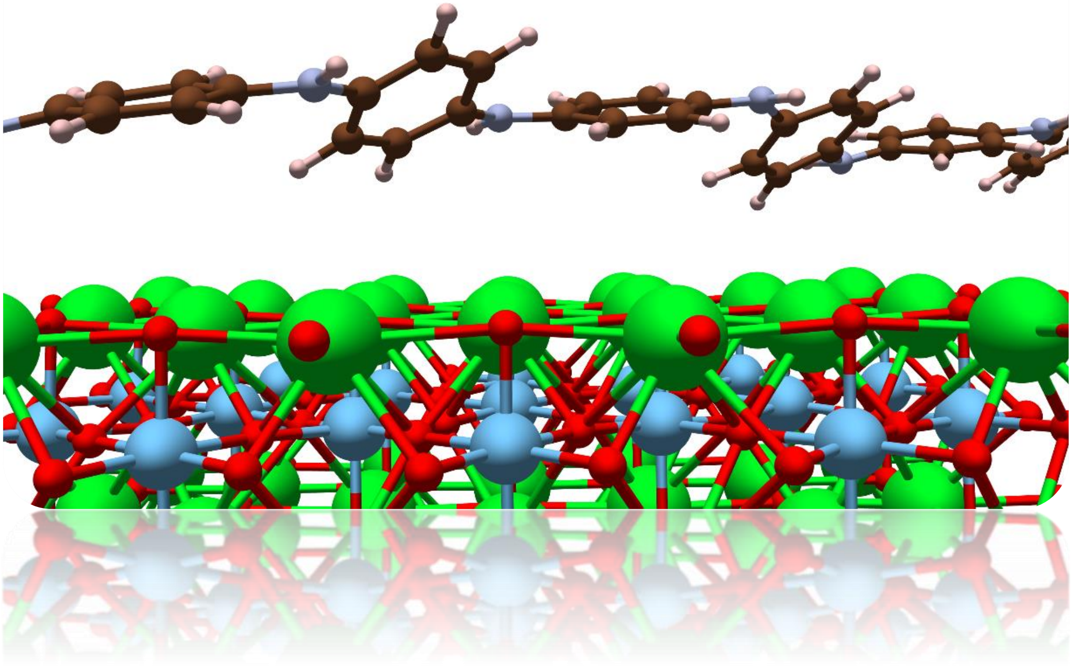
CCP5 ANNUAL GENERAL MEETING

42ND EDITION
AND THE ANIVERSARY OF THE 40TH EDITION

THE UNIVERSITY OF HUDDERSFIELD
5TH – 7TH SEPTEMBER 2022



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Organizing committee

Marco Molinari (M.Molinari@hud.ac.uk)

Alin-Marin Elena (alin-marin.elena@STFC.ac.uk)

David Cooke (D.J.Cooke@hud.ac.uk)

With the help of Nathan Wood, Minh Khoa Ta, Susanna Vigorito, Thomas Smith, and Sidra Munir.

