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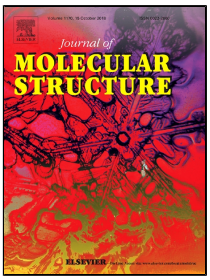

Simulation study on the relationship between the crosslinking degree and structure, hydrophobic behavior for poly (styrene-co-divinylbenzene) copolymer

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Simulation study on the relationship between the crosslinking degree and structure, hydrophobic behavior for poly (styrene-co-divinylbenzene) copolymer

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Keywords

Poly (styrene-co-divinylbenzene), Crosslinking degree, Structure, Hydrophobic behavior, Molecular simulation

ABSTRACT: Molecular dynamics (MD) and Grand Canonical Monte Carlo (GCMC) simulation were employed to investigate the relationship between the crosslinking degree and structure, hydrophobic behavior for poly (styrene-co-divinylbenzene) （P(S-DVB)）copolymer. The structure properties of P(S-DVB) with different crosslinking degree were evaluated by density, fractional free volume (FFV) and glass transition temperature (T_g). The magnitude of the hydrophobicity of P(S-DVB) polymer was quantitatively assessed by solubility parameter, surface energy, interfacial interaction of P(S-DVB) coating-water system and adsorption isotherms. The simulation results identically showed its hydrophobicity decreased with the increase of crosslinking degree. Moreover, the free energy of interaction