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MRET Treated Water as a Special Case of Confined Water (Review)

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ABSTRACT

Water, under nanoscale confinement, exhibits structural, dynamical behaviors that differ profoundly from its unconfined counterpart. The nanoscale confined water exhibits the anomalous reduction of viscosity, dielectric permittivity and conductivity. The significant reduction of the MRET (Molecular Resonance Effect Technology, US Patent # 6022479) water values of electrical conductivity, dielectric permittivity and viscosity confirm the relatively high, long range dynamic structuring of water molecules in activated water produced by the MRET activation process. It allows to consider MRET treated water as a special case of the confined water.

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Introduction

Water is essential for almost every aspect of life on our planet and, unsurprisingly, its properties have been studied in great detail. However, only a minute amount of information remains known about the electrical properties of interfacial and strongly confined water, in which the structure deviates from that of unconfined water. Confined water becomes distinctly layered. The structural change is hypothesized to affect the conductivity of water and particularly its polarizability, which in turn modifies intermolecular forces that play a crucial role in many physical and chemical processes [2].

Another intriguing property of the strongly confined water is an exceptionally low viscosity. This phenomenon can be explained due to the specific polarized oriented formation of the water molecular structure. The described structure, characterized by high intra-layer hydrogen bonding and low inter-layer coupling, typically defines **2D-layered materials or molecular assemblies**, such as specific 2D-Covalent Organic Frameworks (COFs) or hydration layers around hydrophobic molecules. This structure results in strong, stable in-plane interactions and weak, often disordered, interactions between layers. Strong, often long-range hydrogen bonding or covalent bonding holds the 2D sheet together.

Discussion

In hydrated systems, water molecules can form a strongly hydrogen-bonded, structured shell within the layer. Weak van der Waals forces or very weak hydrogen bonding allows for sliding or separation, often leading to distinct separation of, for example, hydration layers around hydrophobic molecules. Certain 2D-COFs are specifically designed with this structure for enhanced stability or functionality. This configuration is also found in the hydration layers of hydrophobic molecules, where the first shell is highly ordered, and the second shell is less coupled. The structural alignment can lead to enhanced molecular properties such as higher proton mobility, distinct phase behaviors on nanoscopic scales, or unique spectroscopic signatures in water layers. [6-8] Low viscosity of water (for example, when the temperature rises or when exposed to specific magnetic fields) is directly related to **breaking the hydrogen bonds** that hold molecules together. Breaking the bonds changes the cluster structure: At low viscosity, the hydrogen bond network becomes less ordered. Bond angles become distorted, and molecules begin to change partners more frequently, making the structure **dynamic** rather than static. Clusters become smaller. Instead of stable frameworks of dozens of molecules (reminiscent of the hexagonal structures of ice), smaller groups—dimers and trimers—predominate. Paradoxically, the destruction of bulky "hollow" clusters allows molecules to move closer together. This increases mobility (fluidity), as molecules can more easily "slide" past each other. In specific cases, such as 1D confinement (within carbon nanotubes of <1 nm), extremely low viscosity is achieved precisely because water forms highly ordered, linear "single-file" chain clusters that act like a conveyor belt, reducing intermolecular friction.

