Boulder School for Condensed Matter and Materials Physics, July 9-August 3, 2012

Polymers in Soft and Biological Matter

Syllabus of the course

The overall logical architecture of the course is based on three mutually interweaving streams.

Stream 1: common basics

Interactions. [3 lectures. **P.Pincus**.] Four fundamental forces in molecular world: Van der Waals, hydrogen bonds, hydro (or solvo) phobic, electrostatic. Hard core repulsion. Inter- and intra- molecular forces versus inter- and intra-particle forces. For VdW: Hamaker constants, Lifshitz theory, retardation. For electrostatics: ions and charged particles versus polar and polarizable ones; pH and pK; screening, correlation energy, linear and non-linear screening, double layer, Debye-Huckel and Poisson-Boltzmann theories; solvation and hydration. Correlation induced attraction of like charges. Effective interactions through the media: hydrophobic, depletion (both for dilute systems and specifically polymers semi-dilute), fluctuations-mediated forces (Casimir-like). Adhesion, wetting, friction, lubrication.

Surfaces and interfaces. [2 lectures. **T.Kuhl**] Rigid and deformable interfaces, surface tension, Young-Laplace equation, wetting and contact angle, capillarity. Oswald ripening, nucleation and growth. Adsorption, Gibbs and Langmuir. Surface force apparatus etc.

Review of basics in experimental techniques in soft matter physics. [4 lectures**]**

- Scattering: (**T. Kuhl**) (Light, X-ray, neutron): static scattering (structure factor, etc.), dynamic scattering (diffusion coefficient determination; dynamic structure factor), multiple scattering in opaque media (DWS), surface/interface techniques, etc.
- Microscopy: (**D. Weitz**) optical, confocal, two-photon, optical coherence tomography, AFM, TEM, STM, etc.
- Rheology: (**D. Pine**) Macro- and micro-rheology – linear rheology: Boltzmann superposition, relaxation modulus, storage and loss moduli, step-strain, creep, oscillatory, etc; non-linear rheology; particle tracking, one- and two-particle, fluorescence correlation, diffusing wave;.
- Microfluidics (**E. Kumacheva**)

Simulations in polymer and soft matter physics. [5 lectures. **D.Frenkel** and **K.Kremer**] Monte Carlo vs. molecular dynamics vs. Brownian dynamics vs. dissipative dynamics: main ideas, advantages and disadvantages. Lattice Boltzmann method. Particularities of charged systems, Ewald summations. Various thermostats and their use for simulations. Multi scale modeling. Examples.

Review of hydrodynamics. [3 lectures. **L.Mahadevan**] Balance laws, constitutive equations and boundary conditions. Symmetry, invariance and how to derive equations for simple and complex fluids. Dimensional analysis and scaling laws. Compressibility, Viscosity, Inertia. Bulk and interfacial flows. Stability and instability. Pattern formation. Low dimensional flows. Analogies to other field theories (electrostatics, elasticity, transport). Porous media, stiff and soft. Introduction to complex fluids - polymers, suspensions, ferrofluids, biofluids. Locomotion in fluids.

Active systems away from detailed balance. [2 lectures. **F.MacKintosh**] Molecular motors. Swimmers, pushers and pullers. Active hydrodynamics. Active semi-flexible gels and their rheology. Cytoskeleton. Topological enzymes.

Total for stream 1: 19 lectures

<u>Stream 2: polymers</u>

Foundations of polymers. [4 lectures. **A.Grosberg and M.Rubinstein**] Hierarchy of energies: covalent bonds and volume interactions. Ideal polymer chain models: freely jointed, rotational isomers, worm-like. Entropic elasticity of single chain and "force spectroscopy" experiments. Confinement. Excluded volume. Theta-point. Coils and globules. Melts and Flory theorem, possible corrections to it. Polymer solutions, classification of regimes. Thermodynamics and phase diagrams of polymer solutions. Thermodynamics of mixtures. Polymers and colloids, polymers and membranes. Peculiarities of semi-flexible polymers. Polymer liquid crystals.

Polyelectrolytes. [3 lectures. **M.Rubinstein**] Counterion distribution near planes (Gouy-Chapman), lines (Onsager-manning), and spheres; Flory & scaling theory of polyelecrolyte chain, Odijk-Skolnick-Fixman & Joanny-Dobrynin persistence length; necklace transitions of lyophobic polyelectrolytes; semidilute polyelectrolyte solutions - statics & dynamics including entanglement mystery; adsorption of polyelectrolytes at charged surfaces (hydrophilic & hydrophobic); polysoaps - hydrophobically modified polyelectrolytes; polysalts - random polyampholytes; adsorption of polyampholytes; block polyampholytes including disproportionation of micelles; complexes of oppositely charged polyelectrolytes and layer-by-layer films.

