



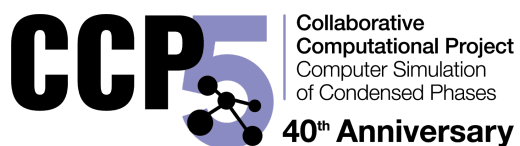
CCP5 AGM 2020

8th September 2020

Due to covid the event is online

Zoom@<https://ukri.zoom.us/j/95912975476?pwd=d1lvc1piYWJqWXFpZ0FXZklidmcydz09>

Live on YouTube@<https://youtu.be/oGZYGKPWZc4>



University of
HUDDERSFIELD
Inspiring global professionals

Organisers

Dr Marco Molinari, University of Huddersfield

Dr Alin M Elena, Daresbury Laboratory, STFC, UKRI

The organizers acknowledge the support received from Georgia Lomas (Daresbury Laboratory) and Jonathan Oldfield (Rutherford Laboratory) with the registration process and the organization of the event.

Programme

Time	Speaker	Title
9:30 - 10:00	Prof Paola Carbone, University of Manchester, CCP5 Chair	Opening/CCP5/CCP5 Prize
10:00 - 10:30	Dr Ali Karimi, Continental AG, Germany, invited	From Material Chemistry to Tire Performance using Multiscale Modeling
10:30 - 11:00	Prof Rosalind Allen, University of Edinburgh, invited	Simulating non-equilibrium phase transitions in the growth of bacterial biofilms
11:00 - 11:30	Email Break	
11:30 - 12:00	Dr Helen Chappell, University of Leeds, invited	Iron Oxide Nanoparticles for the Treatment of Iron Deficiency Anaemia
12:00 - 12:15	Oliver Gittus, Imperial College London	Soft Matter under Thermal Fields: How Non-Equilibrium Coupling Effects Alter Transport Properties
12:15 - 12:30	Dr Jorge Miguel, University of Strathclyde	Accounting for polarization in non-polarizable force fields
12:30 - 12:45	Dr José A. Martinez-Gonzalez, Donostia International Physics Center Spain	Molecular dynamics of interfacial water in contact with model silicon surfaces
12:45 - 14:00	Lunch	
14:00 - 14:30	Dr ViV Kendon, University of Durham	Quantum computing for scientific applications: how to give your simulations a quantum boost
14:30 - 14:45	Dr Colin Freeman, University of Sheffield	Survival of DNA in natural environments
14:45 - 15:00	David McKechnie, University of Strathclyde	Interfacial Concentration Effect Facilitates Heterogeneous Nucleation from Solution
15:00 - 15:15	Dr Charlie Wand, University of Manchester	Computer simulations of epoxy binding on Iron Oxide surfaces
15:15 - 15:45	Email Break	
15:45 - 16:15	Prof Tina Düren, University of Bath, invited	Combining molecular simulation and machine learning: autonomous investigation of porous solids for adsorption

applications

16:15 - 16:30	Jacob Earnshaw, Sheffield Hallam University	Molecular Dynamics Modelling of Polymeric Nanocomposite Thin Films
16:30 - 16:45	Dr Silvia Di Lecce, Imperial College London	Lateral ordering in nanoscale ionic liquid films between charged surfaces enhances lubricity
16:45 - 17:00	Dr Breannan O Conchuir, IBM Research Europe	The Role of Chemical Heterogeneity in Surfactant Adsorption at Solid-Liquid Interfaces
17:00 - 17:10	Good Bye!	

Invited Speakers

Prof Rosalind Allen, University of Edinburgh

Prof Tina Düren, University of Bath

Dr Helen Chappell, University of Leeds

Dr Ali Karimi, Continental AG

Dr Viv Kendon, University of Durham

Abstracts



From Material Chemistry to Tire Performance using Multiscale Modeling

Ali Karimi*

Principal Engineering Material Simulation, Continental Reifen Deutschland GmbH,
Hannover, Germany

The physical phenomena and properties of filled rubber compounds cover a wide range of length and time scales: from Angstroms and sub picoseconds to millimeters and minutes. For this reason, an equally wide range of simulation methods at different levels of resolution and, consequently, including differing degrees of freedom is employed to study them. Different simulation methods that bridge the atomistic description of the system to a coarser level have been developed in order to reach the mesoscopic time and length scales important for many material properties. Here, a short introduction to multiscale simulation approaches in macromolecular chemistry is given.

