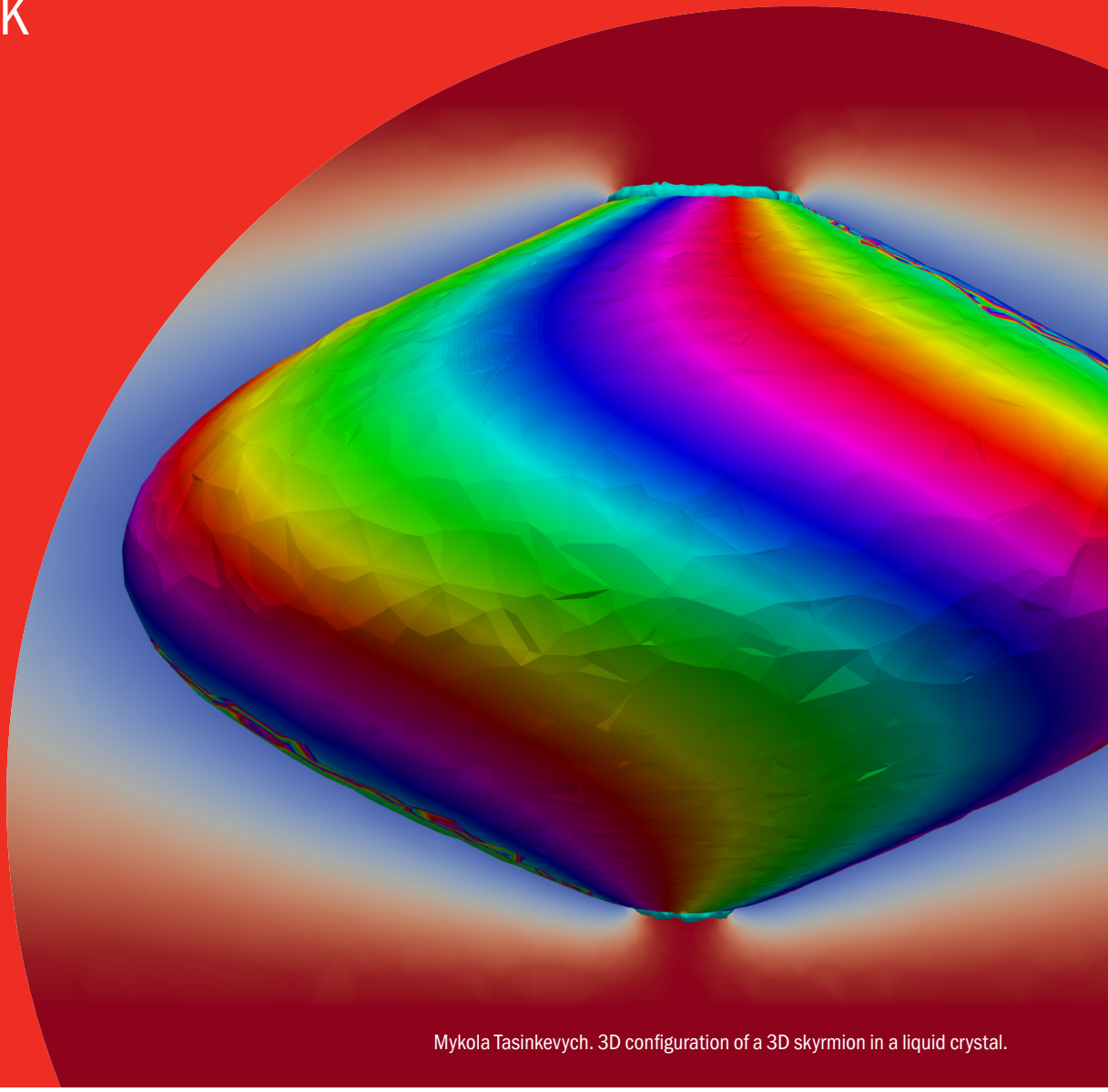
# Advanced School in Liquids and Complex Fluids ‘Solutions in the Snow’

5–8 December 2022
Sheffield Hallam University,
Sheffield, UK



Mykola Tasinkevych. 3D configuration of a 3D skyrmion in a liquid crystal.

iop.org

IOP Institute of Physics

# Programme

## Monday 5 December 2022

| | |
|---|---|
| 1pm | **Registration and Lunch** |
| 2pm | **Welcome** |
| 2:15pm | **Lecture**: Making Complex Fluids Work for Refugees<br>**Professor Tony Ryan OBE** |
| 3:15pm | **Lecture 1**: Elastic neutron scattering: Studying structures over many orders of magnitude<br>**Dr Gregory Smith** |
| 4pm | **Networking and Poster Session** |
| 5pm | **Day concludes** |

