

热力学

凝胶网络中溶剂性质的分子动力学模拟

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摘要 本文利用分子动力学(MD)方法模拟了三种不同结构的凝胶网络系统, 对系统的压力、溶剂的自扩散系数以及溶剂在凝胶不同区域的密度分布等进行了考察。模拟结果表明, 被吸收进入凝胶网络的溶剂的性质与纯溶剂的性质有很大的差别, 但凝胶结构的不均匀性对凝胶网络中溶剂的性质几乎没有什么影响。

关键词 [分子动力学](#) [凝胶网络](#) [扩散系数](#) [密度分布](#)

分类号

Molecular dynamics simulation of properties of solvent in gel network

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Abstract

Three kinds of gel networks with different structures were studied via molecular dynamics (MD) simulation. Both the pressure and the self-diffusion coefficient of the solvent were investigated in detail, as well as the density distribution of the solvent in different regions of gel networks. The simulated results showed that the heterogeneity of gel structures had little influence on the properties of the solvent in the studied gel networks, although there was considerable difference between pure solvent and the solvent in the gel networks.

Key words [molecular dynamics](#) [gel network](#) [diffusion coefficient](#) [density distribution](#)

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