The main challenge of using molecular simulation is always how the macroscopic properties of the material, which are interesting for industrial applications, can be transferred to the atomistic scale and vice versa. Several examples will be shown where the different performances of the automobile tire like the rolling resistance, braking distance or the lifetime of tire are linked to the molecular description of the compound.

Simulating non-equilibrium phase transitions in the growth of bacterial biofilms

Prof Rosalind Allen, University of Edinburgh

Iron Deficiency Anaemia (IDA) affects nearly a sixth of the global population and accounts for numerous disabling symptoms including impaired immune responses, fatigue, poor cognitive development in children, and ultimately maternal and child mortality. Treatment options for IDA include dietary modification, home fortification, oral iron supplementation and intravenous iron (IV). These latter two treatment options are based on the use of nanoparticulate iron-oxides with organic ligand coatings, and are particularly interesting from a structural chemistry perspective.

Here we use the Near and Intermediate Range Diffractometer (NIMROD, ISIS) to carry out neutron diffraction studies, and first principles DFT methods to provide insight into these experimental results. Using Pair Distribution Function analysis, we combine the experimental and theoretical data to elucidate details of the iron-oxide phases and the detailed chemical structure of ferrihydrite, the main inorganic iron-oxide phase of both the supplements and IV irons. Computational modelling is then employed to characterize the interactions between the iron-oxide particle surface and the organic ligands of the coating.

The results include an improved ferrihydrite structure, and an elaboration of the chemical bonding of the organic ligands to the IHAT nanoparticle core. We have also shown how the character of this bonding changes through the digestive tract as pH alters, and provide an explanation for the late absorption of this novel iron supplement, which remains intact through the stomach and small intestine.

As the only nutritional deficiency that affects both developing and developed populations, new treatment options that can overcome potentially dangerous side effects are increasingly important and any chemical insight that can improve the rational design of these drugs will be immensely valuable.

Iron Oxide Nanoparticles for the Treatment of Iron Deficiency Anaemia

Dr Helen Chappel, University of Leeds

Iron Deficiency Anaemia (IDA) affects nearly a sixth of the global population and accounts for numerous disabling symptoms including impaired immune responses, fatigue, poor cognitive development in children, and ultimately maternal and child mortality. Treatment options for IDA include dietary modification, home fortification, oral iron supplementation and intravenous iron (IV). These latter two treatment options are based on the use of nanoparticulate iron-oxides with organic ligand coatings, and are particularly interesting from a structural chemistry perspective. Here we use the Near and Intermediate Range Diffractometer (NIMROD, ISIS) to carry out neutron diffraction studies, and first principles DFT methods to provide insight into these experimental results. Using Pair Distribution Function analysis, we combine the experimental and theoretical data to elucidate details of the iron-oxide phases and the detailed chemical structure of ferrihydrite, the main inorganic iron-oxide phase of both the supplements and IV irons. Computational modelling is then employed to characterize the interactions between the iron-oxide particle surface and the organic ligands of the coating.

The results include an improved ferrihydrite structure, and an elaboration of the chemical bonding of the organic ligands to the IHAT nanoparticle core. We have also shown how the character of this bonding changes through the digestive tract as pH alters, and provide an explanation for the late absorption of this novel iron supplement, which remains intact through the stomach and small intestine.

As the only nutritional deficiency that affects both developing and developed populations, new treatment options that can overcome potentially dangerous side effects are increasingly important and any chemical insight that can improve the rational design of these drugs will be immensely valuable.

Quantum computing for scientific applications: how to give your simulations a quantum boost

Dr Viv Kendon, Durham University

You have probably noticed that new computers are not getting faster, but HPC facilities are becoming more diverse. Dedicated hardware for neural networks and machine learning; GPUs; FPGAs; ASICs; each requiring new skills to programme and integrate with conventional computers. And now, quantum computing is promising to be the latest and greatest innovation to speed up your computations. Computational scientists know that it is never that easy, a lot of hard work goes into simulation advances by any route. There are good theoretical reasons to support the idea that quantum computers can eventually make a bigger difference to many simulations than other types of new hardware.

To facilitate the process of integrating quantum computing into scientific computing, CCP-QC was proposed and funded in the recent call for CCPs. I will give an overview of CCP-QC's plans to work with existing CCPs, HECs, and the quantum computing community. This will include an introduction to current state of the art in quantum computing, and some insights into what we expect will work (and what won't) and why.

