



MAX-PLANCK-INSTITUT FÜR
BIOPHYSIKALISCHE CHEMIE
KARL-FRIEDRICH-BONHOEFFER-INSTITUT
Theoretische und computergestützte Biophysik
37077 Göttingen Am Fassberg 11



Mittwoch, 10. Februar 2010

14.00 Uhr c.t.
Seminarraum T6-E37
Abt.10500

Dr. Paul Whitford

Los Alamos Nat. Lab., USA

Simulating conformational transitions in the ribosome

The ribosome is a massive ribonucleoprotein complex (~2.4 MDa) that harnesses large-scale structural fluctuations to produce unidirectional protein synthesis. Two key conformational changes during translation are accommodation and translocation. Accommodation is the process by which transfer RNA (tRNA) enters the ribosome, and translocation allows the tRNA to move through the ribosome. Here, we address the structure-function relationship that governs accommodation and translocation using all-atom molecular simulations in combination with cryo-electron microscopy (cryo-em) and single-molecule fluorescence (smFRET). Flexible fitting of atomic models to cryo-em density maps provides structures for states that have not been resolved crystallographically. These models are then used as endpoints in simulations and the resulting mechanisms are compared to smFRET measurements. Details of these computational methods and the resulting ribosome dynamics will be discussed.

Helmut Grubmüller, Andrea Vaiana