Day 1			
Time	**Event**	**Presenter**	**Location**
12:00 – 12:45	**Arrival / Registration / Lunch**		Student Hub (JPSG/31)
12:45 – 13:00	**Opening remarks**		JPSG/18
13:00 – 13:30	**Invited:** Present and future of CCP5	Prof. Paola Carbone The University of Manchester	JPSG/18
13:30 – 14:00	**Invited:** What can simulation teach us about crystallisation from solution	Prof. John Harding, The University of Sheffield	JPSG/18
14:00 – 14:15	Predicting thermodynamic properties of adsorption monolayers with lattice models	Dr Pavel Stishenko, Cardiff University	JPSG/18
14:15 – 14:30	Modelling mineral-organic interactions: Adsorption of organic molecules and biomolecules on the alpha-Al_2O_3 (0001) surface	Dr Natalia Martsinovich, The University of Sheffield	JPSG/18
14:30 – 14:45	A first-principles study on the absorption of phosphate on oxygenated graphene	Dr Xue Yong, The University of Sheffield	JPSG/18
14:45 –15:00	Time Series Decomposition of Spontaneous Urinary Bladder Activity: connecting statistical mechanics with the thermodynamics of contractile hollow viscera	Dr Arun Chind, Proshen Health & Risk Consulting Ltd	JPSG/18
15:00 –16:00	**Refreshments**		Student Hub (JPSG/31)
16:00 –16:30	**Invited:** Opportunities and Challenges in Formulation Modelling	Dr Jerry Winter, Unilever	JPSG/18
16:30 – 17:00	**Invited:** Multiscale modelling of perovskite solar cells	Prof. Alison Walker, University of Bath	JPSG/18
17:00 –17:15	Lattice Dynamics of Uranium Dinitride (UN_2)	Dr Joseph Flitcroft, The University of Manchester	JPSG/18
17:15 –17:30	Computational Study of the Formation of Sn-BEA for Liquid Phase Catalysis	Owain Beynon, Cardiff University	JPSG/18
17:30 –17:45	Multiscale Modeling of lithium diffusion and NMR properties solid state electrolytes	Mahmoud Attia, Mansoura University	JPSG/18
17:45 –18:00	On the formation of C_2H_4O isomers on dust surfaces in the ISM	Reetu Reetu, The University of Sheffield	JPSG/18
18:00 - 20:00	**Poster Session 1**		Atrium JPSG/C02
20:00	**Buffet Dinner**		The Keys, Byram St, Huddersfield HD1 1BU

Day 2			
Time	**Event**	**Presenter**	**Location**
09:00 –09:30	**Invited:** Simulation as a tool in materials Chemistry and Physics	Prof. Richard Catlow, University College London	JPSG/18
09:30 – 10:00	**Invited:** Optimisation of sustainable plastics by tuning the filler-polymer interface	Dr Karen Johnston, University of Strathclyde	JPSG/18
10:00 – 10:15	Modelling Organic-Inorganic Interfaces of Urinary Calculi	Rhiannon Morris, University of Leeds	JPSG/18
10:15 – 10:30	Interfacial Free Energies from MD Simulations: Application to $CaSO_4 \cdot xH_2O$	Dr Stephen Yeandel, The University of Sheffield	JPSG/18
10:30 – 10:45	Interfacial Free Energies of Calcium Carbonate with Water from Atomistic Simulations	Emma Armstrong, The University of Sheffield	JPSG/18
10:45 – 11:30	**Refreshments**		Student Hub (JPSG/31)
11:30 – 12:00	**Invited:** Atomistic Modelling of Interfaces	Prof. Steve Parker, University of Bath	JPSG/18
12:00 – 12:15	A DFT study on the stability and vibrational fingerprint of phosphate species on the surfaces of Ceria	Minh Khoa Ta, University of Huddersfield	JPSG/18
12:15 – 12:30	How does lattice thermal conductivity "work"? Insight from first-principles calculations	Dr Jonathan Skelton, The University of Manchester	JPSG/18
12:30 – 12:45	Exploring the phase behaviour of Hard-Sphere Dimers.	Omar-Farouk Adesida, University of Warwick	JPSG/18
12:45 – 13:00	Determining the Phase Diagram of a Machine-Learned Carbon Potential via Nested Sampling	Dr George Marchant, University of Warwick	JPSG/18
13:00 – 14:00	**Lunch**		Student Hub (JPSG/31)
14:00 – 14:30	**Invited:** Nested sampling: what can we learn about an interatomic potential?	Dr Livia Bartok-Partay, University of Warwick	JPSG/18
14:30 – 15:00	**Invited:** The history of CCP5	Prof. Bill Smith, CCP5	JPSG/18
15:00 – 15:15	Using molecular dynamics simulation to predict the aggregation propensity of mAb formulations & accelerate development	Yuhan Wang, University College London	JPSG/18