Combining molecular simulation and machine learning: autonomous investigation of porous solids for adsorption applications

Prof Tina Düren, University of Bath

With millions of different porous materials to choose from, molecular simulations are invaluable for identifying promising candidates for applications such as gas storage or advanced separations. They are significantly cheaper than experimental synthetic approaches, allowing many materials to be assessed in quick succession.

Numerous large-scale screenings of porous materials have been conducted, assessing the performance of hundreds of thousands of structures using molecular simulations. However, they are expensive and can lack accuracy, often relying on finding a compromise between computational costs and calculating the property of interest for all structures precisely. This brute-force approach becomes impractical when considering mixtures of guest molecules, complex guest molecules, and different experimental conditions.

To further reduce the time taken for materials discovery, some research groups have trained machine learning models on the screening data sets, with varying results. A core problem is the focus on traditional machine-learning prediction, where a model is first trained and then used to estimate properties of interest for all structures in the data set. It is only after a large number of simulations have been conducted that the model can be used to identify the top performing materials for the application of interest.

Combining Bayesian optimisation and molecular simulation we have developed a new approach, which we call the Autonomous Materials Investigator (AMI), which allows us to identify the top performing materials of a database without having to calculate the property of interest for 10,000s of individual structures. One of the core attractions of this new methodology is that our model can make recommendations based on limited information, updating itself in-situ from molecular simulation of performance for a given application.

Using the hCOF (hypothetical covalent organic frameworks) [1] and the hMOF (hypothetical metal-organic frameworks) [2] databases, we demonstrate the AMI's impressive efficiency. For example, the AMI identifies 90 of the top 100 performing structures from 69,480 hCOF structures with less than 500 calculations for methane storage. This performance allows us to perform screening for more computationally expensive applications. Finally, our method can also integrate experimental inputs in addition to simulations to allow for further aspects of the materials to be considered during screening.

References

- [1] R. Mercado, R. Fu, A. Yakutovich, et al., *Chem. Mater.*, 30, 5069 (2018)
- [2] C. Wilmer, M. Leaf, C. Leet, et al., *Nature Chemistry*, 4, 83 (2012)

Contributors



Soft Matter under Thermal Fields: How Non-Equilibrium Coupling Effects Alter Transport Properties

Oliver Gittus, Imperial College London

Soft condensed matter is characterized by an energy scale comparable with room temperature thermal energy. Thermal fields can induce a plethora of coupling effects, changing the structure, dynamics and transport properties of these materials. We demonstrate that temperature gradients can be used to manipulate soft matter with two examples. (1) Anisotropic colloids, where an inhomogeneous mass distribution can bias rotational diffusion, altering the Soret coefficient of the colloidal suspension [1]. (2) Liquid and supercritical acetonitrile (a polar fluid), where a temperature gradient can induce an electrostatic field, leading to a decrease in thermal conductivity [2]. These results suggest a variety of potential applications: from using temperature gradients as sensing probes, to thermophoretic transport, to waste heat recovery.

[1] O. R. Gittus, J. D. Olarte-Plata and F. Bresme, *Eur. Phys. J. E*, 42, 90 (2019)

[2] O. R. Gittus, P. Albella and F. Bresme, submitted, (2020)

Accounting for polarization in non-polarizable force fields

Dr Miguel Jorge, University of Strathclyde

Classical non-polarizable models, normally based on a combination of Lennard-Jones (LJ) sites and point charges, are extensively used to model thermodynamic properties of fluids, including solutions and mixture. An important shortcoming of this class of models is that they do not explicitly account for polarization effects - i.e. a description of how the electron density responds to changes in the molecular environment. Instead, polarization is implicitly included, in a mean-field sense, into the parameters of the model, usually by fitting to pure liquid properties (e.g. density). Problems arise when trying to describe thermodynamic properties that involve a change of phase (e.g. enthalpy of vaporization), solutions/mixtures (e.g. solvation free energies), or that directly depend on the electronic response of the medium (e.g. dielectric constant)¹. Fully polarisable models present a natural route for addressing these limitations, but at the price of a much higher computational cost. In this work, we combine the best of those two approaches, by running fast simulations using non-polarizable models and applying post facto corrections to the computed properties in order to account for polarization effects.