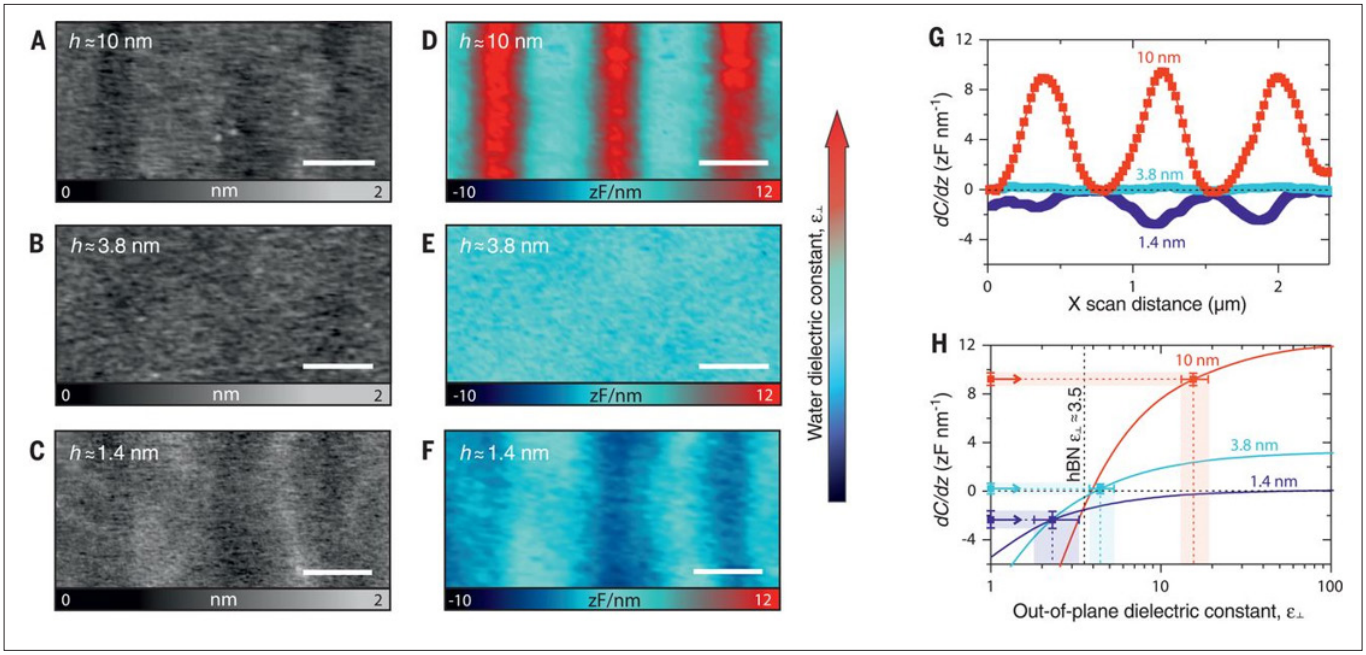

Figure 1: Water confined to sub-nanometer spaces (around 1-2 nm) exhibits an anomalously low out-of-plane dielectric constant (ε1≈ 2-4) and low conductivity, fundamentally differing from bulk water (ε≈80). This "electrically dead" layer, only 2-3 molecules thick, arises because confinement inhibits the rotational freedom of water dipoles, preventing their alignment with an external field [7].

The dielectric constant ε of interfacial water has been predicted to be smaller than that of bulk water (ε≈ 80) because the rotational freedom of water dipoles is expected to decrease near surfaces, yet experimental evidence is lacking. We report local capacitance measurements for water confined between two atomically-flat walls separated by various distances down to 1 nm. The experiments reveal the presence of an interfacial layer with vanishingly small polarization such that its out-of-plane ε is only ~ 2. The electrically dead layer is found to be two to three molecules thick. These results provide much needed feedback for theories describing water-mediated surface interactions and behavior of interfacial water, and show a way to investigate the dielectric properties of other fluids and solids under extreme confinement [7].

Water, under nanoscale confinement, exhibits structural, dynamical behaviors that differ profoundly from its unconfined counterpart. Low-Dimensionality Confinement (often called quantum confinement) is a physical phenomenon that occurs when the motion of charge carriers (electrons or holes) is restricted in one or more dimensions on the nanometer scale. The classification of systems depends on the number of dimensions in which charge carriers can move freely. When water is confined between surfaces (e.g., graphene or hBN) below 1.4 nm, the dielectric constant drops from 80 towards 2.1, a value closer to ice or even lower, depending on the confinement thickness. **Confinement Effect on Conductivity**: While confinement can enhance in-plane conductivity, the *interfacial layer* itself often shows highly **reduced** conductivity perpendicular to the surface. Under confinement, water's electrical properties become highly anisotropic, with the permittivity decreasing perpendicularly but behaving differently parallel to the interface. The reduction is heavily dependent on the hydrophobicity of the confining walls and the ability of water to form a robust, ice-like, or layered structure at the surface.

