AKB 19 Proteins

Time: Wednesday 16:00–16:45 Room: ZEU 260

AKB 19.1 Wed 16:00 ZEU 260

Origin of the twisting in β-sheet structures — •Joel Ireta and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195, Berlin

The potential-energy surface of a single-strand β-sheet is studied using density-functional theory in the Perdew, Burke, and Ernzerhof approximation to the exchange-correlation functional. Infinite polyalanine and polyglycine chains are used to model the single-strand β-sheet structure. The potential-energy surface of polyalanine is found to be asymmetric with respect to twisting. This leads to a left-handed twist of few degrees in the structure. However for polyglycine, the potential-energy surface is found to be symmetric. We find that the asymmetry in the potential-energy surface of polyalanine can not be solely attributed to repulsive interactions between the side group, which is absent in polyglycine, and the helix backbone but to the pyramidalization of the nitrogen atom in the peptide bond. Symmetry with respect to twisting in the potential-energy surface of polyalanine is induced when nitrogen pyramidalization is avoided. In a survey throughout the crystallized structures of proteins listed in the protein data bank, we find indeed a left-handed twisting in the β-sheet conformations.

AKB 19.2 Wed 16:15 ZEU 260

On the balance of the enthalpic and the entropic contributions to the stability of the helix: A DFT-GGA study — •Lars Ismer[1], Joel Ireta[1], Matthias Scheffler[1], and Jörg Neugebauer[2] — [1]Fritz-Haber-Insitut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, D-40237 Düsseldorf

Accurate theoretical studies of the thermodynamic stability of isolated peptide chains may serve as a reliable reference to understand the stability of the secondary structure of proteins. We have therefore calculated the free energy difference needed to fold the fully extended structure (FES) of isolated, infinite polyalanine (Ala) and -glycine (Gly) chains into various helical conformations such as the 3_{10}-, α-, and π-helix. The calculations were done by employing DFT-GGA, plane waves, pseudopotentials and the quasi-harmonic approximation to estimate the finite temperature effects. We find that entropic contributions to the free energy strongly reduce the enthalpic stability of the helices at elevated temperatures, leading to a transition to the FES at $T_c \sim 460$ K for Ala and $T_c \sim 400$ K for Gly. Below T_c the α-helix is the conformation with the lowest free energy. The π-helix shows the strongest temperature dependence resulting in a significant destabilization with respect to the α- and 3_{10}-helix for $T > 0$ K. A detailed analysis showed these thermodynamic trends to be *intrinsic* features of the specific hydrogen bonding network formed by the various helices and to be largely independent of the specific amino acid.

AKB 19.3 Wed 16:30 ZEU 260

Protein structure comparison based on a vectorial structure representation — •Florian Teichert and Markus Porto — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany

A vectorial structure representation has recently been proposed as an equivalent description of globular protein folds. We develop suitable similarity measures for this vectorial structure representation, incoorporating the proper treatment of gaps, based on which we divise a scheme to align protein structures which is conceptually different from existing schemes.

[1]˜F.˜Teichert and M.˜Porto (in preparation)