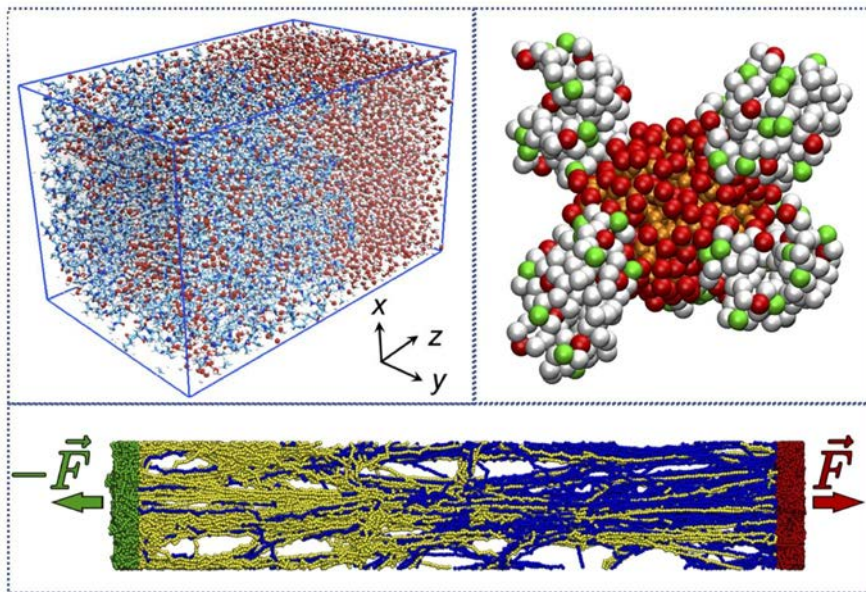


PHYSIKALISCHES KOLLOQUIUM

ANTRITTSVORLESUNG

AM 12. NOVEMBER 2018 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



COMPUTATIONAL PHYSICS OF SOFT AND FLUID MATERIALS

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Macromolecules and complex fluids serve as integral components in the development of modern soft and 'smart' functional materials, e.g., for applications in medicine, liquid phase catalysis, or energy storage devices. From a statistical physics perspective these liquids are typically modelled as classical, interacting many-body systems of varying complexity. While the structural and thermodynamic properties of a 'simple' liquid can still be studied by analytical (statistical mechanics) theory to a wide extent, applied fluid materials display much higher complexity and one typically resorts to particle-resolved (molecular) computer simulations for an accurate treatment. Here, the challenge is to set-up and analyse these 'computer experiments' in a meaningful way and, if possible, to reduce and interpret the large amount of generated data by simple and transparent models. In this way, computer simulations establish an important bridge between theoretical physics and applied material science, providing useful structure-property-function relationships for the rational design of new materials. In this talk I will introduce and discuss these ideas by means of a few illustrative examples of soft and fluid systems of varying complexity, i.e., starting from simple liquids like hard-sphere colloids to fully atomistic models of multi-component electrolytes or polymers relevant for modern applications.