Thus, the confinement effect on the bulk water has three main characteristics such as the reduction of viscosity, dielectric permittivity and conductivity. This phenomenon quite closely resembles the anomalous physical parameters of the bulk water after MRET treatment. The electrical conductivity of MRET activated water at 20◦C in the range of frequencies 0.1Hz- 100 kHz decreased by 77-90% in 30-minute activated water and by 66-70% in 60-min-activated water respectively, compared to non-activated distilled water. The dielectric permittivity in the very low frequency range, 0.1-1000 Hz, decreased by 80-90%, and in the range of frequencies 1-100 kHz and decreased by 18% in the 30 minute activated water; a decrease by 70-85% was observed in the range 0.1-1000 Hz in the 60-min-activated water compared to non-activated water [9].

In the area of very low tangent pressure magnitudes close to zero (the tangent pressure **τ** in the range of **0.004 - 0.005Pa**), the value of viscosity of regular non-activated water in compliance with the phenomenon of *adhesion* sharply increased 150 - 250 times, for instance, to **η=0.22Pa•s** at **τ=0.004Pa**. In the same area of very low tangent pressure, MRET activated water showed the anomalous effect of the decrease of viscosity about 2 times with a slight difference for both times of activation (slightly higher decrease of viscosity for 30-minute activated water when compared to 60-minute activated water). For instance, the value of viscosity of 30 minutes activated water dropped to **η=0.0004Pa•s** at **τ=0.0045Pa**. As a result of such anomalies the level of difference in the values of viscosity for non-activated and MRET activated water in the range of low tangent pressure magnitudes of **0.004 - 0.005Pa** was registered at the level of **300 - 500 times** for 30 minutes activated water and at the level of **200 - 250 times** for 60 minutes activated water [10].

The significant reduction of the MRET water values of electrical conductivity, dielectric permittivity and viscosity confirm the relatively high, long range dynamic structuring of water molecules in activated water produced by the MRET activation process. It allows to consider MRET treated water as a special case of the confined water.

Main types of systems with limitations/confinements:

- **Quantum Wells are 2D Systems:** Motion is limited in one dimension (e.g., thin film). Carriers are free to move in the plane (x, y), but are "locked" along the axis z.
- **Quantum Wires are 1D Systems:** Motion is limited to two dimensions. Carriers can only move along one line (axis z).
- **Quantum Dots are 0D Systems:** their motion is restricted in all three dimensions. Electrons are confined to a tiny volume, making their energy spectrum completely discrete, like an atom ("artificial atoms").

When the size of the structure becomes comparable to **the Bohr radius of an exciton** or the de Broglie wavelength in the material, the energy spectrum ceases to be continuous and becomes discrete.

When water flows through 1D or 2D channels, its behaviour deviates substantially from the well-established principles of hydrodynamics. This is because reducing the dimensionality of any interacting physical system amplifies interaction effects that are beyond the reach of traditional hydrodynamic equations. In low-dimensional water, hydrogen bonds can become stable enough to arrange water molecules into an ordered state, causing water to behave not only like a liquid but also like a solid in certain respects. The dynamic interaction between low-dimensional water transport and ion-coupled structural features lies at the heart of recent advances in the design and investigation of angstrom-scale biomimetic and neuromorphic channels [8].

Key Effects of Confined Water on Biological Systems

Confined water in biological systems—water restricted in nanopores, near surfaces, or within protein cavities—exhibits altered, slower dynamics and unique structural properties compared to bulk water. Essential for biological functions, it maintains protein folding, enables ion transport through membrane channels, and influences molecular recognition, often behaving as a "pre-melting" phase.

Protein Structure and Dynamics: Bound water molecules form a hydration shell crucial for the stability and dynamics of proteins. This water is relatively immobile and essential for enzymatic activity.