I will show how the application of polarization corrections allows for systematic improvements in the accuracy of classical non-polarizable models: i) they eliminate long-standing systematic deviations in predictions of the dielectric constant of liquids across the entire polarity range (from alkanes to water)^{2,3}; ii) they offer a theoretically-grounded explanation as to why the dipole moments of effective non-polarizable models are much lower than real dipole moments in the liquid phase^{4,5}; iii) they offer a route to simultaneously predict the vapourisation enthalpy and the hydration free energy of water⁵; iv) they allow for accurate predictions of thermodynamic properties of mixtures of compounds with different polarity (e.g. alcohols/alkanes), without ad hoc parameter adjustments⁶. I will finish by presenting very recent work on developing a new self-consistent approach for deriving both force field parameters and polarization corrections from simple QM/MM calculations. This paves the way for a new generation of classical models that combine high accuracy with low computational cost.

(1) C. Caleman, P. J. van Maaren, M. Hong, J. S. Hub, L. T. Costa, D. van der Spoel, *J. Chem. Theor. Comput.* 8, 2012, 61-74.

(2) C. Vega, *Mol. Phys.* 113, 2015, 1145-1163.

(3) M. Jorge, L. Lue. *J. Chem. Phys.*, 150, 2019, 084108.

(4) I. V. Leontyev, A. A. Stuchebrukhov, *J. Chem. Phys.* 130, 2009, 085102.

(5) A. W. Milne, M. Jorge, *J. Chem. Theory Comput.* 15, 2019, 1065–1078.

(6) M. C. Barrera, M. Jorge, *J. Chem. Inf. Model.*, 2020, 10.1021/acs.jcim.9b01005.

Molecular dynamics of interfacial water in contact with model silicon surfaces

José A. Martínez-Gonzalez^{1,2} and Victoria Garcia-Sakai¹

¹ISIS, Rutherford Appleton Lab, SFTC, Didcot, Oxfordshire, Great Britain

²Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain.

Silicon and silicon-based/coated materials have been proposed as in-vivo biomaterials. For example, silicon products are used in the composition of medical instrumentation, i.e, dialysis tubing, pacemaker leads, or singular in developing new sensors or for drug-delivery applications [1, 2]. When these materials are in contact with blood or introduced into the body, a close strong interaction with water appears, and a specific aqueous interface is created[3], [4]. This 'interfacial water' has become a subject of substantial interest, addressing open questions relating to how its behaviour changes depending on the hydrophobicity of the surface. The dynamical behaviour of interfacial water with TiO₂ and SiO₂ powders has been probed by various spectroscopic methods [5–7] including neutron scattering and infrared. And although, QENS has also been used to study confined water in different materials, such as MCM-41, not has been applied extensively to the case of silicon surfaces.

The work presented here aims to study, from a theoretical perspective, how the different surface interaction (more or less hydrophobic) change the behaviour of water not only in the nearest region but also at greater distances. Silicon-(100) surfaces terminated in hydrogen, hydroxyl groups and without any termination are the selected systems. MD simulations were performed using DLPOLY v4.0 package with Tersoff potential to the silicon surfaces and the flexible SPC-type model to water (SPC-FW) [8]. All simulations were carried out with constant temperatures and pressure. Any constraint algorithm for hydrogen vibration was used for SPC-FW. MDANSE package was used to obtain the measurable $I(q,\omega)$ from MD simulations which is the starting point for further analysis (relaxation time, dynamical structure factors, ...).

[1] H. A. Santos, Porous silicon for biomedical applications. Elsevier, 2014.

[2] S. E. Saddow, Silicon carbide biotechnology: a biocompatible semiconductor for advanced biomedical devices and applications. Elsevier, 2012.

[3] M. A. Bag and L. M. Valenzuela, Int. J. Mol. Sci., 18, 8, (2017).

[4] J. M. Morais, F. Papadimitrakopoulos, and D. J. Burgess, AAPS J., 12, 188–196, (2010).

[5] E. C. Spencer et al., J. Phys. Chem. A, 113, 2796–2800, (2009).

[6] A. A. Levchenko et al., J. Phys. Chem. A, 111, 12584–12588, (2007).

[7] E. Mamontov et al., Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys., 79, 051504, (2009).

[8] J. A. Martínez-Gonzalez, N.J. English, and A A. Gowen, AIP Advances, 7, 115105 (2017).

Survival of DNA in natural environments

Dr Colin Freeman, University of Sheffield

The preservation and survival of DNA in the natural environment remains a key scientific question. The DNA extracted from sediments provides information on evolution and human development such as diet and food processing. This rich source of information is compromised by our understanding of the decay of the DNA which is controlled by the environmental conditions. A major component of these conditions are mineral surfaces where the DNA can be bound. We present a combined molecular dynamics and atomic force microscopy study on the binding of DNA chains to calcite mineral surfaces. Our study demonstrates that strong binding can occur via direct interactions and also facilitated by ions in the surrounding solution. Exploration of surface topography shows that steps on the surface dominate binding profiles. We combine the two methods to examine the decay process of the DNA molecules on the surface. This data is then used to speculate on DNA preservation in sediments.

