Short Training Course - ECIS2022

"Advanced Characterization and Modelling techniques for Colloids"

2-3 September 2022, FORTH, Heraklion

<u>Motivation</u>: Properties of soft matter systems result from balance of different interactions acting on a range of length scales. Their proper characterization requires appropriate tools and techniques allied to pertinent interpretation. Techniques continuously evolve to adapt to the more challenging questions on more complex materials. This short course aims to provide an up to date introduction to optical microscopy, scattering and rheometry as tools for characterization of soft materials and an introduction on the capabilities of numerical simulations for the microscopic understanding of the behavior, and the prediction of structure-property relations, of soft matter systems.

The course will take place at FORTH in Heraklion, in a hybrid manner. Participants may follow the course on-site or online. The course will consist of 4 half-day sessions and will include hands on demonstration of experiments (microscopy, rheometry, scattering) and simulations at the Polymer & Colloid lab (for on-site participants).

Deadline for registration 15 May 2022. A maximum number of 50 on-site and 20 on-line participants will be accepted.

<u> Program – Syllabus:</u>

1stday (Friday, 2 September): Experimental rheology (Jan Vermant) and Computer Simulations (Roseanna Zia & Vangelis Harmandaris)

(1) Rheology: Jan Vermant

9.00 – **10.30**: Rheology basics: Landmark observations and rheological material functions for suspensions – Linear viscoelasticity: what is it good for? Brownian hard spheres and beyond.

30 min break

11.00 - **12.30**: Stable dispersions: Shear thinning and thickening in colloidal suspensions - Gelation: The ugly ducks in rheology - the yield stress and thixotropy - Advanced rheometrical tools for non-linear rheology and structure probing.

Lunch break 12.30 -14.00

(2) Computer Simulations: Roseanna Zia & Vangelis Harmandaris

14.00 – 15.30: Introduction to computational modelling and simulation methods for complex molecular systems: Mathematical modeling and simulation methods, Molecular interactions: From atoms to colloids, Monte Carlo methods, Molecular dynamics simulations, Brownian dynamics, Fluctuations and time correlations, Hierarchical simulations across spatiotemporal scales

Simulations of colloids and interfaces: Interfaces and Interphases, Friction and gradient of dynamics at interfaces, Structural properties: Phase diagram of colloids, Structure and morphology of polymer and/or colloids at interphases, From atoms to macroscopic properties

30 min break

16.00 -17.30: Making simulations and experiments "talk" to each other: Brief overview of microscopic forces (hydrodynamic, entropic, enthalpic; short vs. long range), Reprise: The connection between microscopic forces, structure, phase behavior, & rheology, Equilibrium and dilute suspensions: a relatively easy task to match colloidal interactions in models to experiments, Gels, glasses, dense self-assembly: paving a new road

30 min break

18.00 -**18.45**: Outlook and future opportunities: Physics based models at very large scales, Machine and deep learning overview, Physics-based machine learning & opportunities

2nd day (Saturday, 3 September) Scattering and Microscopy (Stefan U. Egelhaaf and Roberto Cerbino)

(3) Scattering techniques: Stefan U. Egelhaaf

9.00 - 10.30: Light Scattering techniques: Static light scattering (average intensity, interference, form and structure factor with simple models, SLS set-ups, examples)

30 min break

11.00 - 12.30: Dynamic light scattering: fluctuations, correlation function, intermediate scattering function, homo-/heterodyne scattering with simple cases (sizing/polydispesity; diffusion versus directed motion) and not so simple cases (concentrated suspensions), DLS set-ups, examples

Neutron and x-ray scattering (briefly) Still waves but different radiation-matter interaction, set-ups, examples

Lunch break 12.30 - 13.30 - lab tour 13.30 - 14.30

(4) Microscopy and applications: Roberto Cerbino

14.30 - 16.00: Anatomy of a microscope: from light sources to detectors (a primer), Mechanisms of sample contrast: scattering (absorption, dephasing, birefringence) vs fluorescence, Diffraction-limited microscopy: bright-field, dark-field, phase-contrast, DIC, wide-field, confocal, light-sheet, digital holographic microscopy, Basics of superresolution microscopy: single-molecule localization (PALM/STORM, PAINT) vs REversible Saturable Optical Fluorescence Transitions (STED)

30 min break

16.30 -18.00: Soft matter microscopy, Direct space experiments: particle localization and tracking in 2D and 3D (correlation, MSD, van Hove, rotational tracking, errors and artifacts), ensemble-averaged approaches (spatio-temporal image correlations, PIV), nanoscopy and applications, Reciprocal space experiments: Digital Fourier Microscopy, Differential Dynamic Microscopy and applications, Microscopy-based microrheology: passive (one- and two-points) microrheology, active microrheology, Poking while watching: microscopy meets rheology

18.00 - 19.00: Round table - Discussion

19.00: Departure for dinner to nearby village of Agios Myronas