- **Hydrophobic Interactions**: Confined water enables protein folding and aggregation. The structured nature of this water allows it to facilitate the interactions that give proteins their 3D shape.
- **Ion Transport:** In nanopores and membranes, confined water regulates the movement of ions. Its high dielectric constant and restricted movement can assist in selective permeability.
- **Biological Force and Pressure:** Confined water can generate significant pressure, equivalent to as much as 1,000 atm. This allows cells to store energy and create force to manage chemical reactions.
- **Pre-melting Phase:** In very small restricted spaces, water can enter a "pre-melting" phase, behaving as both a liquid and a solid. This state is critical for understanding water-protein interaction.

Key Physical Effects:

- **Increasing the band gap:** As the structure size decreases, the energy of the first level increases. This leads to a "blue shift" —*the* absorption and emission of light occur at higher energies (shorter wavelengths).
- **Discreteness of levels:** Instead of wide energy zones, clearly separated energy levels are formed.
- **Density of States Variation:** The distribution of available energy states changes dramatically with the dimensionality (step-like for 2D, peak-like for 1D, and delta-like for 0D).
- **Slower Dynamics:** The motion of water molecules confined near biological membranes or inside proteins is significantly slower than in bulk water.
- **Lowered Freezing Point:** Confined water often remains liquid far below (0°C), often down to (-45°C) before forming special types of ice, which helps in preventing cell damage at low temperatures.

From a fundamental perspective, the interactions of water and solutes with a confining surface dramatically modify the liquid's structure and, consequently, both its thermodynamical and dynamical behaviors, breaking the validity of the classical thermodynamic and phenomenological description of the transport properties of aqueous systems. Additionally, man-made nanopores and porous materials have emerged as promising solutions to challenging problems such as water purification, biosensing, nanofluidic logic and gating, and energy storage and conversion, while aquaporin, ion channels, and nuclear pore complex nanopores regulate many biological functions such as the conduction of water, the generation of action potentials, and the storage of genetic material [1].

This "biological" water acts more like a structural component of the cell rather than just a solvent, influencing cellular osmoregulation, hydration, and overall functioning.

How can the nanoscale confinement and its special case, such as MRET treatment, affect structural characteristic of water molecules? Large water molecular cluster formation (such as in liquid water or ice) causes a **distortion of the intramolecular covalent bonding angle** (H-O-H) from the isolated, gas-phase value of roughly 104.5°-105°, but it generally acts to change it toward a more symmetric, tetrahedral angle closer to 109.5°. The formation of hydrogen bonds, especially in large, dense clusters, weakens the covalent O-H bonds, but the specific, long-range alignment often causes the tetrahedral angle to open slightly. The covalent bond angle of 114.5° (or values close to it in the range 114.5°- 114.1°) in the scientific literature is often associated not with the internal covalent angle of one molecule, but with **the angle of the acceptor hydrogen bond** in specific cluster configurations. In the hydrogen bonded networks, the water clusters represent ring-concentrated regions where different constitution of ring structures implies structural heterogeneity closely related with the arrangement of hydrogen bond networks. The spatial distributions of clusters suggest microscopic local structures between clusters [3].

Specific angles in clusters (114.5°): In some models (e.g., in studies of 2222 type clusters) the angle between the vector O-H acceptor molecule and the line connecting the oxygen centers (H-O...O), can reach 114.1°- 114.5° such high values are characteristic of "strained" geometries in multi-particle interactions, where the molecule is simultaneously both a donor and an acceptor of several bonds.

These observations suggest that the nature of the O−H···O hydrogen bond in water clusters is determined by the inductive effects originated by the different spatial arrangements of the water molecules in the studied clusters [4].

The results show that the cooperative effects of hydrogen bonding in small water clusters arise from a compromise between: 1) the deformation energy (i.e., the energy necessary to modify the

electron density and the configuration of the nuclei of the isolated water molecules to those within the water clusters), and 2) the interaction energy (Eint) of these contorted molecules in (H2O) n. Whereas the magnitude of both deformation and interaction energies is enhanced as water molecules are added to the system, the augmentation of the latter becomes dominant when the size of the cluster is increased [5].

