L-11 **Session A, Wednesday, 15.06., 9^{00} - 9^{40}**

Structural Biology Using Light Sources Helps Combat Infectious Diseases and Antibiotic Resistance

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Many aspects of protein function, including molecular recognition, assembly and catalysis, depend on the 3D atomic structure. X-ray crystallography remains the most powerful method capable of providing atomic information on interactions of proteins with other macromolecules and small ligands. Modern light sources and dedicated macromolecular crystallography (MX) beamlines have expanded our competence in determining macromolecular structures. New strategies developed allow data collection from highly demanding crystals using mini-beams and reduce radiation damage. Genome sequencing projects have accelerated significantly and now include studies of many human pathogens. Expanded protein sequence space allows comprehensive approaches to studies of the entire cellular systems. Structural Genomics efforts took advantage of these innovations and contributed a complementary array of the rapid, highly integrated and cost effective methods in molecular and structural biology and created structure determination pipelines. When combined with MX synchrotron facilities, advanced software and computing resources, these pipelines resulted in significant acceleration of protein structure determination and expanded the range of projects. Structure determination pipelines can be applied to emerging diseases. Several examples of application of light sources to important biology challenges will be discussed. Structures obtained through X-ray crystallography combined with biochemical assays and numerical simulation can help to construct a model of the enzymes catalytic pathways. Structures of complexes with ligands in combination with *in vitro* and *in vivo* inhibition studies can provide important insights into the interactions that modulate selectivity and potency of inhibitors that could serve as lead compounds for drug development.

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L-12 **Session A, Wednesday, 15.06., 9^{40} - 10^{20}**

Monte Carlo structure factors for self-assembling polymers

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We present Monte Carlo data for self-assembling multiblock copolymer melts and solutions.

We use experimentally determined Flory–Huggins interaction parameters, χ, to quantify the interactions between ionic and nonionic monomers. Analysis of the experimental data indicate that χ between poly(styrenesulfonate) and polystyrene is about 5, a value that is orders of magnitude larger than that obtained in mixtures of nonionic polymers. Our model predicts that clustering of ionic monomers in the disordered state results in stabilization of the disordered phase and the product $p2\chi N$ is well above the mean-field value of 10.5 at the order–disorder transition (N is the total number of monomers per chain). Network morphologies and hexagonally packed cylinders are observed in the ordered state at large p values while more traditional lamellar phases are found at small values of p. Simulations indicate that complex morphologies such as gyroid and perforated lamellae are obtained in symmetric block copolymers wherein the volume fraction of the B block, ϕB, is about 0.5, while simple unperforated lamellae are obtained in asymmetric block copolymers wherein ϕB is about 0.25. This result is very different from the well-established phase behavior of nonionic block copolymers but consistent with experimental results. We also make a number of additional predictions, still awaiting an experimental verification, such as the emergence of the hexagonal phase in the weak segregation limit, and a remarkable insensitivity of the product $p\hat{}2\chi N$ (N is the total number of segments in a copolymer chain) at the order–disorder transition to ϕB.

L-13 **Session A, Wednesday, 15.06., 11^{40} - 12^{20}**

Structural studies of chitinases from extremophiles

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Proteins from extremophiles hold the secret of protein stability and enzymatic efficiency. We have analysed chitinases from cold-adapted and thermophilic bacteria, compared them and looked for the features that give those ezymes their special characteristics.