Polymer networks and gels. [2 lectures. **Y.Rabin**] Rubber elasticity. Equilibrium swelling and collapse of networks. Sol-gel transition, gelation versus percolation, preparation of polymer gels. Dependence of gel properties on preparation procedure. Peculiarities of networks of semi-flexible polymers. Polyelectrolyte gels. Osmotic pressure of counterions. Collapse of polyelectrolyte gels.

Polymer dynamics. [3 lectures. **T.McLeish**] Rouse dynamics. Hydrodynamics and Zimm model. Reptation. Viscoelasticity, cooperative diffusion, etc. Reptations of branched polymers, dynamics of mixing, other applications.

Brushes and micelles. [2 lectures. **E.Zhulina**] Brushes of all sorts of geometries, including polyelectrolyte ones. Micelles, including spherical, rod-like or worm-like, and bilayers. Self-assembly and CMC. Polyelectrolyte brushes - planar, cylindrical, spherical, effect of salt, multivalent counterions.

Block-copolymers. [1 lecture. **E.Zhulina**] The idea of microphase segregation, strong and weak segregation regimes, possible symmetries, phase diagrams. Block-copolymers in selective solvents. Two blocks, three blocks, and multi-blocks.

Biopolymers. [1 lecture. **A.Grosberg**] Peculiarities of biological macromolecules as polymers. Proteins, nucleic acids, polysaccharides. Hierarchy of structures (primary, secondary, ternary). Connections to genomics and proteomics. Types of secondary structures and physics of their formation – helix-coil transitions in a variety of settings: homo- and heteropolymers, single strand and double (and multi) strands, etc. DNA folding will be discussed in virus part, protein folding in protein part.

Disordered polymers. [1 lecture. **A.Grosberg**] Quenched and annealed sequences. Microphase segregation in quenched random heteropolymers. Polyampholytes.

Semi-flexible polymers. [1 lecture. **F.MacKintosh**] Peculiarities of semi-flexible polymers in terms of their single chain entropic elasticity, their propensity for nematic ordering, their network properties, their collapse behavior.

Total for stream 2: 18 lectures

<u>Stream 3: soft and biological matter</u>

Liquid crystals. [3 lectures. **N.Clark**] Nematics (and cholesterics), smectics of various types. Phase transitions**.** Frank constants and textures. Defects in liquid crystals. Liquid crystals of semi-flexible polymers and elastomers.

Membranes and their fluctuations [3 lectures, **S. Safran**]: Self assembly of amphiphiles into micelles, microemulsions, and membranes; membrane curvature energy; thermal fluctuations of membranes; 2d persistence length and renormalization of bending energy; fluctuation-induced interactions of membranes; inhomogeneous membranes - spontaneous vesicle formation, membrane inclusions and their interactions.

Physics of colloids. [5 lectures. **P.Chaikin, D.Pine, D.Weitz**] Colloidal stability; colloidal sols, micro- and macroemulsions, foams; phase diagrams, colloidal crystals, Wigner crystals; colloidal “molecules”. Dynamics: phoresis, sedimentation. Polymers in colloidal systems. DLVO. Kinetics of aggregation. Floculation, droplet formation in shear, diffusion and convection. Non equilibrium phase transitions, colloids of complex shapes, DNA covered colloids, “life”.

Biology and Soft Matter by Numbers. [1 lecture, **Y.Rabin]**

Proteins. [3 lectures, **E.Shakhnovich**] The goal here should be not so much to reviewthe field in its entirety, but to highlight its relation to the rest of the course, i.e., to polymers and soft matter. Possible topics include but not limited to: primary, secondary, ternary structures; folding and folding phenomenology, latent heat and cooperative/first order de- and re-naturation; random polypeptides and libraries – theory and experiment; selection of sequences; protein evolution – review of proteomics data.

Viruses. [2 lectures, **R.Bruinsma**] Possible review more or less of the same style as proteins. Caspar-Klug crystallography, classification, RNA and DNA viruses, RNA secondary and tertiary structure, compact forms of DNA, pressure of genome, ejection dynamics, self-assembly of protein shells and viruses, elasticity of shells, von Karman theory and buckling instability, higher viruses, their lipid coat and life cycles.

Membranes, the Nernst Potential, and the Action Potential. [1 lecture, **R.Bruinsma**] The lecture will discuss first how a potential difference develops across lipid bilayers: the Nernst Potential, which is the basis of bio-electricity. Then it will review the classical Goldmann-Katz equation for the rest-potential of cells, extending the Nernst Potential concepts. The last part of the lecture will discuss the Cable Equation and how a discharge of the rest-potential develops a traveling pulse, the Action Potential, that is the basis of communication between neurons.

Total for stream 3: 18 lectures