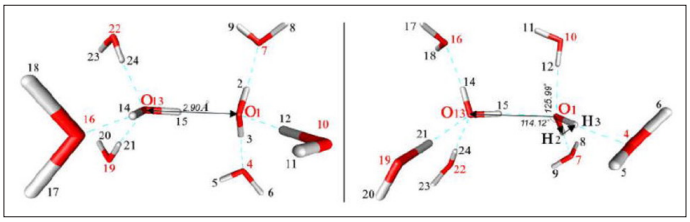

Figure 2: A 2222 cluster (maximum number of neighbors). The O - O distance is shown as 2.90 Å, and the HO---O (HO from the acceptor molecule, latter O is the central donor oxygen) angle as 114.12°. The dihedral angle formed by the central acceptor water plus the central donor oxygen is 125.99° [6].

Fig.2 illustrates the 2222 cluster, and it gives the initial values of the principal distances and angles. The constrained cluster was very close to the unconstrained cluster in all parameters: unconstrained bond lengths ranged from 0.9611 to 0.9699 Å, constrained value 0.9641 Å for all four O-H covalent bonds. The "unconstrained pair" was defined by taking the initial central pair, freezing all oxygen atoms (2 to 8 oxygens), and optimizing the hydrogens only. These conditions produced the very limited ranges of distance and angle that are defined as unconstrained here. Bond angles were 105.21 to 105.61. (unconstrained), 105.40 (constrained); the dihedral defined as d4 above was frozen at zero for the unconstrained as well as the constrained dimer, but is in any case <1°. Variables were scanned with and without the constraints. This gives O - O distance 2.90056 Å vs. 2.90046 Å (constrained). The angle defined by the two donors and the H covalently bonded on the acceptor (a3 above) was 114.08° vs 114.12° (constrained). The dihedral given by the two oxygens and the two hydrogens on the acceptor molecule (d3 above) was 126.1° vs 126.0° on the constrained pair. Other results were also very close: Energy, -152.96350 H vs. -152.96306 H (constrained) (We use energy units of Hartrees (H), or millihartrees (10-3 H, written mH) throughout this paper. 1 mH ≈ kBT, where kB = Boltzmann's constant, T = temperature (K)), at approximately 300 K, where most simulations of biological interest are done. Electron density at bond critical point is 0.02464 vs. 0.02430 (constrained) [6].

Increasing the number of molecules in a cluster enhances the covalent nature of hydrogen bonds (cooperativity effect), which leads to charge redistribution and further deformation of the geometry of each individual molecule.

Conclusion

The formation of large water molecular clusters causes a slight increase in the water molecule's H-O-H covalent bond angle (closer to the ideal tetrahedral angle of 109.5°) compared to an isolated water molecule (104.5°), primarily driven by the cooperative strengthening of hydrogen bonds and charge redistribution. As the hydrogen-bonded network grows (dimer, trimmer, larger clusters), the angular strain within the cluster decreases, often leading to more tetrahedral coordination, particularly in three-dimensional, cage-like structures, unlike the special case of the confined water. In specific cases, such as 1D confinement (within carbon nanotubes of <1 nm), extremely low viscosity is achieved precisely because water forms highly ordered, linear "single-file" chain clusters that act like a conveyor belt, reducing intermolecular friction. The anomalous characteristics of the confined water such as extremely low viscosity, decreased dielectric permittivity and conductivity allow us to consider MRET treated water as a special case of the confined water. The reviewed results of the current scientific investigations allow us to conclude that MRET treatment of the bulk water leads to the formation of extremely large molecular clusters with a high range of cooperation. This new configuration leads to charge redistribution and further deformation of the geometry of each individual molecule. As a result, the MRET treatment of water can leads to the specific external angles in clusters which can reach 114.5° depending on the type of neighbor (donor/acceptor).

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