15:15 – 15:30	The role of surface ionisation and topology in the hydration-induced swelling of Graphene Oxide (GO) membranes	Mohd Rafie Bin Shaharudin, The University of Manchester	JPSG/18
15:30 – 15:45	Topological network analysis of thin ionomer membranes	Prof. James Elliott, University of Cambridge	JPSG/18
15:45 – 16:30	**Refreshments**		Student Hub (JPSG/31)
16:30 – 16:45	Towards High-throughput simulations of polymers plasticizers	Lois Smith, The University of Manchester	JPSG/18
16:45 – 17:00	Composites made of Polyaniline and $SrTiO_3$: Thermoelectric Abilities	Nathan Wood, University of Huddersfield	JPSG/18
17:00 – 17:15	Machine Learning Force Fields for Multicomponent Organic Liquids: Applications for Battery Electrolytes.	Dr Ioan-Bogdan Magdau, University of Cambridge	JPSG/18
17:15 – 17:30	Molecular Fluid Dynamics	Dr Edward Smith, Brunel University London	JPSG/18
17:30 – 18:00	**Invited:** Properties of condensed matter from fundamental physical constants	Prof. Kostya Trachenko, Queen Mary University of London	JPSG/18
18:00 – 20:00	**Poster Session 2**		Atrium JPSG/C02
20:00	**Seated Dinner & Awards**		The Keys, Byram St, Huddersfield HD1 1BU

Day 3			
Time	**Event**	**Presenter**	**Location**
09:00 – 09:30	**Invited:** Diffusion in Oxides and Halides – Insights and Surprises from Simulations	Prof. Neil Allan, University of Bristol	JPSG/18
09:30 – 09:45	A first-principles study of the impact of Frenkel and Schottky defects on the thermal properties of ceria	Thomas Smith, University of Huddersfield	JPSG/18
09:45 – 10:00	High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation	Ioanna Pallikara, The University of Manchester	JPSG/18
10:00 – 10:15	Alkali metal nitrates: a new model for crystallisation	Vittoria Fantauzzo, The University of Sheffield	JPSG/18
10:15 – 10:30	**Invited:** Epoxy-resins: insights from molecular simulations for the development of better coatings	Prof. Flor Siperstein, The University of Manchester	JPSG/18
10:45 – 11:40	**Refreshments**		Student Hub (JPSG/31)
11:30 – 12:00	**International:** Materials Modelling Activities at CHPC: Collaboration with CCP5	Dr Happy Sithole, CHPC-South Africa	JPSG/18
12:00 – 12:15	Wettability of graphite under 2D confinement	Zixuan Wei, The University of Manchester	JPSG/18
12:15 – 12:30	Ethylenediamine series as additives to control the morphology of magnetite	Dr David Cooke, University of Huddersfield	JPSG/18
12:30 – 12:45	The influence of water, carbon dioxide and hydrogen peroxide on the morphology of cerium oxide nanoparticle	Dr Marco Molinari, University of Huddersfield	JPSG/18
12:45 – 13:00	**Concluding Remarks**		JPSG/18
13:00	**Departure**		

Talks abstracts

Present and future of CCP5

Presenter: Prof. Paola Carbone
University of Manchester Invited talk 1

An introduction to the CCP5 and the new network consortium CCP5++, what we stand for and what are the plans for the future

What can simulation teach us about crystallisation from solution

Presenter: Prof. John Harding
University of Sheffield Invited talk 2

CCP5 began with the simulation of liquids and only a few years later added the simulation of the structure and properties of crystals. Simulating the interface between the two is much harder, but when we consider how ionic solids crystallise from solution we cannot avoid the complexities of the aqueous interface. These can include interface dipoles, complex reconstructions, partially dissolved species and ordering of the water by the crystalline solid. There are also formidable problems of length and timescales to be considered that make the use of ab initial methods problematic. The alternative of using classical forcefields presents problems of how to obtain a robust, accurate representation. We shall dip our toes into the water, form our interface and see what happens.

