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A DFT-GGA based thermodynamic analysis of the secondary structure of proteins LARS ISMER, JOEL IRETA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Maxp-Planck-Gesellschsft, JÖRG NEUGEBAUER, Theoretische Physik, Universität Paderborn — Studies of the thermodynamic stability of the secondary structure of proteins are important for understanding the protein folding process. We have therefore estimated the free energy change to fold a fully extended structure (FES) into the α-helical conformation for isolated infinite poly-glycine (Gly) and -alanine (Ala) chains. The calculations have been performed employing DFT-GGA, a plane-wave pseudo-potential approach and the harmonic approximation. Our results reveal [1], that this approach leads to a significantly improved description of thermodynamic data with respect to previous studies based on empirical force fields. Further we find, that the enthalpy to transform an α-helix into an FES strongly reduces with increasing temperature: at room temperature the free energy difference for Gly is close to zero within the numerical error bar (0.5 kcal/mol), whereas for Ala the α-helix is by 1.0 kcal/mol more stable. We conclude, without recoursing to any empirical input parameters, that an isolated Ala-FES will even at room temperature spontaneously fold into an α-helix.

1. L. Ismer, J. Ireta, S. Boeck and J. Neugebauer submitted to Phys. Rev. E

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