## Tuesday 6 December 2022

| | |
|---|---|
| 9am | **Lecture 2**: Elastic neutron scattering: Studying structures over many orders of magnitude<br>**Dr Gregory Smith** |
| 9:45am | **Workshop**: Elastic neutron scattering: Studying structures over many orders of magnitude<br>**Dr Gregory Smith** |
| 10:30am | **Morning Break** |
| 11am | **Lecture 1**: Theory of inhomogeneous liquids in and out of equilibrium: density functional theory and its dynamical extensions<br>**Professor Andrew Archer** |
| 11:45am | **Lecture 2**: Theory of inhomogeneous liquids in and out of equilibrium - density functional theory and its dynamical extensions<br>**Professor Andrew Archer** |
| 12:30pm | **Lunch** |
| 1:30pm | **Flash poster presentations** |
| 3pm | **Afternoon Break and Poster Session** |
| 5pm | **Day concludes** |

## Wednesday 7 December 2022

| | |
|---|---|
| 9am | **Workshop**: Theory of inhomogeneous liquids in and out of equilibrium: density functional theory and its dynamical extensions<br>**Professor Andrew Archer** |
| 9:45am | **Lecture 1**: Colloids at liquid interfaces - interactions, rheology, and materials<br>**Dr Job Thijssen** |
| 10:30am | **Morning Break** |
| 11am | **Lecture 2**: Colloids at liquid interfaces - interactions, rheology, and materials<br>**Dr Job Thijssen** |
| 11:45am | **Workshop**: Colloids at liquid interfaces - interactions, rheology, and materials<br>**Dr Job Thijssen** |
| 12:30pm | **Lunch** |
| 1:30pm | **Q&A Session** |
| 2:15pm | **Sessions conclude**<br>**Gather belongings and walk to museum** (for those attending) |
| 3pm | **Tour at Kelham Island Museum** |
| 4pm | **Free time** |
| 7pm | **Conference Dinner**<br>Piccolino Restaurant |

## Thursday 8 December 2022

| | |
|---|---|
| 9am | **Lecture 1**: Theory and modelling of liquid crystal materials<br>**Professor Nigel Mottram** |
| 9:45am | **Lecture 2**: Theory and modelling of liquid crystal materials<br>**Professor Nigel Mottram** |
| 10:30am | **Morning Break** |
| 11am | **Workshop**: Theory and modelling of liquid crystal materials<br>**Professor Nigel Mottram** |
| 11:45am | **Lecture 1**: Computer simulation - its impact on our understanding of liquids and complex fluids<br>**Professor Mike Allen** |
| 12:45pm | **Poster Prize and Closing Remarks** |
| 1pm | **Conference concludes** |

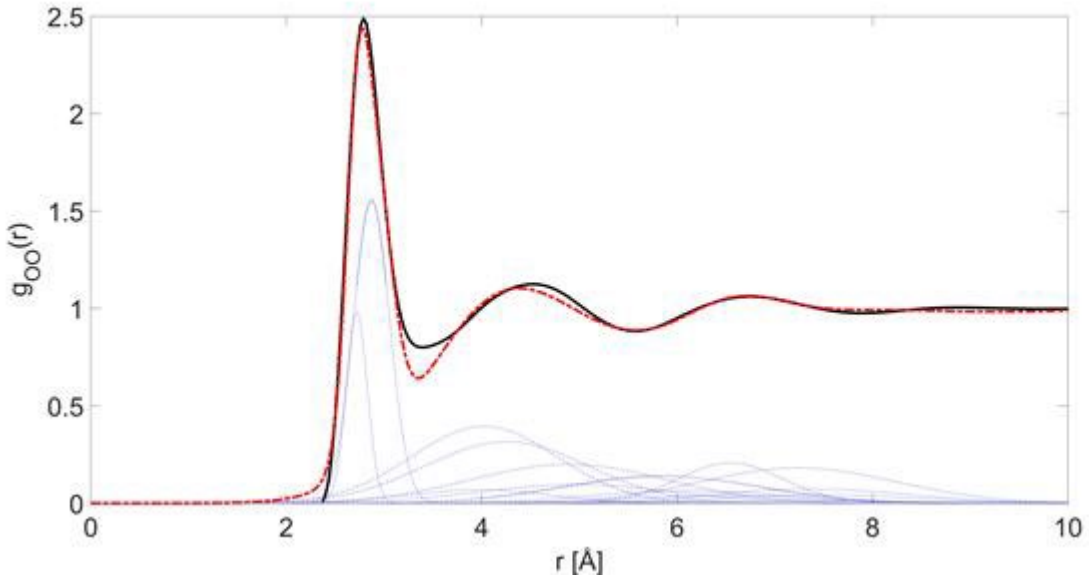
# Abstracts

1

## The Short-Range Order in Liquid Water and Amorphous Ice

**Neta Ellert**[1], Guy Makov[1], Eyal Yahel[2]
*[1]Materials Engineering Department, Ben-Gurion University of the Negev, Beer-Sheva, Israel, [2]Physics Department, Nuclear Research Centre-Negev, Beer-Sheva, Israel*

