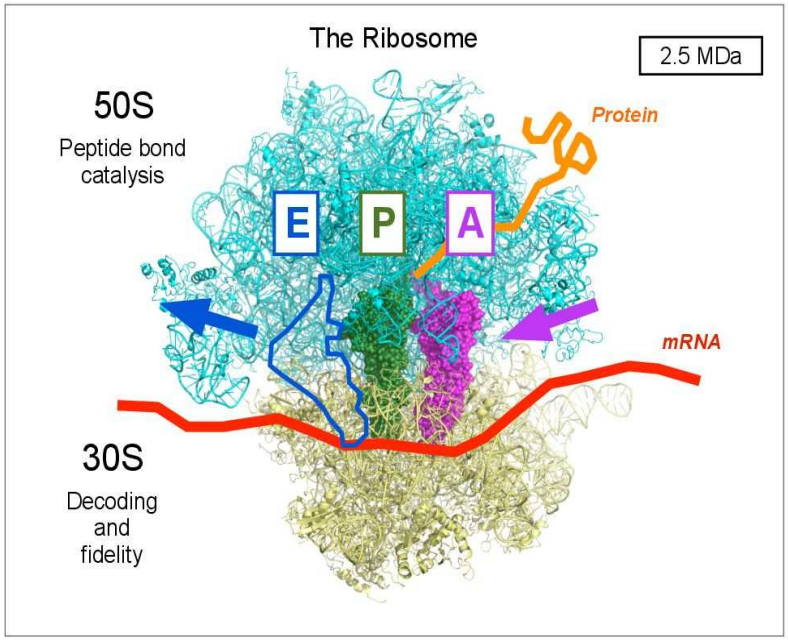
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg
Physikalisches Institut

PHYSIKALISCHES KOLLOQUIUM

AM 10. DEZEMBER 2012 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



FORCES AND CONFORMATIONAL DYNAMICS IN BIOMOLECULAR NANOMACHINES

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Proteins are biological nanomachines. Virtually every function in the cell is carried out by proteins -- ranging from protein synthesis, ATP synthesis, molecular binding and recognition, selective transport, sensor functions, mechanical stability, and many more. The combined interdisciplinary efforts of the past years have revealed how many of these functions are effected on the molecular level. Computer simulations of the atomistic dynamics play a pivotal role in this enterprise, as they offer both unparalleled temporal and spatial resolution. With state of the art examples, this talk will explain the basics of this method, the type of questions that can (and cannot) be addressed, and its (current) limitations. The examples include aquaporin selectivity, mechanics of energy conversion in F-ATP synthase, the mechanical properties of viral capsids, and tRNA translocation within the ribosome. We will further demonstrate how atomistic simulations enable one to mimic, one-to-one, single molecule experiments such as FRET distance measurements, and thereby to enhance their accuracy. We will, finally, take a more global view on the 'universe' of protein dynamics motion patterns and demonstrate that a systematic coverage of this 'dynasome' allows to predict protein function more reliably.