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Potential Energy Landscape of the Liquid-Liquid Phase Transition in Water and the transformation between Low-Density and High-Density Amorphous Ice N. GIOVAMBATTISTA, CUNY-Brooklyn College, F. SCIORTINO, Universita di Roma La Sapienza, F. W. STARR, Wesleyan University, P. H. POOLE, St. Francis Xavier University — The potential energy landscape (PEL) formalism is a valuable approach within statistical mechanics for describing supercooled liquids and glasses. We use the PEL formalism and computer simulations to study the transformation between low-density (LDL) and high-density liquid (HDL) water, and between low-density (LDA) and high-density amorphous ice (HDA). We employ the ST2 water model that exhibits a LDL-HDL first-order phase transition and a sharp LDA-HDA transformation, as observed in experiments. Our results are consistent with the view that LDA and HDA configurations are associated with two distinct regions (megabasins) of the PEL that are separated by a potential energy barrier. At higher temperature, we find that LDL configurations are located in the same megabasin as LDA, and that HDL configurations are located in the same megabasin as HDA. We show that the pressure-induced LDL-HDL and LDA-HDA transformations occur along paths that interconnect these two megabasins, but that the path followed by the liquid and the amorphous ice differ. We also study the liquid-to-ice-VII first-order phase transition. The PEL properties across this transition are qualitatively similar to the changes found during the LDA-HDA transformation, supporting the interpretation that the LDA-HDA transformation is a first-order-like phase transition between out-of-equilibrium states.

N. Giovambattista
CUNY-Brooklyn College

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