The short-range order in water and amorphous ice was determined from experimentally measured partial radial distribution functions by applying the Quasi Crystalline Model (QCM), an approach to analysing the short-range order in liquids and amorphous systems, which employs a structural model to determine the short-range order of a liquid directly from the radial distribution function. This model uses a reference lattice structure to generate a hypothetical amorphous radial distribution function that is compared with the radial distribution function obtained from experiments or simulations. The short-range order of the amorphous system is identified with the specific reference lattice producing the best fit for the data.
Three partial radial distribution functions were analysed for water at several pressures and temperatures and for three amorphous ices. It was found that at low temperatures and pressures, the short-range order of water is similar to that of the hexagonal ice (Ih) structure. At higher pressures and low temperatures, the short-range order of water becomes similar to that of tetragonal ice III structures with c/a ratio of 0.8. At higher temperatures of 573K, the short-range order obtained was similar to that of rhombohedral ice II. For amorphous ice states, we found that the three amorphous ices, distinguished by their densities: Low-Density Amorphous (LDA), High-Density Amorphous (HDA), and Very-High-Density Amorphous (VHDA)– correspond to three different SRO, namely ice Ih, tetragonal ice III and ice II, respectively.
An example for a successful fit of the partial O-O radial distribution function at ambient conditions is shown in the figure attached.

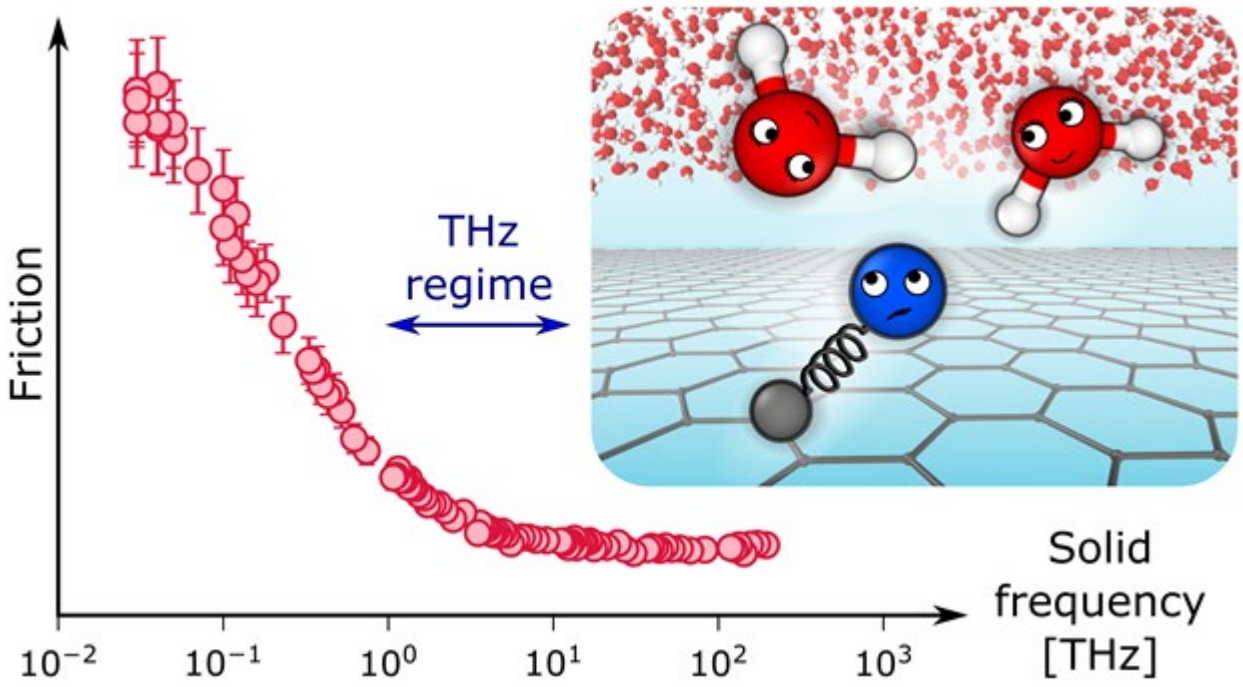


2

# Classical quantum friction at water--carbon interfaces

**Anna Bui**[1], Fabian L. Thiemann[2,1,3], Angelos Michaelides[1], Stephen J. Cox[1]
[1]*University Of Cambridge, U.K.*, [2]*University College London, U.K.*, [3]*Imperial College London, U.K.*

