

Towards a Coarse-Grained Description of HYADD Hydrogels

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HYADD, a biocompatible hydrogel of a polysaccharidic backbone functionalized with hydrophobic side chains, is a promising substitute of pure hyaluronic acid for several medical applications. The typical size and relaxation timescales of the system do not allow to use atomistic molecular dynamics as an effective simulation tool to investigate HYADD properties. A coarse-graining strategy will be presented, with an emphasis on the problems related to the parametrization of the coarse-grained interaction parameters, and on the limitations of actual atomistic forcefields for sugars. The results from a preliminary simulation of the coarse-grained system will be also shown.