



Wednesday, February 14th, 2018, 16:15h

Technische Universität Berlin
EW-Building, Room EW 201 (!)
Hardenbergstrasse 36, 10623 Berlin

Prof. Dr. Pablo G. Debenedetti
Princeton University, NJ, USA Isf

„Computational Investigation of the Phase Behavior of Supercooled Water“

Supercooled water exhibits numerous anomalies in its thermodynamic properties. The existence of a metastable phase transition between two liquid phases has been proposed as a thermodynamically-consistent interpretation [1] of experimental data. One of the most interesting scientific controversies of the past few years originates in the claim that the liquid-liquid transition in molecular models of water is really a misinterpreted crystallization transition [2]. Several other free energy studies [3], provide conclusive evidence contradicting this claim. Until very recently, the origin of the discrepancy was not understood. Analysis of the hybrid Monte Carlo code used by Limmer and Chandler sheds light into the origin of the discrepancy.

[1] Poole et al., Nature, 360, 6402, 1992

[2] Limmer and Chandler, J. Chem. Phys., 135, 134503, 2011; J. Chem. Phys., 138, 214504, 2013

[3] e.g., Liu et al., J. Chem. Phys., 131, 104508, 2009; Sciortino et al., Phys. Chem. Chem. Phys., 13, 19759, 2011; Liu et al., J. Chem. Phys., 137, 214505, 2012; Poole et al., J. Chem. Phys., 138, 034505, 2013; Palmer et al., Nature, 510, 385, 2014; Smallenburg and Sciortino, Phys. Rev. Lett., 115, 015701, 2015

We cordially invite everybody who is interested.

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