Generalized-ensemble sampling of protein folding and aggregation

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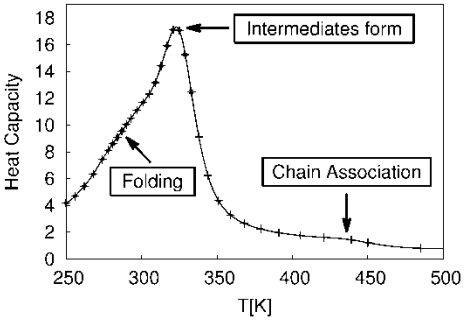
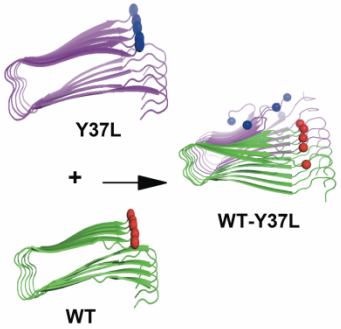
A detailed knowledge of the processes by that proteins fold, self-assemble or aggregate is crucial for an understanding of disease pathways and the working of drugs at the level of cells. As these fundamental processes are difficult to trace in experiments, there is a need for reliable computational tools that complement experiments in studying folding and aggregation of proteins. In this talk, I will describe some of the methods and techniques that are transforming computer simulations into virtual microscopes. As examples on how high performance computing can probe the molecular mechanism of cells I will discuss the folding of proteins that can take more than one structure and the formation of amyloid oligomers and fibrils that are associated with various diseases.





Selected Publications:

- Hansmann, U.H.E., *Parallel Tempering Algorithm for Conformational Studies of Biological Molecules*, Chem. Phys. Lett. **281** (1997) 140.
- Eisenmenger, F., U.H.E. Hansmann, Sh. Hayryan and C-K Hu: *[SMMP] A Modern Package for Simulation of Proteins*, Comp. Phys. Comm. **138** (2001) 192
- Mohanty, S., J.H. Meinke, O. Zimmermann and U.H.E. Hansmann, *Simulation of Top7-CFr: a transient helix extension guides folding*, Proc. Natl. Acad. Sci. USA, **105** (2008) 8004.
- W.M. Berhanu, F. Yasar and **U.H.E. Hansmann**, *In Silico cross seeding of Aβ and amylin fibril-like oligomers*, ACS Chem. Neurosci., **4** (2013) 1488.