BP 4: Protein Structure and Folding

Time: Monday 17:30–19:30 Location: H43

BP 4.1 Mon 17:30 H43

MODELS FOR PROTEIN FOLDING — •PEDRO OJEDA[1], NAN-YOW CHEN[2], AURORA LONDONO[3], and MARTIN GARCIA[1] — [1]Theoretische Physik, FB 18, Universitaet Kassel, Kassel, Germany — [2]Institute of Physics, Academic Sinica, Nankang, Taiwan — [3]Department of Molecular Biology, IPICYT, S.L.P., Mexico

The problem of predicting the native structure of a protein for a given sequence is of great interest due to its relevance to many fields in Biology. Up to now two kinds of models were developed to qualitatively explain some aspects of the folding-problem, but the complete solution of the problem is still missing. One of those models is called *deterministic* because it considers all atoms and all interactions. The simulations require sophisticated computer resources. Another approach is called *stochastic* because it makes use of the so called Markov processess. This method has the advantage of requiring only a personal computer to obtain the solution.

In this work we employ Monte Carlo scheme and consider an *Off-lattice model* in which the degrees of freedom are the so-called Ramachandran angles. The potential energy is calculated as in PRL 96, 078103 (2006).

Using this method we were able to predict the native structure of diferent proteins.

BP 4.2 Mon 17:45 H43

Exact Solution of the RNA Folding Problem with Loop Entropy — •Thomas R. Einert, Paul Näger, and Roland Netz — Physikdepartment (T37), Technische Universität München, 85748 Garching, Deutschland

We discuss the equilibrium statistical mechanics of the secondary structure of an RNA molecule taking into account the loop entropy. We derive a recursion relation for the restricted partition $Z(N, M)$ function of an RNA of length N with M free backbone segments, M being a measure for the spatial extension of the molecule. The additional index M enables us to include loop entropy costs (characterized by the loop exponent c) and allows us to study stretching of the RNA. As an advantage over previous iterative formulations, our iteration equation can be solved in polynomial time. In the homopolymeric case, the recursion relation is solved analytically with generating functions methods. A phase transition is present only in the range $2 < c < 2.47...$ and is characterized by non-universal critical exponents . Explicit results for the force-extension curve are obtained.

BP 4.3 Mon 18:00 H43

Intrinsic structural properties of mesoscopic models for protein folding and aggregation — •Michael Bachmann[1,2], Stefan Schnabel[1], Christoph Junghans[1], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10/11, D-04109 Leipzig, Germany — [2]Computational Biology & Biological Physics, Lunds Universitet, Sölvegatan 14A, SE-223 62 Lund, Sweden

In this talk, the importance of mesoscopic models for soft materials is illustrated for folding processes of protein-like heteropolymers [1] and their aggregation [2]. In addition, it is shown that the conformational transitions accompanying folding and aggregation processes of naturally finite systems are similar to phase transitions, but not in a strict thermodynamic sense. In particular, the aggregation studies reveal the advantages of a microcanonical analysis, compared to the standard canonical approach.

[1] S. Schnabel, M. Bachmann, and W. Janke, Phys. Rev. Lett., in print; J. Chem. Phys., in print.

[2] C. Junghans, M. Bachmann, and W. Janke, Phys. Rev. Lett. **97**, 218103 (2006).

BP 4.4 Mon 18:15 H43

Analyzing knots in protein structures — •Virnau Peter[1], Mirny Leonid[2], and Kardar Mehran[3] — [1]Uni Mainz — [2]Harvard-MIT Division of Health Sciences and Technology — [3]Massachusetts Institute of Technology, Department of Physics

Although globular homopolymers display an abundance of knots (Virnau et al, J. Am. Chem. Soc. 127, 15102 (2005)), only about one in a thousand protein structures are knotted. Can this absence of entanglement be explained in terms of statistical mechanics or is there an evolutionary bias? Do knots in proteins serve a purpose and how do they actually fold? To elaborate on this, we will present an overview of knotted proteins from the current version of the Protein Data Bank (Virnau et al, PLOS Comp Biol 2, e122 (2006)). We will also discuss some particularly intriguing examples of this set and the evolutionary context in which knots appear.