Interfacial Concentration Effect Facilitates Heterogeneous Nucleation from Solution

David McKechnie, University of Strathclyde

Crystal nucleation from solution plays an important role in environmental, biological, and industrial processes. Nucleation studies are often performed in small scale experimental setups such as microfluidics and microplates, where small volumes of solution are in contact with an oil at a high surface area to volume ratio. It is widely accepted that nucleation from solution often occurs heterogeneously at interfaces. With this high ratio, heterogeneous nucleation could dominate, and the properties of the interface may influence the results. We use a combined experimental and computational approach to investigate the nucleation of glycine from aqueous solution at oil-solution and air-solution interfaces [1]. Experimentally we found that the presence of oil greatly enhanced the nucleation rate of glycine from aqueous solution, with 85% of samples nucleating within three days with an oil layer compared to 3% without the oil layer. This is surprising as the hydrophobic, non-polar oil (tridecane) would not be expected to interact with hydrophilic, highly polar glycine. Classical molecular dynamics (MD) simulations reveal a stark difference in the solution composition at oilsolution and air-solution interfaces, with a 21% increase in concentration at the oil-solution interface, and a 49% decrease in concentration at the air-solution interface. As the nucleation rate is very sensitive to solution concentration, we propose that this interfacial concentration effect facilitates heterogeneous nucleation. Further work will use a model surface to investigate how interfacial properties influence the interfacial concentration, and hence heterogeneous nucleation.

[1] D. McKechnie et al., *J. Phys. Chem. Lett.* 2020, 11, 6, 2263–2271

Computer simulations of epoxy binding on Iron Oxide surfaces

Charlie Wand¹, Simon Gibbon² and Flor Siperstein¹

¹ Department of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK

² AkzoNobel Research & Development, Northallerton, North Yorkshire, DL7 7BJ, UK

Epoxy resins have a wide range of applications as polymer adhesives and protective coatings, from aerospace and marine applications through to nontoxic interior coatings in the food industry [1]. In all cases, the performance of the final solid-polymer system is dependent on the physicochemical properties of the interface and the interaction between the polymer and the solid substrate. However, experimental methods to characterize this interaction are limited and mostly deteriorative to the interface. Computer modelling provides a tool to investigate the surface-polymer interface at an atomistic level.

Here we perform atomistic molecular dynamics simulations to investigate the binding of a diglycidyl ether of bisphenol A (DGEBA) on Iron Oxide surfaces (Figure 1) and investigate the effect of number of repeat units in DGEBA on the binding energy ($\Delta E_{binding}$) defined as;

$$\Delta E_{binding} = E_{\substack{adsorbate \\ surface}} - (E_{adsorbate} + E_{surface})$$

Where $E_{\substack{adsorbate \\ surface}}$ is the energy of the adsorbed DGEBA on the surface and $E_{adsorbate}$, $E_{surface}$ are the energy of the adsorbate and surface in vacuum respectively.

In epoxy resin applications the composition of the solid substrate is highly varied, with pre-treatments and production processes leading to a non-uniform surface chemistry and roughness. To reflect this, we investigate two Iron Oxides surfaces, hematite (Fe_2O_3) and magnetite (Fe_3O_4) and the influence of surface hydroxylation. We find that binding is stronger for DGEBA on hematite than magnetite, in agreement with previous literature findings [2] and suggest causes of this trend based on the surface termination.

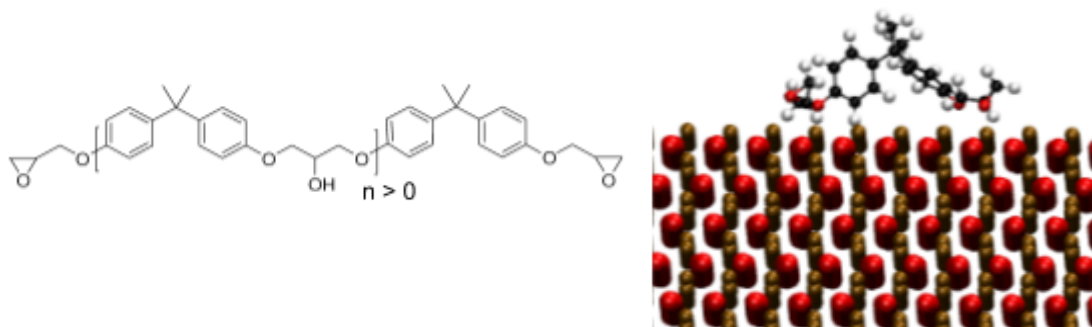


Figure 1: Left: Structure of diglycidyl ether of bisphenol A (DGEBA). Right: n=0 DGEBA adsorbed onto an iron terminated Fe_2O_3 (0001) surface

This work was done with support from the EPSRC Prosperity Partnership SusCORD (EP/S004963/1).

