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传递现象

氨基酸扩散系数的分子动力学模拟

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摘要 采用分子动力学模拟的方法模拟了298. 15 K正则系综下甘氨酸、丙氨酸等12种氨基酸在水中的扩散过程，扩散系数的计算采用微分-区限变分法。计算结果表明：相同浓度下按不同分子数样本计算得到的扩散系数有较大差别，且分子数越多则模拟结果越接近于实验值。5种氨基酸在水中的扩散系数与文献值相对比，误差小于7%。还用同样的方法模拟了氧气在水中的扩散过程，模拟结果与实验结果吻合也较好。实验表明采用分子模拟手段可以获得具有工业应用价值的扩散系数，从而有助于计算传质学的发展。

关键词 分子动力学模拟；氨基酸；扩散系数

分类号

Molecular dynamics simulation of amino acid diffusion coefficient

Abstract

By using molecular dynamics (MD) simulation, the diffusion of 12 amino acids, such as glycine and alanine was simulated at 298. 15 K with constant NVT ensemble trajectory, and the diffusion coefficients were calculated with differentiation-interval variation. The results showed that the diffusion coefficients of the same solution differed greatly when they were calculated with different molecule-number samples, and the one which was calculated with the sample with the maximum number of molecules was closest to the experimental value. Comparing calculated diffusion coefficients of 5 amino-acids in water with the values reported in literature showed an error less than 7%. Furthermore，the diffusion of oxygen in water was simulated with the same method, and satisfactory results in good agreement with the experimental value were obtained. This paper is aimed to show that the diffusion coefficients for industrial use can be calculated with the MD simulation method, which would be helpful to the development of computational mass transfer theory.

Key words molecular dynamics simulation；amino acid；diffusion coefficient

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