Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Effect of hydrogen bond cooperativity on the behavior of water

KEVIN STOKELY, Boston University — Four scenarios have been proposed for the low–temperature phase behavior of liquid water, each predicting different thermodynamics. The physical mechanism which leads to each is debated. Moreover, it is still unclear which of the scenarios best describes water, as there is no definitive experimental test. Here we address both open issues within the framework of a microscopic cell model by performing a study combining mean field calculations and Monte Carlo simulations. We show that a common physical mechanism underlies each of the four scenarios, and that two key physical quantities determine which of the four scenarios describes water: (i) the strength of the directional component of the hydrogen bond and (ii) the strength of the cooperative component of the hydrogen bond. The four scenarios may be mapped in the space of these two quantities. We argue that our conclusions are model-independent. Using estimates from experimental data for H bond properties the model predicts that the low-temperature phase diagram of water exhibits a liquid–liquid critical point at positive pressure.

Kevin Stokely
Boston University

Date submitted: 27 Nov 2010 Electronic form version 1.4