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中文题名	液态水的氢键网络结构与粘性机理研究
英文题名	Research on Hydrogen Bond Structures of Liquid Water and the Mechanism of Structural Response on Viscosity
中文关键词	水沙动力学;液态水;粘性;氢键网络结构
英文关键词	water-sediment dynamics;liquid water;viscosity;hydrogen bond network
中文文摘	<p>液态水是最常见的流体，拥有一系列特殊的物理和化学性质，这些性质主要归因于水分子之间所形成的氢键结构。氢键相互连接形成三维氢键网络，其中存在环结构、片元、团簇等结构，这些结构对外界条件变化很敏感，同时，水分子氢键网络的微观结构也是影响宏观输移性质的重要因素。本文提出了基于水分子氢键网络结构研究液态水宏观性质的理论和方法，通过温度、离子溶液、剪切作用等环境变量影响水分子结构，定量分析不同工况下水分子结构与粘性之间的响应机制。主要内容包括以下三个方面。（1）提出一种基于图论的液态水氢键网络分层团簇搜索方法，分别定义氢键、环结构、片元、团簇为第一、第二、第三和第四级结构。该算法能基于图团体检测搜索获得拥有特征结构的“有限”团簇结构。水分子团簇形态具有分形的特征，并且偏好于特定拓扑连接方式，并且发现其与氢键网络密度涨落存在密切的关系，团簇代表高密度区域。（2）利用分子动力学研究了温度、离子溶液、剪切作用下水分子结构的变化规律，定量分析其通过结构变化造成粘性改变的物理机制。温度导致水分子热运动加剧，削弱氢键网络连接性，导致粘性减少。离子通过替代作用影响水分子-离子团簇（离子第一壳层）内的水分子氢键结构，水分子-离子团簇的静电效应与离子占据空间阻碍扩散的体积效应共同引起氢键网络重塑，进而导致粘性的变化。高剪切作用通过对水分子结构产生压缩轴破坏-延伸轴形成的各项异性影响，破坏水分子氢键网络，进而导致粘性减小，出现剪切稀释。（3）总结出粘性与温度、离子溶液、剪切作用等多个环境因素之间的具体表达式，通过理论推导、经验拟合等方法分析了在不同温度、离子溶液、剪切作用等外界条件下粘性对氢键网络结构变化的响应机制，发现两者之间存在幂律关系，定量揭示了液态水微观结构与宏观性质之间的联系。</p>
外文文摘	<p>Liquid water is the most common fluid in nature, with a series of special physical and chemical properties that are mainly attributed to the formation of hydrogen bonds between water molecules. Hydrogen bonds form a complex three-dimensional hydrogen bond network, within which there are many structures such as rings, fragments, and clusters. These structures are highly sensitive to changes in external conditions. Meanwhile, the microscopic structure of the hydrogen bond network is also a crucial factor for influencing macroscopic transport properties. This article proposes a theory and methodology for studying the macroscopic properties of liquid water based on the hydrogen bond network structure of water molecules. By analyzing the impact of environmental factors such as temperature, ionic solutions, and shear effects on the structure of water molecules, this study quantitatively analyzes the response of water structures on viscosity under different conditions. The main content includes the following three aspects. (1) A hierarchical clustering method for the hydrogen bond networks of liquid water based on graph theory is proposed. Hydrogen bonds, rings, fragments, and clusters are defined as the first, second, third, and fourth levels of structure, respectively. This algorithm can search for "finite" clusters with characteristic structures based on graph community detection. The morphology of water clusters exhibits fractal characteristics and the clusters prefer specific topological connections. At the same time, there is a close relationship between water clusters and hydrogen bond network density fluctuations, and the clusters represent high-density regions. (2) Molecular dynamics simulations are used to investigate the changes of water structures under the influence of temperature, i</p>

	<p>onic solutions, and shear effects, and quantitatively analyze the physical mechanisms that lead to changes in viscosity by structural changes. Temperature increases the thermal motion of water molecules, and it weakens the connectivity of hydrogen bond network, resulting in a decrease in viscosity. Ions affect the hydrogen bond structure of water molecules within water-ion clusters (the first shell of ions) via substitution effects. This effect, combined with the spatial hindrance of ions, leads to the rearrangement of the hydrogen bond network and ultimately changes in viscosity. Shear effects have anisotropic effects on water structures, and destroy the hydrogen bond network of water molecules, leading to shear thinning where the viscosity of liquid water decreases with increasing shear rate. (3) The correlations between viscosity and many environmental factors such as temperature, ionic solutions, and shear are summarized. By using induction and derivation methods, it is found that the response of viscosity to hydrogen bond structures under different temperatures, ionic solutions, and shear conditions is a power law relationship, revealing the relationship between the microscopic structure and macroscopic properties of liquid water.</p>
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