Predicting thermodynamic properties of adsorption monolayers with lattice models

Presenter: Pavel Stishenko
Co-author: Andrew Logsdail; Amit Chaudhari
Cardiff University

Delegate talk 1

Lattice models have long been employed to understand thermodynamics and process kinetics of adsorption monolayers (adlayers). Langmuir's isotherm and Ziff-Gulari-Barshad model of CO oxidation are essential parts of heterogeneous catalysis and surface science curricula. But for many interesting adsorption systems construction of lattice models is non-trivial and laborious. Low symmetry of adsorbent surface and adsorption complexes, long-range lateral interactions, many-body interactions, multiplicity of adsorbate species, and complex phase behaviour greatly complicate both model building, parametrization, and doing computations with it. The Surface Science Modelling and Simulation Toolkit (SuSMoST) [1] comprise Python libraries and utility scripts that greatly simplify routine of building, parametrization, and investigation of adsorption systems. Taking on the input sketches of the relevant adsorption complexes, SuSMoST scripts are able to enumerate all possible non-equivalent allocations of pair of adsorption complexes up to desired cut off radius, as well as all possible unit cells (phases) of the adlayer up to desired unit cell size. These generated structures can be used to build a lattice model, parametrize it, to construct a convex hull in the space of mixing energy and surface coverage. For parametrized models SuSMoST libraries support Metropolis Monte Carlo calculations with parallel replicas and weighted histograms support. SuSMoST includes Python package for numerically-exact calculation of the partition function using tensor-network algorithms (tensor renormalization and transfer-matrix). With SuSMoST one can evaluate equilibrium surface coverages, adlayer structures, phase transitions (critical values of temperature and chemical potentials). Interesting systems and phenomena studied with SuSMoST are hydroxylation of oxygen-terminated MXenes [2], Devil's stair case of phase transitions in a metal-organic adlayer [3], influence of surface defects on stability of adlayers phase's [4], chlorine chemisorption on anatase surface.

References:

[1] S. S. Akimenko, G. D. Anisimova, A. I. Fadeeva, V. F. Fefelov, V. A. Gorbunov, T. R. Kayumova, A. V. Myshlyavtsev, M. D. Myshlyavtseva and P. V. Stishenko, J Comput Chem, 2020, 41, 2084–2097

[2] T. R. Kayumova, I. P. Kolganov, A. V. Myshlyavtsev, P. V. Stishenko and A. I. Fadeeva, Surface Science, 2022, 717, 121984.

[3] A. I. Fadeeva, V. A. Gorbunov, O. S. Solovyeva, P. V. Stishenko and A. V. Myshlyavtsev, J. Phys. Chem. C, 2020, 124, 11506–11515.

[4] A. I. Fadeeva, V. A. Gorbunov, P. V. Stishenko, S. S. Akimenko and A. V. Myshlyavtsev, Applied Surface Science, 2021, 545, 148989.

Modelling mineral-organic interactions: Adsorption of organic molecules and biomolecules on the alpha-Al_2O_3 (0001) surface

Presenter: Natalia Martsinovich
Co-author: Aneesa Ahmad
University of Sheffield

Delegate talk 2

Binding of organic molecules on oxide mineral surfaces is a key process in soil preservation due to its ability to protect soil organic carbon from microbial degradation. To understand the nature and strength of sorption of organic carbon in soil, we investigated the binding of small organic molecules and larger polysaccharide biomolecules (typical building blocks of soil organic carbon) on alpha-Al_2O_3, a common soil mineral which is known to strongly bind organic matter. The calculations of adsorption on the alpha-Al_2O_3 (0001) surface were carried out using density functional theory (DFT) with empirical dispersion correction. First, adsorption of small organic molecules containing of a variety of functional groups was investigated and compared to the binding of water. Amine, amide and carboxylic acid functional groups were found to bind to this surface more strongly than water. Alcohol, ether, thiol and ester groups had binding energies very similar to that of water, while hydrocarbons were found to bind less strongly. Carboxylic acids were the strongest bound adsorbates in this study. Dissociated adsorption configurations were usually more favourable than molecular adsorption; hydrogen bonding was also found to make a significant contribution to the strength of adsorption. Thus, a number of organic functional groups were identified, such as amine, amide and carboxylic acids, which are able to bind to the alpha-Al_2O_3 (0001) surface more strongly than water and are likely to adsorb on this mineral surface under ambient conditions. Informed by these insights into adsorption of small molecules, we modelled adsorption of biomolecules - fragments of polysaccharides which naturally occur in soil: cellulose, chitin, chitosan and pectin. Pectin, which contains hydroxyl and carboxylic groups, and chitosan, which contains hydroxyl, amine and amide groups, were found to bind strongly, consistent with the strong binding of the functional groups present in these molecules. Cellulose, which contains only ether and hydroxyl groups, showed the least strong adsorption among the biomolecules studied. Our results show that biomolecules containing acid, amine and amide groups, such as pectin and chitosan, bind strongly to soil minerals and therefore are likely to be stable in soil.

