

WATER: FROM AB-INITIO SIMULATIONS TO COARSE GRAINED MODELS

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The unusual properties of water, including the thermodynamic anomalies of the liquid, the existence of more than one amorphous ice form, and the abnormal mobility of the water ions, derive from the tetrahedral network of hydrogen bonds that hold the molecules together. Computer simulations are an essential tool to understand the microscopic origin of these fascinating properties, complementing experiment and theory.

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