

Katedra chemie Přírodovědecké fakulty UJEP

zve studenty, akademiky a odbornou veřejnost na přednášku

What can we learn from doing computer simulations of simple water models?

kterou přednese vážený host

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Termín a místo konání:

POZOR ZMĚNA!

4. září 2024 v 10:00

(konec do 11:00 včetně diskuse)

učebna CP-3.23 v budově CPTO

Anotace přednášky:

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) and rose models of water.