

THEORY OF PHASE TRANSITIONS IN POLYPEPTIDES AND PROTEINS%0A

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ON THE THEORY OF PHASE TRANSITIONS IN POLYPEPTIDES

The phase transitions of this or a similar nature occur or can be expected in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA,

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In the previous chapter a novel and general theoretical method for the description of phase transitions in finite complex molecular systems was introduced. In particular, it was demonstrated that for polypeptide chains, i.e., chains of amino acids, one can identify specific twisting degrees of

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The developed theory is free of model parameters and is based solely on fundamental physical principles. We apply the developed formalism to the description of thermodynamical properties of alanine polypeptides of different lengths. We analyze the essential thermodynamical properties of the system, such as heat capacity, phase transition temperature, and latent heat of the phase transition

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To study thermodynamic properties of the system one needs to investigate its potential energy surface with respect to all degrees of freedom. There is a number of different methods for calculating

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There are nearly 100 000 different protein sequences encoded in the human genome, each with its own specific fold. Understanding how a newly formed polypeptide sequence finds its way to the correct fold is one of the greatest challenges in the modern structural biology.

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