作者	倪科
中文题名	液态水层流粘性的微观机理研究
英文题名	Research on the microscopic mechanism of the viscosity of liquid water in lamin
	ar flow
中文关键词	液态水,层流,粘性,氢键
英文关键词	viscosity, hydrogen bond, liquid water, laminar flow
中文文摘	粘性作为液态水的重要物理特性,反映了水抵抗剪切作用的能力,决定了溶质输送和能量传 递的效率。传统上认为水的粘性主要由分子间作用力和分子热运动产生的动量交换而产生。 粘性的测量实验结果表明,粘性受温度和压强的影响。不过在粘性的测量实验中均要求雷诺 数(Re)非常小,在一定流速下会失效。自然界中的流动均具有一定的速度,为了研究液态 水运动时溶质输移过程的合理预测,需考虑不同流动状态对液态水粘性的影响。本文选取 简单的流动状态——层流,对液态水粘性的微观机制以及层流中粘性的变化规律进行研究, 主要内容包括以下四个方面。(1)利用量纲分析法和量子化学从头计算法建立液态水粘性和 氢键结构变化之间的定量关系,采用回归分析法定量计算了分子间作用力和分子热运动产生 的热量交换在不同温度下对粘性的贡献。研究结果表明,在较低温度下,液态水粘性由氢键 结构的变化产生;随着温度的升高,液态水内氢键变化加快,氢键平均寿命减小,粘性也随 之减小。在较高温度下的分子热运动产生的动量交换对液态水粘性的影响不能忽略,当温度 逐渐升高直到水的沸点,分子热运动引起的动量交换对粒态水粘性的影响不能忽略,当温度 逐渐升高直到水的沸点,分子热运动引起的动量交换对粘性的贡献越来越大,甚至超过 50%。 (2)利用红外光谱法开展液态水层流的观测实验,借助于液态水粘性的氮心不同温度下液 态水粘性随 Re 的增大均呈现先增大后减小的规律,不同 Re 下液态水粘性的变化幅度随着温 度的升高而减小。(3)利用分子动力学模拟法验证了不同温度下液态水粘性随 Re 的变化规 律,并对不同温度和 Re 条件下氢键结构因子进行了统计,发现同一温度下氢键的平均结构 与层流流动状态无关,因而氢键结构的变化可以通过氢键结构因子和 Re 这两个独立变量来 反映,进而可以液态水层流粘性可以表达成二者的函数形式。(4)将神经网络方法与分子动 力学方法进行结合,应用于水分子团簇结构的能量和动力学的计算过程中。研究结果表明, 神经网络方法在兼顾精度的同时可以有效改善计算效率,从而可以应用于大体系的计算。
外文文摘	As one of the most important physical properties of liquid water, viscosity ref lects the resistance of water to shear stress and determines the efficiency of solute transport and energy transfer. It is widely accepted that the viscosity of water is mainly caused by the exchange of momentum between intermolecular fo rces and molecular thermal motion. Large amounts of experiment results for visc osity measurements convey the idea that viscosity is affected by temperature an d pressure only. However, Reynolds number (Re) is required to be very small in the experiments for viscosity measurements, which will fail at higher flow rate s. In natural world, water always flows at a certain rate, which is far from st ationary state. Therefore, it is necessary to take into account the effects of flow state on the viscosity of water, for the purpose of accurate calculation o f water flow and reasonable prediction of the solute transport process. In this paper, we choose a simple flow type, laminar flow, to study the microscopic me chanism of the viscosity of liquid water, as well as the change of viscosity in laminar flow. The main contents include four aspects as follows. Firstly, the quantitative relationship between the viscosity of liquid water and the change of hydrogen bonding structure is determined by using dimensional analysis and a b initio calculation, and regression analysis is used to quantitatively calcula te the contribution of two factors, namely intermolecular forces and momentum e xchange of molecular thermal motion, to the viscosity of liquid water at differ ent temperatures. The results show that at lower temperatures, the viscosity of

	liquid water is generated by the change of hydrogen bonding structure. As the
	temperature increases, the change of hydrogen bonds in liquid water is accelera
	ted with a decrease of the average lifetime of hydrogen bonds, so the viscosity
	decreases as well. The influence of momentum exchange of molecular thermal mot
	ion should not be neglected. When the temperatures increases, this factor plays
	a more and more important role in contributing to the total viscosity, with a
	contribution of over fifty percent at the boiling point of water. Secondly, the
	infrared (IR) spectroscopy experiments for laminar flow of liquid water is con
	ducted. The measurement of viscosity is replaced by the detection of O-H stretc
	hing vibration in liquid water by means of quantitative correlation between the
	viscosity of liquid water and the structure of hydrogen bonds. The results sho
	w that the viscosity of liquid water increases with the increase of Re at diffe
	rent temperatures, and the maximum change of viscosity at different Re decrease
	s as the temperature increases. Thirdly, the variation of viscosity of liquid w
	ater with Re at different temperatures is verified by molecular dynamics simula
	tion. The structure factor of hydrogen bonds is statistically analyzed as well.
	There seems to be no connection between the average structure of hydrogen bond
	s and the flow rate of laminar flow at the same temperature. Therefore, the cha
	nge of hydrogen bonding structure can be reflected by the two independent varia
	bles, the structure factor of hydrogen bonds and Re. The viscosity of liquid wa
	ter in laminar flow can be expressed as a functional form of the two variables.
	Finally, neural network method is combined with molecular dynamics method to c
	alculate the energy and dynamics of the structure of water clusters. The result
	s show that the neural network method can effectively improve the computational
	efficiency while taking into account the accuracy, so it can be applied to the
	calculation of large-scale systems.
答辩日期	2019. 09. 07