A first-principles study on the absorption of phosphate on oxygenated graphene

Presenter: Xue Yong
Co-author: Natalia Martsinovich
University of Sheffield

Delegate talk 3

Phosphorus is one of the most essential nutrients for plant growth and crop production. However, excess phosphorus in soil can be detrimental to the environment and the plant. Improved phosphorus management would promote the development of profitable and sustainable crop production. [1] However, due to the lack of proper affordable technology, it is currently hard to measure the amount of phosphorus in the soil, therefore a sensor technology needs to be developed. Graphene is a promising sensor material; experiments showed that incorporation of single-layer and multilayer graphene in sensors resulted in significantly improved sensor performance. [2] Therefore, in this work, we investigate oxygenated graphene containing epoxide and hydroxyl groups (labelled "graphene epoxide" and "graphene hydroxides") as a sensor material for detection of phosphate in the soil through density functional theory (DFT) calculations. This work provides quantitative insight into how different phosphate species (PO_4^{3-} , $OHPO_3^{2-}$, $(OH)_2PO^-$, $(OH)_3PO$) can be adsorbed on the graphene. All the considered phosphate compounds can be physisorbed onto the pristine graphene, graphene epoxide, and graphene hydroxides. Compared with pristine graphene and graphene epoxide, graphene hydroxides show stronger adsorption for all the phosphate species because of hydrogen bonding interactions between the phosphate and the hydroxide groups. The adsorption becomes stronger with the number of formed hydrogen bonding interactions. PO_4^{3-} in general, tends to sit on top of C atoms while P-O bonds point to the centre of the aromatic rings. $OHPO_3^{2-}$ would like to sit on the C and the OH- group points away from the graphene surface. For $(OH)_2PO^-$ and $(OH)_3PO$, they sit similarly on C atoms, while the OH groups parallelly point up and down to the graphene surface. A specific arrangement of hydroxyl groups on graphene is identified, which is able to trap phosphate species. All phosphate species transfer some electron density to the graphene surfaces. We anticipate that a suitably designed graphene hydroxide would be an ideal sensor for charged phosphate. Such sensors will enable the transition toward sustainable and affordable agriculture.

References:

[1] Franklin D. Roosevelt, Message to Congress. May 20, 1938 [3] [2] He et al. ACS Appl. Mater. Interfaces 2017, 9, 14, 12719–12727

Time Series Decomposition of Spontaneous Urinary Bladder Activity: connecting statistical mechanics with the thermodynamics of contractile hollow viscera

