Fluidics
chaired by Jeff Wood/Hai Le The – room 6

11.45-12.00	*Molecular dynamics simulations of ionic liquids for energy storage devices* Ranisha Sitlapersad (MSM)
12.05-12.20	*The reduction of Taylor dispersion by AC-electroosmotic mixing for the improvement of liquid chromatography* Eiko Westerbeek (BIOS)
12.25-12.40	*Surface Reaction Driven Flow* Abimbola Ashaju (SFI)
12.45-13.00	*Particle aggregates via droplet evaporation on superhydrophobic fractal-like substrates* Carola Seyfert (PoF)

Molecular dynamics simulations of ionic liquids for energy storage devices, Ranisha Sitlapersad (MSM)
Supercapacitors offer a promising technology for energy storage, in the form of electrochemical double-layer capacitors (EDLCs). Using ionic liquids (ILs) as electrolytes in EDLCs has several advantages over conventional electrolytes, such as: a large electrochemical window, that allows a higher operating voltage; a high thermal stability; non-flammability; and, a very low vapour pressure. Unfortunately, the application of ILs in supercapacitors yields a lower power density in comparison to commercial supercapacitors. The power density is related to the mobility of the ions in the bulk, in the electrode's pores and near the various interfaces. In this study, we explore the properties of ILs at these locations, through atomistic molecular dynamics simulations, in order to optimise EDLCs based on ILs. We present bulk simulations of [BMIM][BF4] and a 50-50 mixture of [BMIM][BF4] and [BMIM][Cl]. In addition, we present simulations of the ionic liquids confined between two copper electrodes, both neutral and charged. We observed a strong layering of the ions near the electrodes, which decreases the power density, since the ions are highly immobile near the electrodes. Potentially these results could explain the poor power density of IL supercapacitors. Understanding and solving this problem is the direction of future research.

The reduction of Taylor dispersion by AC-electroosmotic mixing for the improvement of liquid chromatography, Eiko Westerbeek (BIOS)
Liquid chromatography is a widely used separation technique for a variety of applications. The need for high quality separations is most prominent in the life sciences, where identification of target substances relevant in disease mechanisms is performed down to the femtomole level. One of the effects which limits the performance of liquid chromatography is band broadening due to Taylor dispersion. In this project we aim to design a system, which fulfills the different needs for traditional open liquid chromatography systems as well as is able to reduce the Taylor dispersion by AC-electroosmotic mixing perpendicular to the pressure driven flow.

Surface Reaction Driven Flow, Abimbola Ashaju (SFI)

The autonomous motion of catalytic bimetallic nanorods within an aqueous peroxide solution has been reported in literature. A single nanorod consists of a bimetallic couple that catalyzes the decomposition of an aqueous solution such as hydrogen peroxide, thereby creating the necessary gradients (electric, concentration) that actuate motion. This bimetallic catalytic system can be immobilized to generate convective flow that was quantified by a numerical study. In this work, we focus on experimental and numerical analysis that provides fundamental insight on the key elements including the generated electric field, reaction kinetics and mass transport that impact the overall diffusio-electroosmosis phenomena. The surface reactivity pattern characterized by the dimensionless Damköhler number, that releases and depletes protons is related to the fluid flow. Such surface induced convective fluid flow can be harnessed in systems to reduce mass transport limitations.

Particle aggregates via droplet evaporation on superhydrophobic fractal-like substrates, Carola Seyfert (PoF)

Sessile droplets on superhydrophobic substrates are common in nature and technology. In the case of droplets containing solid particles, the evaporation of the solvent turns into an effective tool to aggregate any non-volatile content. The high contact angles and unpinned contact lines of the droplets, induced by hydrophobicity, can lead to a complete recovery of the solid solute in form of aggregates. Under the right conditions, the solid remainder takes the form of highly compact and spherically shaped aggregates, featuring a minimal contact area with the supporting substrate. We investigate the evaporation of colloidal droplets on a new kind of superhydrophobic, micro-structured substrate, featuring fractal-like glass pillars. Such substrates present an intricate geometry with non-flat top surfaces of the pillars. Different sizes and concentrations of monodisperse polystyrene particles lead to various shapes of particle aggregates after the evaporation of the solvent.