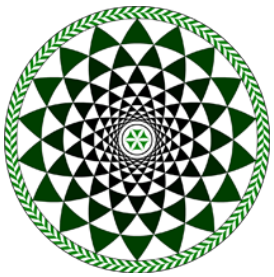

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Diffusive properties and intermolecular interactions of water molecules in neighborhood of polymer chain as seen by various simulations techniques.

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Polymers, which exhibit lower critical solution temperature (LCST) are a good substrates to design stimuli-responsive materials with many applications such as micro-valves, chemical indicators, drug delivery systems, lenses and many others [1,2]. In such systems three fundamental types of water may be distinguished: “bulk”, primary and secondary bounded water [3]. Knowledge about diffusion of various types of water is crucial because it determines rapidness of volume phase transition (VPT) resulted from distortion of metastable equilibrium in intermolecular interactions being of answer on external stimuli. Currently, experimental techniques allow only to determine averaged diffusive properties of water in complex systems. In this work two simulation techniques were applied: Quantum Mechanic (QM) and Monte Carlo (MC). QM method was used to optimize polymer-water systems and to study electrostatic interactions between molecules. Poly(vinylmethylether) (PVME) was chosen as a model thermo-responsive polymer because of its simple chemical structure. The MC method - DLL model [4] was used to examine diffusion of various types of water molecules. Influence of polymer chain lengths, and concentration on water diffusivity is discussed for athermal case, where only excluded volume interactions are taken into account. The water mobility in various distances from polymer chain is also shown.

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