The unique structural features of water, ranging from ambient liquid up to supercritical, extreme-pressure conditions: Insights from classical and *ab initio* molecular dynamics simulations.

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Abstract

The complex behavior of water has motivated the scientific community to develop novel theories and methodologies to provide deeper insight into the molecular causes of its anomalies compared to most liquids. A molecular understanding of the water properties is crucial in numerous processes in chemistry, physics, geosciences, biology, and life evolution. Despite long-lasting research efforts, new intriguing properties are still being described and even the phase diagram of water, although systematically explored in the past, is far from being complete. From a theoretical point of view, the investigation of these characteristic structural features of water and the temperature and pressure effects upon them could be achieved by employing multi-scale modeling techniques, ranging from classical or *ab initio* molecular simulation techniques to coarse-graining methods. Our recent multi-scale simulation studies of water [1-7] at a very wide range of temperatures and pressures will be systematically presented, aiming to shed some light on the unique structural features of water at ambient liquid up to supercritical, extreme-pressure conditions.

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