# IN QUEST OF A WATER MODEL DESCRIBING HYDRATION OF BIOLOGICAL MACROMOLECULES


## Summary

The first model of liquid water at atomic resolution was proposed as early as in 1933. Since that time a vast amount of data concerning both microscopic and macroscopic parameters describing hydration phenomena has been collected. Majority of experimental and theoretical studies pointed out that the main driving force of the so called "hydrophobic interactions" is an entropic effect connected with the solute-induced reorganization of solvation shells. Water molecules surrounding apolar solutes were shown to organize in ice-like structures, the properties of which, in particular molecular packing, proton relaxation rates, distribution and strength of intermolecular H-bonds, differ significantly from those determined for the bulk water. Dozens of models were proposed to describe properties of aqueous solutions at different length-scales, but up to 1999 there was no uniform theory of water for the scales varying from nanometers up to millimeters/centimeters, Recently developed LCW model, by K. Lum, D. Chandler and J. D. Weeks, is the first one, which could be applied to a wide range of phenomena including atom hydration, macromolecule solvation, surface wetting, etc.