19. Structural and dynamic behavior of atomistic water models in the supercooled regime

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Several atomistic water models reproduce the properties of water reasonably well at ambient conditions. However, at lower temperature the simulations results show discrepancies with some of the properties observed experimentally. Most notably, no spontaneous crystallization is observed even at large degree of supercooling. In this work we present a systematic study of the supercooled regime using a variety of models, including TIP4P-Ew, TIP4P-2005, TIP5P-Ew and Six-Site. We found that all the models show the same qualitative picture characterized by a maximum in the heat capacity followed by a dramatic kinetic slowdown as the temperature decreases even further. These results are consistent with a liquid-liquid phase transition in the metastable regime, as suggested by several authors. After comparing the diffusion coefficient of the different models with the experimental values using a rescaled temperature, we conclude that the TIP5P-Ew produces the better description of supercooled water. Finally, we use this model to quantify the cage effect by the distribution of mean square displacements of the water molecules, the hydrogen bond and cage self correlation functions obtaining the characteristic time scales of relaxation for different supercooled temperatures.