

Water: from deep undercooling to ultrahigh pressure

Roberto Car,

Princeton University, Princeton, New Jersey 08544, USA

The structure and dynamics of water change dramatically with mutated thermodynamic conditions, from glassy polymorphs, to metastable and stable liquids, all the way to superionic ice forms at extreme pressure and temperature. The huge range of time scales that characterizes these different states of matter cannot be spanned by a unique simulation approach, but requires models with different levels of coarse graining, ranging from continuous random networks and empirical force fields to ab-initio molecular dynamics approaches.