

## Structural Heterogeneities and Walrafen Pentamers in Liquid Water

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We investigate the degree to which a pentamer-cluster as a unit structure can offer insights regarding local heterogeneities of water. A pentamer-cluster forms from five water molecules, one of which is located at the center of a tetrahedron and the other four are hydrogen bonded to it. The thermodynamic behavior of water may be related to the local arrangements of the molecules, which are strongly affected by the formation of hydrogen bonds. We identify minimum energy configurations of two pentamers interacting via the hydrogen bond and the Lennard-Jones potentials of the oxygen atoms. We observe that the minimum energy configurations are associated with specific configurations corresponding to high-density and low-density local structures. The high-density local structure resembles the local structure of ice VII, and the low-density local structure resembles the local structure of hexagonal ice. In the high-density configuration, the 3.4 Å distance between second neighbors is enhanced, as expected from experimental and molecular dynamic simulation results of high-density water. The interaction between the pentamers can be represented by a double-well potential in one dimension, where the outer well is deeper than the inner well. The outer and the inner wells correspond to the hydrogen bond and the Lennard-Jones interactions of the pentamers respectively. Using this potential, we calculate the loci of the temperature of maximum density and the compressibility maximum.