[1] Friedrich, Jörg. *Metal-Polymer Systems: Interface Design and Chemical Bonding*. John Wiley & Sons, 2017.

[2] Bahlakeh, Ghasem, et al *J. Phys. Chem. C* **120** 20 (2016): 11014-11026.

Molecular Dynamics Modelling of Polymeric Nanocomposite Thin Films

Jacob Earnshaw, Doug Cleaver, Alexander Hamilton and Michal Krompiec

Sheffield Hallam University

The organic-inorganic nature of the silsesquioxanes, $\text{RSiO}_{1.5}$, provides a basis for the development of materials with unique macro-scale properties. Within our work, we focus on the cubic polyhedral oligomeric silsesquioxane (POSS) structure. Each POSS cube is characterised by the distinctive silica core that is functionalised with organic moieties at the vertices. A wide variety of functional groups may be utilised as the grafted organic species, lending to the rich chemistry available to this species.

Here we use Molecular Dynamics simulations to elucidate the atomistic and molecular level mechanisms that contribute to the observed material properties. We have simulated both synthetically relevant and as yet to be synthesised structures. (include something more specific about current mixed system work). By analysing the inter-molecular packing and intra-molecular interaction and behaviour, we have determined strong sensitivities of microscopic and macroscopic properties to the choice of functionalising moieties. We also determine that the quality of charge description is paramount for the quantitative matching of experimental thermomechanical behaviour.

Lateral ordering in nanoscale ionic liquid films between charged surfaces enhances lubricity

Silvia Di Lecce¹, Alexei Kornyshev¹, Michael Urbakh² and Fernando Bresme¹

¹Department of Chemistry, Imperial College London, W12 0BZ, United Kingdom

²School of Chemistry, Faculty of Exact Sciences and the Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel

The ability to control and manipulate friction is extremely important in many research fields such as biomedicine, engineering, chemistry, physics, and nanotechnology [1]. Indeed, friction is responsible for significant energy losses on the industrial scale as well as for material fatigue, degradation and mechanical failure. In nanoscale devices, the friction losses and the material wear can be minimized by placing a thin nanometric liquid film between the sliding surfaces. Ionic liquids (ILs) are being actively investigated as lubricants given their unique thermophysical properties: chemical and thermal stability, low vapour pressure and low melting temperature [2]. Furthermore, the structural and dynamic properties of ILs can be modified through electric field, opening new avenues to develop tunable lubrication devices [3–6].

We systematically investigate the impact of IL composition and molecular structure on friction, by using grand canonical non-equilibrium molecular dynamics [3, 7]. Using both coarse grained and atomistic models of 1-*n*,2-methyl-imidazolium tetrafluoroborate [C_{*n*=2..6}MIM][BF₄] ILs, we show that the friction force depends significantly on the chain length of cation and the surface charge [7]. The nanofilm is less compressible and show lower friction forces when the IL contains cations with shorter aliphatic chain. At high loads, we observe maxima in the friction force at specific surface charges, where the slippage plane vary from the IL-electrode interface to the interior of the film.

We extend our analysis considering imidazolium cations and widely used anions, featuring difference molecular structures, spherical (BF₄), elongated surfactant-like (C₂SO₄) and elongated with a more delocalized charge (NTf₂). Our results show that surface charge and anion geometry enables the crystallization of BF₄, and NTf₂ nanofilms, resulting in friction forces lower than the one obtained for C₂SO₄ which forms disordered layers. We identify the formation of crystal-like structure as a new mechanism to tune the friction response with electric fields.