BP 4.5 Mon 18:30 H43

Why are pi-helices so seldomly observed in proteins ? — Lars Ismer[1], Joel Ireta[2], and •Joerg Neugebauer[1] — [1]Max-Planck-Institut fuer Eisenforschung, Max-Planck-Strasse 1, D-40237 Duesseldorf — [2]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

Three different helical secondary structure motifs are observed in proteins: the alpha-, the 3-10-, and the pi-helix. While the alpha- and the 3-10-helix show occurences of about 80 % and 20 % respectively, the pi-helix is, however, only found in exceptional cases. The existing explanations herefore given in literature are rather qualitative and based on empirical assumptions. We here present a free energy analysis of infinitely long poly-L-alanine and -glycine helices which is based on DFT-GGA and the harmonic approximation and which is free of any empirical input parameters. We show, that the rarity of the pi-helix can be explained as an entropic effect, which is intrinsic and exists even in the absence of any environmental aspects, like solvents. By means of elasticity theory we show that the origin of the instability is due to geometric peculiarities of the pi-helix and independent of the amino acid sequence.

BP 4.6 Mon 18:45 H43

Protein structure reconstruction from a vectorial structure representation — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK

We illustrate an approach to reconstruct the folded protein structure from its vectorial representation, a process which is indeed very similar to actual protein folding in the sense that it also employs a 1D quantity to determine the 3D folded structure. This has been prompted by the recent proof that the contact matrix of a protein structure can be reconstructed from its vectorial representation [1], from which the 3D structure can in turn be efficiently recovered [2]. Here, we take one step further and present a reconstruction procedure that uses directly a 3D structure description (the tube model [3]) and a cost function based on the vectorial structure representation. Although no full reconstruction has been achieved yet, the contact matrix overlap to the target structure reaches up to 75%. These simulations are used to investigate the 'energy landscape' of this model by means of enhanced sampling techniques including umbrella sampling. They provide a novel approach to investigate protein energy landscapes, which is conceptual different from usually applied Gō-type techniques.

[1] M. Porto *et al.*, Phys. Rev. Lett. **92**, 218101 (2004).
[2] M. Vendruscolo *et al.*, Fold. & Des. **2**, 295 (1997).
[3] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).

BP 4.7 Mon 19:00 H43

A generalized vectorial protein structure representation and its application in structure comparison — •Florian Teichert[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular "Severo Ochoa", (CSIC-UAM), Cantoblanco, 28049 Madrid, Spain

A structural profile was recently proposed for single-domain protein structures [1]. We have extended this representation to include a consistent description of both single- and multi-domain folds [2], thus considerably broadening its applicability in bioinformatics. For one possible application, a so-called structure alignment scheme, we use this extended structural profile to compare three-dimensional protein folds and locate segments where similarities or differences exist. The benefit of our alignment scheme is that it is more general than existing algorithms. A first assessment shows that its performance is comparable with existing techniques. Yet, even more important, it constitutes a promising starting point for the analysis of structure/structure, se-

quence/structure, and sequence/sequence alignments within the same scheme.

[1] M. Porto, U. Bastolla, H.E. Roman, and M. Vendruscolo, Phys. Rev. Lett. **92**, 218101 (2004) *(4 pages)*.
[2] F. Teichert and M. Porto, Eur. Phys. J. B **54**, 131-136 (2006).

BP 4.8 Mon 19:15 H43

Electronic structure of proteins: extended building block model — •Volodymyr Maslyuk[1], Ingrid Mertig[1], Thomas Bredow[2], Michael Mertig[3], Denis Vyalikh[4], and Serguei Molodtsov[4] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle, Germany — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, D-53115 Bonn, Germany — [3]Max-Bergmann-Zentrum für Biomaterialien, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

We report a novel approach for the calculation of the electronic density of states of proteins of huge biomolecules. The proposed model is based on the consideration of individual amino acids in the corresponding conformation of the peptide chain. The densities of sates (DOS) of the building blocks additively contribute to the electronic structure of the entire protein complex aligned at the charge-neutrality level [1] of the protein. The derived results agree well with experimental data obtained by means of photoemission (PE), resonant PE, and near-edge x-ray absorption spectroscopy. The model was applied to describe the electronic spectra of the surface protein layer (S-layer) of Bacillus sphaericus NCTC 9602. [1] H. Vázquez et al., Europhys. Lett. 65, 802 (2004); H. Vázquez et al., Appl. Surf. Sci. 234, 108 (2004); H. Vázquez et al., Phys. Rev. B 71, 041306(R)(2005).