Friction at water--carbon interfaces remains a major puzzle with theories and simulations unable to explain experimental trends in nanoscale waterflow. A recent theoretical framework---quantum friction (QF)---proposes to resolve these experimental observations through nonadiabatic coupling between dielectric fluctuations in water and graphitic surfaces. Here, using a classical model that enables fine-tuning of the solid's power spectrum, we provide evidence from simulations in general support of QF. In particular, as the principal peak in the solid's power spectrum begins to overlap with water's Debye and librational modes, we find an increase in friction comparable to that proposed by QF. At the microscopic level, we find that this contribution to friction manifests more distinctly in the dynamics of the solid's charge density than that of water. Our results advocate for experimental verification of QF by probing the carbon substrate's electronic response, rather than water's structure or dynamics.



3

# The role of lubricant ridge size on drop dynamics in Slippery Liquid Infused Porous Surfaces (SLIPS)

**Hossein Abdolnezhad**[1], Ciro Semprebon[1]
[1]*Department Of Mathematics, Physics And Electrical Engineering, Faculty Of Engineering And Environment, Northumbria University, Newcastle upon Tyne, U.K.*

Slippery liquid-infused porous surfaces (SLIPS), inspired by the slippery properties of the Nepenthes pitcher plant, have been introduced to increase the mobility of liquids by minimizing the liquid–solid contact. The SLIPS are composed of lubricating liquid film that is impregnated with micro-nano-porous matrix. The low frictional force of the SLIPS enables them to exhibit anti-biofouling, anti-icing, and self-cleaning properties as well as corrosion prevention and drag-reduction with broad implication for industry including biomedical devices, fuel transportation and food packaging.
When a droplet is placed on such slippery surfaces a lubricant ridge is formed. When a drop is fixed in space the lubricant ridge grows slowly over time, as the lubricant is driven from the surrounding by a pressure imbalance. The growth rate depends both on the lubricant viscosity and the thickness of the lubricant layer and continues until either the ridge reaches a size comparable to the drop size, or the lubricant available is gathered. When the drop is moving, however, the growth dynamics is deeply altered by drop motion, leading to a symmetry breaking front / rear, a different growth law, and velocity dependent steady states with smaller ridge sizes. In this experimental work we systematically describe these phenomena at varying of lubricant thickness, viscosity and drop velocity. Furthermore, we evaluate how the relative size of the lubricant ridge impacts the drop motion.

4

# Barium Hexaferrite Ferrofluid in Ethylene Glycol

Yusra Ahmed, Alison Paul, Alenka Mertelj, Darja Lisjak, Daniel Zabek
*[1]School of Engineering, Cardiff University, Cardiff, CF24 3AA, U.K., [2]School of Chemistry, Cardiff University, Cardiff, CF10 3AT, U.K., [3]Department of Complex Matter, Jozef Stefan Institute, SI-1000, Ljubljana, Slovenia, [4]Department of Material Synthesis, Jozef Stefan Institute, SI-1000, Ljubljana, Slovenia, [5]School of Engineering, Cardiff University, Cardiff, CF24 3AA, U.K.*

Keywords: barium hexaferrite, ferrofluid, ethylene glycol.

Abstract: When suspended in an isotropic liquid, recently discovered barium hexaferrite nano-platelets form a ferromagnetic-ferrofluid which exhibits interesting magnetic properties [1]. Manufacturing the barium hexaferrite nano-platelets via hydrothermal synthesis remains of fundamental interest and allows for optimisation of structural, magnetic, and morphological properties, which all impact on ferrofluid properties. We have developed a hexadecyltrimethylammonium bromide surfactant assisted manufacturing method for ethylene glycol based ferrofluids with barium hexaferrite nano-platelets concentrations between 10 - 200 mg/ml. The advantage of the proposed ethylene glycol-based ferrofluid is low volatility, low toxicity, and high thermal stability opening the way into a vast number of thermal, electrical, medical, and analytical applications. A hexagonal nano-platelet morphology with a typical diameter between 80 - 120 nm was identified by Scanning Electron Microscopy (SEM). Ferrofluid stability was determined by zeta potential measurements, with a zeta potential of 39.3 mV. Saturation magnetisation of high-density dry particles and concentrated fluids were measured using a Vibrating Sample Magnetometer (VSM), where they exhibited superior magnetic and thermal properties compared to previously used butanol based ferrofluids [1].

