SM&FT 2017 - The XVII Workshop on Statistical Mechanics and nonpertubative Field Theory

Contribution ID: 61 Type: not specified

The BioPhys scientific activity

Friday, 15 December 2017 11:30 (20 minutes)

Experiments are devised to answer theoretical questions and theory is a necessary prerequisite to analyze data and extract useful information. The complexity of biological systems makes extremely difficult to construct models and identify simple questions to ask to experiments. On the other end, models in many cases look overwhelming complicated. In this situation Molecular Dynamics simulation, from ab initio to classical all atoms or coarse grained calculations, may provide foundation for theory and models that cannot only help in asking the right questions but also to assess and interpret experimental data. I will briefly illustrate some of the many interesting results that are being obtained by the research groups participating to the BioPhys IS.

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