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Structural and Dynamic Properties of Bulk and Confined Water

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INTRODUCTION

The structural and dynamic properties of bulk water are now mostly well understood in some ranges of temperatures and pressures. In particular, in many investigations using different techniques, such as X-ray diffraction, neutron scattering, nuclear magnetic resonance (NMR), differential scanning calorimetry (DSC), molecular dynamics (MD), and Monte Carlo (MC), simulations have been performed in the deeply supercooled regime (1–10), and in a situation where the effects due to the hydrogen bonding are dominant.

However, in many technologically important situations, water is not in its bulk form, but instead attached to some substrates or filling small cavities. Common examples are water in porous media, such as rock or sand stones, and water in biological material as in the interior of cells or attached to surfaces of biological macromolecules and membranes. This is what we define here as the "confined" or the "interfacial water."

Water in confined space has attracted a considerable interest in the recent years. It is commonly believed that the structure and dynamics of water are modified by the presence of solid surfaces, both by a change of hydrogen bonding and by modification of the molecular motion, which depends on the distance of water molecules from the surface.

Understanding of the modification from bulk liquid water behavior when water is introduced into pores of porous media or confined in the vicinity of metallic surfaces is important to technological problems, such as oil recovery from natural reservoirs, mining, heterogeneous catalysis, corrosion inhibition and numerous other electrochemical processes. Water in porous materials, such as Vycor glass, silica gel, and zeolites, has been actively under investigation because of its relevance in catalytic and separation processes. In particular, the structure of water near layer-like clay minerals (11–12), condensed on hydroxylated oxide surface (13), confined in various types of porous silica (14–22) or in carbon powder (23) has been studied by neutron and/or X-ray diffraction.

In the field of biology, the effects of hydration on equilibrium protein structure and dynamics are fundamental to the relationship between structure and biological function (24–30). In particular, the assessment of perturbation of liquid water structure and dynamics by hydrophilic and hydrophobic molecular surfaces is fundamental to the quantitative understanding of the stability and enzymatic activity of globular proteins and functions of membranes. Examples of structures that impose spatial restriction on water molecules include polymer gels, micelles, vesicles and microemulsions. In the last three cases, since the hydrophobic effect is the primary cause for the self-organization of these structures, obviously the configuration of water molecules near the hydrophilic-hydrophobic interfaces is of considerable relevance.