Interpreting Single Molecule Folding Experiments: Insights from Molecular Simulation

by Dr. Robert Best

Dept. of Chemistry
University of Cambridge

Abstract:
A unique capability of single molecule experiments is the unambiguous resolution of conformational sub-states of biomolecules and their rates of interconversion. However, these experiments usually probe a single observable, such as a distance, and therefore specific structural information is limited. I will describe how coarse-grained molecular simulations can be used to fill in some of the details. First, I will show how coarse-grained models can be used to suggest structures for the misfolded states of titin polyproteins which are observed in single-molecule FRET experiments. The structures of the misfolds explain their unusual stability, and are also consistent with earlier measurements by AFM. Secondly, I will consider the analysis of folding kinetics in single molecule pulling experiments, focussing mainly on the interpretation of the one-dimensional models which are commonly used to interpret experimental kinetic data.

Friday, October 28th, 2011, 13:00

Room PH 127

Contact:

Prof. Dr. Matthias Rief, mrief@ph.tum.de, phone: 089/289-12471