Kink Formation Dynamics
in a Single α-helical Protein

Nevena Ilieva[1], Antti Niemi[2,3], Xubiao Peng[2], Adam Sieradzan[4]

[1] Institute of Information and Communication Technologies – BAS, Bulgaria
[2] Department of Physics and Astronomy, Uppsala University, Sweden
[3] School of Physics, Beijing Institute of Technology, P. R. China
[4] University of Gdańsk & Technical University of Gdańsk, Poland
nevena.ilieva@parallel.bas.bg

Protein folding remains an open problem despite the progress in understanding the process rate and the success in folding prediction for some small proteins. The reason is the absence of a constructive theoretical framework, both general and specific enough.

In earlier papers, we have argued that protein-folding dynamics can be described in terms of solitons of a generalized discrete non-linear Schrödinger equation (GDNLSE) obtained from the energy function in terms of bond and torsion angles κ and τ [1]. The soliton manifestation is the pattern helix – loop – helix in the secondary structure of the protein, which explains the importance of understanding loop formation in helical proteins and the kink assignment to it [2]. We propose a new mechanism for this process based on the energy transmission along the chain — a disturbance in the latter leads to energy accumulation sufficient to form a kink. We present first insights into the process dynamics by all-atom molecular-dynamics analysis of unfolding of a single alpha-helical protein – one chain of the core structure of gp41 from the HIV envelope glycoprotein (PDB ID: 1AIK). We suggest an adequate quantification of the side-chain orientation dynamics and also identify some force-field related artefacts.

References

[1] A. Krokhotin, A.J. Niemi, and X. Peng, *Soliton concepts and protein structure*, Phys. Rev. **E85**: 031906, 2012.

[2] A.K. Sieradzan, A.J. Niemi, X. Peng, *Peierls-Nabarro barrier and protein loop propagation*, Phys. Rev. **E 90**: 062717, 2014.