



INSTITUT ZA FIZIKU

ZAJEDNIČKI SEMINAR IF i HBD

27. siječnja 2016. (petak) u 11:00 sati (točno)

Institut za fiziku, Bijenička cesta 46, Predavaonica III krilo

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PMF – Sveučilište u Splitu

Molecular structuring in liquid mixtures

Water and associating liquids constitute the environment where the vast majority of biological processes take place. The physical principles behind the structuring in molecular liquids are also responsible for the large scale associations and the assembly of biological complexes. For that reason, we analyze the microstructure of several liquid mixtures by means of statistical physics. Through computer simulations, we're able to follow the evolution in structure with the change in molar fraction of one component and access static properties such as pair correlation functions and atom-atom structure factors. The investigation is supplemented by Kirkwood-Buff integrals, cluster size distribution analysis and snapshots from the simulations. In this presentation we will focus on two key concepts, definition of simple and complex ordered mixtures and atom-atom structure factors as the signature of the domain formation in complex liquids. We will also discuss connection between domains in molecular liquids and larger scale assemblies such as microemulsions and micelles.

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L. Zoranić is working as assistant professor at the University of Split, Faculty of Science, Department of Physics. Her current research topics are micro-heterogeneous liquids and interaction of the antimicrobial peptides with membrane, mostly studied by classical molecular dynamic simulations. Large part of her work includes teaching diploma and doctorate students at the University of Split. Currently she is the principal investigator of the installation research project "Multi-scale description of meso-scale domain-formation and destruction" funded by the Croatian Science Foundation.