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**Effect of Water Concentration on the Molecular Structure of Polyacrylate Gels** SRIRAMVIGNESH MANI, FARDIN KHABAZ, RAJESH KHARE, Texas Tech Univ — Recent studies have suggested pervaporation to be a promising alternative method for separation of aqueous solution of alcohol compared to distillation based separation processes. The ability to tune the hydrophobic/hydrophilic character makes polyacrylate gels attractive candidate materials for separating water-alcohol mixture by pervaporation. Experimentally, it is observed that the amount of water absorbed in the gel i.e. the degree of swelling of the gel shows a large variation with polymer chemistry. Relatively few studies exist highlighting the effects of water concentration on the membrane separation efficiency which in turn is directly related to the internal molecular structure of the water rich membranes. In this regard, an all-atom molecular dynamics (MD) simulation is employed to study water structure in polyacrylate gels. As a first step, polyacrylate copolymer systems with varying degree of hydrophobicity are prepared using the simulated annealing polymerization technique. Atomistic structures of gels containing different amounts of water are also prepared. Effect of water content on the acrylate-water system microstructure is determined by characterizing the packing of water molecules as well as the hydrogen bonding in these systems. In addition, the change in dynamics of water molecules due to the interactions with polymer is captured by monitoring the auto-correlation function of their dipole vector.

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