

Liquid Water Diffusion at Molecular Level

ScienceDaily (Feb. 24, 2012) — Researchers at the universities of Granada and Barcelona have described for the first time the diffusion of liquid water through nanochannels in molecular terms; nanochannels are extremely tiny channels with a diameter of 1-100 nanometers that scientists use to study the behavior of molecules (nm, a unit of length in the metric system equal to one billionth of a meter that is used in the field of nanotechnology).

This study might have an important impact on water desalination and filtration methods. Two articles published in *Science* state that the introduction of graphene membranes and carbon nanolayers will revolutionize water desalination and filtration processes, as water diffuses rapidly through these materials when their pores are 1nm in diameter.

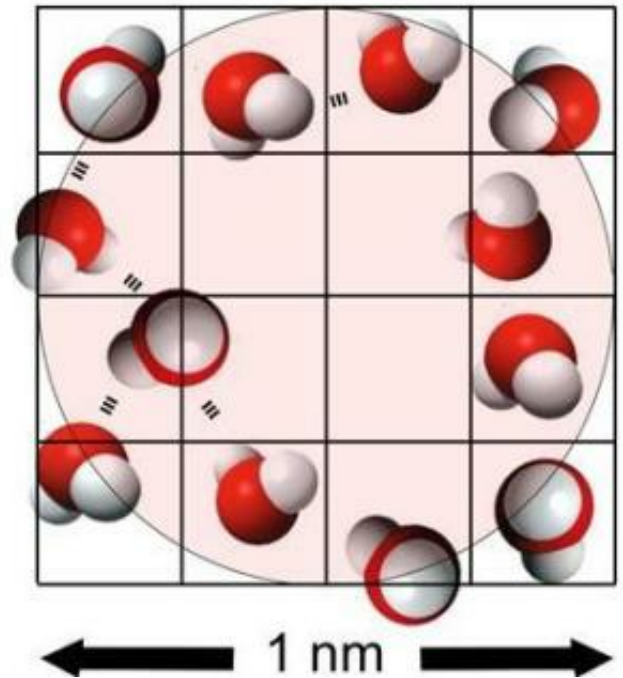
Liquid water exhibits a range of unusual properties that other chemical compounds do not have: up to 65 abnormalities. Some of these abnormalities have been known for 300 years, such as the fact that water expands below 4°C.

Many of the abnormalities found in water have a dynamic nature -- e.g. water molecules move faster as density increases -- as a result of the properties of the hydrogen bond networks that form between water molecules; hydrogen bonds lead to the formation of tetrahedral structures wherein a central atom is located at the center with four molecules located at the corners. However, this geometrical structure changes with pressure and temperature and, until now, changes in the molecular structure and properties of liquid water had not been described.

A Mystery to Solve

Particularly confusing are the results on the diffusion of water confined between two hydrophobic plates. Neither experiments nor computer-based models have clarified whether confinement increases or reduces the mobility of water molecules. However, it seems that the mobility of water molecules relies on ducts having a diameter above or below 1nm.

In a study published in the journal *Physical Review*, professors Francisco de los Santos Fernández (University of Granada) and Giancarlo Franzese (University of Barcelona) described the behavior of water



Potential arrangement of 12 water molecules and their HBs within the cooperative 1nm region. (Credit: Image courtesy of University of Granada)

confined between two hydrophobic plates. In their study, Franzese and Fernandez used models to demonstrate that the diffusion of nanoconfined water is unusually fast, as a result of the competition between the formation and breaking of hydrogen bonds, and the free volume available for cooperative molecule rearrangement.

In nanochannels above 1 nm in diameter, macroscopic diffusion of water only occurs if there is a cooperative rearrangement of molecules, which leads to HB breaking within a cooperative region of 1nm in size. On the other hand, diffusion increases in nanochannels below 1 nm, as fewer HBs need to be broken. Thus, this study proves that the interplay between hydrogen bond breaking and cooperative rearranging within regions of 1-nm determine the macroscopic properties of water.

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Journal Reference:

1. Francisco de los Santos, Giancarlo Franzese. **Relations between the diffusion anomaly and cooperative rearranging regions in a hydrophobically nanoconfined water monolayer.** *Physical Review E*, 2012; 85 (1) DOI: [10.1103/PhysRevE.85.010602](https://doi.org/10.1103/PhysRevE.85.010602)

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