XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Combining Spectral and Scattering Data to Determine Liquid Water Structure

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Abstract: I will discuss recent experimental and simulation data of liquid water and the picture of fluctuations between high-density (HDL) and low-density (LDL) liquid this has led to [1,2]. I will especially focus on the temperature dependence in the O-O pair-distribution function at intermediate range (< 18 Å), which has recently been measured with good statistics [3-5], as well as x-ray spectroscopic and scattering data and simulations with far-reaching implications for our understanding of structure and dynamics in water. Finally, I will discuss recent experiments following the liquid-liquid (HDL to LDL) transition in ultraviscous water [6].

Key-words: Liquid water, x-ray scattering, x-ray spectroscopy, simulations

Support: This work has been supported by the Swedish Research Council through grant number VR 2016-04875

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