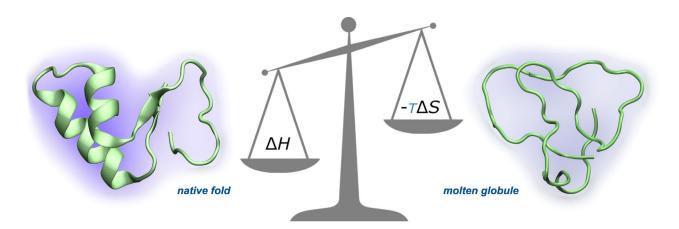


## PHYSIKALISCHES KOLLOQUIUM

AM 20. JANUAR 2025 UM 17 UHR C.T. IM GROßEN HÖRSAAL



## MICROTUBULES' BENDS, CRYO-COOL RIBOSOMES, AND WET PROTEINS HELMUT GRUBMÜLLER MAX PLANCK INSTITUT GÖTTINGEN

The extraordinary diversity and complexity that evolution has produced over the course of around one to two billion years is simply amazing. We are fascinated by the very complex and highly specialized organs that are familiar to us – such as the eye, muscles, and brain. Nevertheless, evolution has achieved its masterpieces much earlier on the molecular level: Without similarly complex biological macromolecules such as proteins, life would be impossible. Combining atomistic computer simulations and statistical mechanics approaches, we are beginning to gain a better understanding of how these highly specialized 'molecular machines' perform their very diverse functions.

We will survey some of the current approaches and challenges of the field. First, we will show how microtubules generate mechanical forces within cells, with a particular focus on the switch between growth/polymerisation and shrinking/depolymerisation phases, driven by GTP hydrolysis. Non-equilibrium atomistic simulations of entire plus-end microtubule tips revealed a tug-of-war between intrinsic microfilament bending and lateral interactions. Second, non-equilibrium shock-freeze simulations of solvated ribosomes reveal how much of the room temperature structural ensemble of these RNA/protein complexes is preserved in single particle cryo-electron microscopy experiments. Third, we will turn our attention towards biomolecular solvation shells, which contribute markedly to protein stability. A new method, permutation reduction, provides access to spatially resolved statistical mechanics of protein solvation.

AKTUELLE INFORMATIONEN FINDEN SIE HIER: WWW.PHYSIK.UNI-FREIBURG.DE

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