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A simulation study of a polypeptide model of a hydrogel SONGUL KUTLU, Lehigh Physics Department, SIDDIQUE KHAN, U Penn Department of Medical Physics, JASON HAAGA, JAMES GUNTON, Lehigh Physics Department
— Hydogels are water insoluble, cross linked polymers that are capable of swelling substantially in aqueous conditions. The crosslinked nature of a hydrogel makes it strong mechanically. Hydrogels has many applications such as in drug delivery, tissue engineering, contact lenses and wound dressing. The preparation of hydrogels through molecular self-assembly gives microscopic information about the material properties. Some of the hydrogels are environmentally responsive to pH and temperature. MAX1 is a chemically synthesized responsive hydrogel which is the chain of valine and lysine aminoacids flanking a tetrapeptide VDPPT. Therefore, the general structure of MAX1 is: VKVKVKVK-VDPPTKVKVKVKV-NH2. In this poster we present preliminary Monte Carlo simulation results which shows that the structure of a single MAX1 peptide is a random coil shape. We will also present preliminary Monte Carlo dimer simulation results for the MAX1 peptide chains in order to study the conformational variations at dimer level. In addition, we also propose a coarse-grained model that we will use to study the self-assembly of these polypeptide chains, in order to understand the formation of hydrogels.

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