



You are cordially invited to

Simple Two-Dimensional model of Water; Simulation and Theoretical studies of Bulk and Solutions

given by

Prof. Dr hab. Tomaž Urbič

Faculty of Chemistry and Chemical Technology, University of Ljubljana

on September 6, 2024, at 11:00

at the Institute of Physics PAS, Leonard Sosnowski Auditorium

Duration: 45 min + Q&A

The event will also be available on ZOOM, [at this link](#)

Abstract of the talk:

The structures and properties of biomolecules like proteins, nucleic acids, and membranes depend on water. Water is also very important in industry. Overall, water is an unusual substance with more than 70 anomalous properties. The understanding of water is advancing significantly due to the theoretical and computational modeling. There are different kinds of models, models with fine-scale properties and increasing structural detail with increasing computational expense, and simple models, which focus on global properties of water like thermodynamics, phase diagram and are less computationally expensive. Simplified models give a better understanding of water in ways that complement more complex models. Here, we review the modelling of properties of water on different levels, the two-dimensional Mercedes-Benz (MB) models of water.

You are also welcome to join expert discussions on statistical-mechanical models of water after this talk.

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About the speaker:

Prof. Dr hab. Tomaž Urbič graduated from Physics at the Faculty of Mathematics and Physics, University of Ljubljana, in 1998, was awarded his PhD at Faculty of Chemistry and Chemical Technology, University of Ljubljana in 2003. In 2004/05 he spent one year at UCSF, San Francisco USA as a visiting researcher (Fulbright Grant). His main research interests are computer simulation and theoretical methods for liquids, fluids, solutions as well as quantum chemical calculation of properties of various materials and modeling of chemical reactions in microchannels.