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Sampling the energy landscape of proteins and protein aggregates

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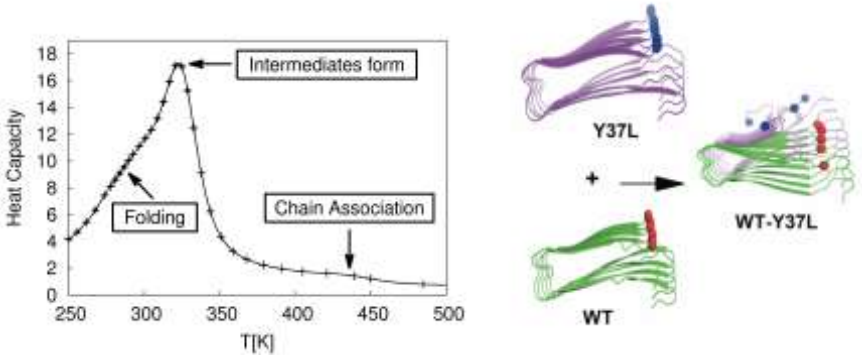
A detailed knowledge of protein structure and function is of critical importance in many medical and biotechnological applications. Despite decades of research, the relationship between amino acid sequence and structure/function of proteins is still only poorly grasped. Hence, there is a need for reliable computational tools that complement experiments in studying folding and interaction of proteins, leading to new insight into the molecular machinery of cells. Unfortunately, the complex form of the forces within and between proteins leads to a rough energy landscape with a large number of local minima acting as traps. The resulting difficulties in sampling the energy landscape increase exponentially with the size of the system. Remarkable progress has been made over the last decade in overcoming this sampling-problem. Examples are generalized-ensemble and replica exchange techniques developed by us and others. However, these methods and algorithms need to be advanced further to allow detailed description of fundamental processes of protein folding, aggregation and interaction in a cell. I will describe our recent progress and discuss some applications focusing on folding of proteins with multiple funnel landscapes and the formation of amyloid oligomers and fibrils.



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.
- Kouza, M., S. Gowtham, M. Seel and U.H.E. Hansmann, *A numerical investigation into possible mechanisms by that the A629P mutant of ATP7A causes Menkes Disease*, Physical Chemistry - Chemical Physics, **12** (2010) 11390.