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Development of a Polarizable Protein-like Coarse Grained Model
SAI JANANI GANESAN, SUDI JAWAHERY, SILVINA MATYSIAK, University of Maryland, College Park — The use of coarse grained simulations to explore larger biological systems and longer timescales has become increasingly popular. One of the major drawbacks of most coarse grained protein models is the absence of polarization effects and hence the inability to reproduce accurate electrostatic screening. The inclusion of polarization effects to amino acids will allow us to characterize the role of dipole-charge interactions in driving secondary structural preferences. We have formulated a polarizable coarse-grained protein-like model using the Drude oscillator approach. The root of the model is based on the coarse-grained MARTINI force field. We apply the new model to polyalanine peptides and observe secondary structure changes in different solvent environments, caused due to changes in dipole interactions. We also explore the effects of adding charged amino acids like Lysines, on conformational preferences of the polyalanine system. Extensions of the current model to more complex systems will also be presented.

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