

عنوان مقاله:

Dynamic Behavior of Poly(N-isopropylacrylamide) in Aqueous Media as a Function of Temperature: Molecular Dynamics simulation

محل انتشار:

كنفرانس بين المللي توسعه فناوري در مهندسي شيمي (سال: 1398)

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خلاصه مقاله:

In this research work, the dynamic behavioral changes of Poly(N-isopropylacrylamide) (PNIPAm) with 32 repeating units in water was investigated at different temperatures via molecular dynamics (MD) simulations. The built models of PNIPAm/water solutions were at a dilute concentration regime. The considered temperature range was from below to above the PNIPAm lower critical solution temperature (LCST), 305 K. This study was implemented to measure the influence of temperature on the dynamic behavior of PNIPAm chain as a thermoresponsive polymer in water

کلمات کلیدی: Poly(N-isopropylacrylamide), PNIPAm, MD simulation, Dilute polymer solution, Dynamic behavior

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