

Are concepts of percolation and gelation of possible relevance to the behaviour of water at very low temperatures?




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Abstract

It is proposed that the unusual low-temperature behavior of liquid water may be interpreted using a simple model based upon connectivity concepts from correlated-site percolation theory. Emphasis is placed on examining the physical implications of the continuous hydrogen-bonded network (or “gel”) formed by water molecules. Each water molecule A is assigned to one of five species based on the number of “intact bonds” (the number of other molecules whose interaction energy with A is stronger than some cutoff V_{HB}). It is demonstrated that in the present model the spatial positions of the various species are not randomly distributed but rather are correlated. In particular it is seen that the infinite hydrogen-bonded network contains tiny “patches” of four-bonded molecules. Predictions based upon the putative presence of these tiny patches for K_T , C_p , and α_p are developed as examples.

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