化学学报 1996 54 (4): 331-337 ISSN: 0567-7351 CN: 31-1320/06

液态水的分子动力学模拟

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 用分子动力学(MD)模拟方法在150~376K的温度范围内对液态水的微正则系统进行了研究。考察了液态水的结构及其性质。模拟采用了由从头算得出的柔性水-水相互作用势MCYL。对时间和空间的平均得出了液态中水分子几何构型及温度改变所引起的液态水结构变化。对径向分布函数gOH, gOO, gHH及配位数的分析表明, 在所考察的温度范围内, 每个水分子与相邻分子形成的氢键数为2~3, 水分子在参与的2个氢键中同时作为授受体。结合对振动谱的研究表明在低温时液态水形成的网络结构可能随温度的升高而形成小的簇结构。

关键词 水 热力学性质 从头计算法 分子动力学 国家教委高等学校博士学科点专项科研基金 势函数

分类号 0643

Molecular dynamics simulation of liquid water

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Abstract The microcanomical ensemble of liquid water was studied by using molecular dynamics simulation at temperatures ranging from 150 to 376K. The structure and the thermodynamic properties were investigated. Flexible water-water interaction potential MCYL was used in the simulation. The effects of temperature on the geonetry of water molecules and on the structure of liquid water were averaged over both the time and space. The analysis of the radial distribution functions shows that there are 2~3 hydrogen bonds formed for each water molecule, and the molecule in liquid form acts both as donor and receptor. The studies on the vibrational spectra indicate that network structure of water at lower temperature mingt turn into the small chuster structure as temperature goes higher.

Key words WATER THERMODYNAMIC PROPERTIES AB INITIO CALCULATION MOLECULAR DYNAMICS POTENTIAL FUNCTIONS

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