

NANOMACHINES AT WORK

HELMUT GRUBMÜLLER

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We will describe four routes towards revealing molecular dynamics and function of biological macromolecules such as proteins, combining high performance atomistic simulations, cryo- electron microscopy, statistical mechanics, and Bayesian approaches.

(1) We address how microtubules switch between growing and shrinking phase. (2) For shock freezing of fully solvated ribosomes we quantify how much of their structural heterogeneity and dynamics is preserved in cryogenic electron microscopy samples. (3) We show for the protein crambin that more than half of the solvent entropy contribution arises from induced water-water correlations. (4) We address structure refinement from single molecule femtosecond XFEL diffraction images.

FRIDAY,
20.10.2023

2:00 PM

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SEMINAR ROOMS I-III
&
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