNA bundling and packing into the cell nucleus. We present a coarse-grained, implicit solvent representation of rigid ds-DNA molecules in the presence of divalent counterions. In order to include solvation effects arising from the discrete nature of the water molecules, short-ranged corrections are added to the pairwise interaction potentials such that the structure of counterions is consistent with results from corresponding explicit solvent simulations. The effective force between two DNA strands generated by these potentials provides an excellent match to that observed in the explicit solvent model. Importantly, this interaction features multiple minima and reproduces the like-charge attraction effect between DNA molecules observed in full atomistic simulations at significantly reduced computational expense. This result proves that it is possible to capture complex multibody interactions between polyelectrolyte strands with two-body potentials.

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