References:

[1] Shuai et al., 2016. Spontaneous liquid crystal and ferromagnetic ordering of colloidal magnetic nanoplates. Nature communications, 7(1), pp.1-8.

5

# Structural Role of Titanium in Glass and Glass Ceramic Materials

**Esther Giron Lange**[1,2,3]
[1]*University of Bath, U.K.,* [2]*Institut Laue Langevin, France,* [3]*Corning Inc., USA*

Titanium glasses were studied aiming a better understanding of the nucleation process in glass and glassceramic materials. Two species of glass, namely a Phosphate glass containing Titanium and Niobium, TiO2-NbO2-P2O5, and a Spinel glass-ceramic, were measured using neutron diffraction at the D4c instrument at the Institut Laue-Langevin (ILL) and x-ray diffraction at the ID15a beamline at the European Synchrotron ESRF. The analysis of their pair distribution functions (PDF) following the method described by Fischer et al. resulted on the preliminary determination of the distances between pairs of atoms and their coordination numbers. Numerous consistency checks are performed during the data processing and analysis to indicate the reliability of these results. In addition to these systems more samples of the same families, i.e. the Phosphate and the Spinel, are being prepared with varying concentrations and annealing stages to extend and complement the analysis.

Nucleation and crystal growth within amorphous materials are of increasing interest among industry due to the potential versatility of their designs. Titanium glasses are important because the presence of this metal has been observed to play a structural role on the crystal growth process. The goal of this research is to develop a model that explains how Titanium affects the crystallisation taking place within the glass in order to effectively design and produce new glass-ceramics. However, the study of glasses is not easy and careful manipulation of the measured data is required in order to identify the differences on the structure of the materials. In this study, the complementary of x-rays and neutrons together with the negative neutron scattering length of Titanium are exploited in order to maximise the information extracted from the data. Results from the two families will be presented, comparing the neutron and x-ray diffraction results, explaining the key steps on the data processing and pointing the main features that can be extracted from the data.

6

# Liquid bridges suspended between horizontal cylinders

**Mrs Agnes Bokanyi-Toth**[1], Dr Dmitri Tseluiko[1], Prof Andrew J. Archer[1], Dr Hemaka Bandulasena[1]
[1]*Loughborough University, Loughborough, U.K.*

The fluid flow in liquid bridges suspended between two horizontal cylinders was studied using (i) experiments, (ii) simulations of the equations of hydrodynamics and (iii) by developing a simplified theory. This theory is a reduced-order two-dimensional dynamical model based on Onsager's variational principle, which is equivalent to the minimum energy dissipation principle in Stokesian hydrodynamics. The model equations are implemented in MATLAB, to investigate the liquid bridge interface both in the presence and absence of gravity. For symmetric and non-symmetric configurations, we show both analytically and numerically that the equilibrium contact angle minimises the free energy and the minimum of the Rayleighan function gives the dynamics.

We validate this simple model by comparing with results obtained by solving the full governing equations via COMSOL Multiphysics simulations, which shows good agreement with the Onsager model results. Several solution methods were tested in COMSOL, including the Phase Field and Moving Mesh Method. For our problem, the results from Phase Field Method are best, although all methods can suffer from some inaccuracy due to failure to exactly conserve the volume of the liquid. This can be remedied by using mesh refinement, at the cost of a significant increase of the computational time.

Additionally, we consider the (three-dimensional) liquid bridge dynamics under the influence of varying electric potentials between the supporting cylinders and examine electrokinetic effects with the Finite Element Method. A stability analysis is also performed for the case of a 600V electric field. To validate our model predictions, we developed our own experimental setup and filmed the dynamics of both electrified and non-electrified liquid bridges. Pure oil droplets (i.e. a nonconducting liquid) were suspended between the parallel electrodes and observed under high (up to 5000V) electric fields. The experiments were performed with three different oils, all exhibiting the same behaviour as predicted by our COMSOL simulations, namely that the electrified drop moves up and develops a stable, flatter interface. In the absence of the electric field, the liquid bridge returns to its initial shape, which hangs lower.

Since capillary bridges are a model of Plateau border cross-sections in a liquid foam, by understanding the dynamics in such geometry, we gain better insight in electrokinetic phenomena in foams. Thus, this project is contributing to tackling key problems related to the control and stability of liquid foams.

# Advanced School in Liquids and Complex Fluids 'Solutions in the Snow'

5–8 December 2022

Sheffield Hallam University, Sheffield, UK



IOP Institute of Physics