References

- [1] M. Urbakh, J. Klafter, D. Gourdon and J. Israelachvili. Black and C. Smith, *Nature*, 430, 525-528 (2004).
- [2] R. Hayes, G.G. Warr and R. Atkin, *Chem. Rev.*, 115, 6327–6426 (2015).
- [3] O.Y. Fajardo, F. Bresme, A.A. Kornyshev, M. Urbakh, *Sci. Rep.*, 5, 7698 (2015).
- [4] J. Sweeney, F. Hausen, R. Hayes, G.B. Webber, F. Endres, M.W. Rutland, R. Bennewitz and R. Atkin, *Phys. Rev. Lett.*, 109, 155502 (2012).
- [5] O.Y. Fajardo, F. Bresme, A.A. Kornyshev, M. Urbakh, *J. Phys. Chem. Lett.*, 6, 3998–4004 (2015).
- [6] A.M. Smith, K.R. J. Lovelock, N. Nand Gosvami, T. Welton and S. Perkin, *Phys. Chem. Chem. Phys.*, 15, 15317 (2013).
- [7] S. Di Lecce, M. Urbakh, A.A. Kornyshev, F. Bresme, *ACS Appl. Mater. Interfaces*, 12, 4105–4113 (2020).

The Role of Chemical Heterogeneity in Surfactant Adsorption at Solid-Liquid Interfaces

J. Klebes^{1,2}, S. Finnigan^{1,3}, D. J. Bray⁴,

R. L. Anderson⁴, W. C. Swope⁵, M. A. Johnston⁶ and **Dr Breannan O Conchuir**¹

¹*IBM Research Europe, The Hartree Centre, Daresbury WA4 4AD United Kingdom*

²*School of Mathematics, University of Leeds, LS2 9JT, United Kingdom*

³*Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, Wood Lane, London W12 0BZ, United Kingdom*

⁴*The Hartree Centre, STFC Daresbury Laboratory, Warrington, WA4 4AD, United Kingdom*

⁵*IBM Almaden Research Center, San Jose, California, United States*

⁶*IBM Research Europe, Dublin, Ireland*

Chemical heterogeneity of solid surfaces disrupts the adsorption of surfactants from the bulk liquid. While its presence can hinder the performance of some formulations, bespoke chemical patterning could potentially facilitate controlled adsorption for nanolithography applications. Although some computational studies have investigated the impact of regularly patterned surfaces on surfactant adsorption, in reality many interesting surfaces are expected to be stochastically disordered and this is an area unexplored via simulations. In this talk we describe a new algorithm for the generation of randomly disordered chemically heterogeneous surfaces and use it to explore the ad-sorption behaviour of four model non-ionic surfactants. Using novel analysis methods we interrogate both the global surface coverage (adsorption isotherm) and behaviour in localised regions. We observe trends in adsorption characteristics as surfactant size, head/tail ratio, and surface topology are varied and connect these to underlying physical mechanisms. We believe that our methods and approach will prove useful to researchers seeking to tailor surface patterns to calibrate non-ionic surfactant adsorption.

This work was supported by the STFC Hartree Centre's Innovation Return on Research programme, funded by the Department for Business, Energy & Industrial Strategy

Participants

Full Name	Company Name
Ahammad N K, Thabassum	IISER Mohali
Allan, Neil	University of Bristol
Allen, Michael	University of Bristol & University of Warwick
Allen, Rosalind	University of Edinburgh
Alvarez, Dinais	Universidad de Sucre, Colombia
Andrade, Marko	Universidad Mayor de San Simón
Anwar, Jamshed	Lancaster University
Azevedo, Aline	IFRJ
Bakumenko, Maryna	Taras Shevchenko National university of Kyiv
Barrera, Maria Cecilia	University of Strathclyde
Bresme, Fernando	Imperial College London
Briquet, Ludovic	Johnson Matthey Technology Centre
Brukhno, Andrey	Computational Chemistry, SCD, STFC/UKRI
Campoli, Lorenzo	SPBSU
Carbone, Paola	The University of Manchester
Cardona, Javier	University of Strathclyde
Cardoso, Marcio	Federal University of Rio de Janeiro
Cen, Jiayi	The University of Manchester
Chappell, Helen	University of Leeds
chergui, yahia	Boumerdes University IGEE Institute
Chiricotto, Mara	Universify of Manchester

Clayson, Ivan	UCL
Combariza, Aldo	Universidad de Sucre, Colombia
Cournia, Zoe	Biomedical Research Foundation Academy of Athens
Crossley-Lewis, Joe	University of Bristol
Dalal, vikram	IIT Roorkee
Dawson, James	University of Huddersfield
Delgado Callico, Laia	King's College London
Dhakad, Ambuj	National Institute of Science Education and Research Search form Search Bhubaneswar
Di Bari, Daniele	University of Perugia and University of Grenoble Alpes
Di Lecce, Silvia	Imperial College London
DINE, Khaled	faculty of technology, university of saida
Doan, Huan	University of Bristol
Düren, Tina	University of Bath
Earnshaw, Jacob	Sheffield Hallam University
Elena, Alin	Daresbury Laboratory STFC
Ewen, James	Imperial College London
EYUPOGLU, Ozan	Istanbul Medipol University, School of Pharmacy, Biochemistry Department
Fantauzzo, Vittoria	University of Sheffield
Fisher, Hayden	University of Southampton
Flitcroft, Joseph	Univeristy of Sheffield
Freeman, Colin	University of Sheffield
Gallo, Marco	TecNM
Geatches, Dawn	STFC

Gibbon, Simon	AkzoNobel
Gittus, Oliver	Imperial College London
Gomes Souza Jr, Fernando	Universidade Federal do Rio de Janeiro
González Pérez, Ramón	Universidad de Guanajuato
González, Minerva	
Gregorio, Joao	UNIVERSITY OF STRATHCLYDE
Harding, John	University of Sheffield
Hendrikse, Rachel	University of Leeds
Heyes, David	Royal Holloway University of London
Hills, Oliver	University of Leeds
Horsch, Martin Thomas	UK Research and Innovation
Hourahine, Ben	The University of Strathclyde
Hughes, Zak	University of Bradford
hutereau, martin	university college london
Jackson, Robert	Keele University
Jorge, Miguel	University of Strathclyde
Julliard, Marcel	Macquarie University
Keal, Thomas	STFC Daresbury Laboratory
khan, Sara	Hazara university, Pakistan
Leslie, Maurice	Daresbury Laboratory (retired)
Lima, Nathali	Univerdade Federal do Rio de Janeiro
Logsdail, Andrew	Cardiff Catalysis Institute
Lu, You	UKRI STFC Daresbury Laboratory
Mandhani, Shruti	Sheffield Hallam University

Marinova, Veselina	University of Sheffield
MARTINEZ-GONZALEZ, JOSE ANGEL	DIPC-CFM
Masters, Andrew	University of Manchester
McCready, Connaire	University of Strathclyde
McKechnie, David	University of Strathclyde
Meyer, Jan	Covestro Deutschland AG
Mirzad Rafael, Effran	The University of Manchester
molinari, marco	University of Huddersfield
Morbec, Juliana	Keele University
Morris, Rhiannon	University of Leeds
Moxon, Samuel	University of Huddersfield
O Conchuir, Breannan	IBM
Olarte-Plata, Juan D.	Imperial College London
Padilla, Carlos A.	
Pallikara, Ioanna	University of Manchester
Parker, Steve	University of Bath
Patti, Alessandro	The University of Manchester
Purton, John	STFC
R, Shashank Krishna	Bishop Heber College (Bharathidasan University)
Reyes Chaparro, Andrés	CINVESTAV
Saheer, VC	KMM Govt Women's College KNR
Salimi Parvaneh, Leila	
Santander, Carlos	Pontifica Universidad Catolica de Chile
Sarwar, Misbah	Johnson Matthey Technology Centre

Seaton, Michael	UKRI STFC Daresbury Laboratory
Shaharudin, Mohd Rafie	the university of manchester
Shen, Xiangjian	Zhengzhou University
Simperler, Alexandra	Simperler Consulting
Simperler, Alexandra	Goldbeck Consulting
Skelton, Jonathan	University of Manchester
Smith, Edward	Brunel University London
Smith, Thomas	University of Huddersfield
Spensley, Neil	3DS
Symons, Benjamin	University of Manchester
Tariku, Semahegn Abayneh	Department of Physics, Addis Ababa University
Teh, Hung-Hsuan	University of Pennsylvania
Terranova, Umberto	University of Buckingham
Todorov, Ilian	STFC
Tolladay, Mat	University of Bath
Trachenko, Kostya	Queen Mary London
Tse, Joshua	University of Huddersfield
Underwood, Tom	University of Bath
Velarde Salcedo, Marco Vinicio	Universidad Autónoma del Estado de México
Wand, Charlie	The University of Manchester
Wei, Zixuan	The University of Manchester
Williams, Chris	University of Manchester
Wood, Nathan	University of Huddersfield
Yeandel, Stephen	University of Sheffield

[Yong, Chin](#)

STFC, Daresbury Laboratory

[Zarkadoula, Eva](#)

Oak Ridge National Laboratory