Presenter: Arun Chind
Proshen Health & Risk Consulting Ltd., Delegate talk 4

The walls of hollow viscera such as the gall bladder and urinary bladder are a composite of several structures including elastic elements (such as elastin and collagen) and smooth muscle. The smooth muscle component is recognised to be necessary for the active contraction of the viscera, allowing expulsion of content. The value of spontaneous contractions for the function of hollow viscera are not known. Recent advances in statistical mechanics have recognised smooth muscle as a form of active matter. In order to characterise the spontaneous smooth muscle activity using time series statistics, archival recordings of spontaneous activity of the rabbit urinary bladder were converted to digital form for statistical analysis. The time series were tested for stationarity, cyclicality, trend, autocorrelation and partial autocorrelation to allow model selection and fitting. Investigations have revealed that the spontaneous contractions form a stationary autocorrelated time series with downward trend, seasonality and cyclicality. The Unobserved Components Model (UCM) with seasonality 15 and cyclicity 2 was found to provide the best fit for this data. The features of the spontaneous activity time series provide evidence of fluctuation-dissipation phenomena in the rabbit urinary bladder. The spontaneous activity (wall fluctuations) is hypothesised to assist in the exchange and dissipation of energy in the wall of the urinary bladder in the storage phase of the micturition cycle. These findings help to harmonise the dynamics of active soft matter with classical statistical mechanics including gas dynamics. This study of time series decomposition of spontaneous bladder activity helps make the link between statistical mechanics and thermodynamics. The findings in this work offer the promise of generalisation of the theoretical framework to spontaneous activity in other contractile-propulsive soft tissue structures and active matter.

Opportunities and Challenges in Formulation Modelling

Presenter: Dr Jeremy Winter
Unilever Invited talk 3

Models relating formulation composition and processing to product performance are becoming an increasingly important part of the innovation process. For a variety of pragmatic reasons, most of the models in actual use are data-driven. This talk will survey some examples of the use of approaches driven by underlying physics and chemistry and will try and provide a road-map for their wider application in future.

Multiscale modelling of perovskite solar cells

Presenter: Prof. Alison Walker
Co-author: Samuel McCallum; Jamie Lerpiniere
University of Bath
Invited talk 4

This talk is an overview of my group's work on mesoscale simulation of charge transport in perovskite semiconductors used as light harvesting layers in solar cells. I will show how we bridge the microscope and continuum simulations with an ensemble Monte Carlo, MC, approach for inorganic semiconductors using semi-classical Boltzmann transport theory. We are using our MC code to understand the mobility-limiting mechanisms in perovskite semiconductors along with transient behaviour. As the code has a number of materials parameters as input, e.g. electron-phonon coupling strengths and effective masses, typically many time consuming and resource hungry runs are required. I will describe how, with the aid of a CCP5 bursary, we are developing a methodology for combining our code with Machine Learning, ML, techniques to make the MC simulations more effective and efficient at exploring scenarios otherwise requiring a prohibitively large number of simulation runs.

Lattice Dynamics of Uranium Dinitride (UN_2)

Presenter: Joseph Flitcroft
Co-author: M. Molinari; J.M. Skelton
University of Manchester
Delegate talk 5

Nuclear power is a proven technology for providing stable electrical power generation without producing greenhouse gasses. However, incidents such as the Fukushima-Daiichi accident show that public confidence in new reactors requires new materials that will enhance the safety of nuclear power stations without compromising on power output. Uranium Nitrides are a potential nuclear fuel material for Generation IV reactors which will support an increased accident tolerance. Uranium nitrides have superior physical properties, viz. a higher melting point, thermal conductivity, and metal density, compared to current oxide fuels. A key property of a nuclear fuel material is its thermal transport, as the ability to remove the excess heat generated by fission events in the fuel rods is important to prevent a core meltdown. Therefore, developing a comprehensive understanding of the thermal transport in fuel materials at the atomic level is of paramount importance. We have used density functional theory calculations to model the structure and phonon dispersion of UN_2. The phonon calculations revealed a dynamical instability, which lead via a tetragonal intermediate to a lower-energy, phonon stable orthorhombic structure, where the nitrogen atoms are distorted from the idealised positions in the cubic fluorite structure. We have further investigated the effect of these structural changes on the physical properties, and found that the lower-symmetry stable structures show a marked reduction in lattice thermal conductivity compared to the fluorite phase.

Computational Study of the Formation of Sn-BEA for Liquid Phase Catalysis

Presenter: Owain Beynon
Co-author: Alun Owens; Andrew J. Logsdail
Cardiff University
Delegate talk 6

Lewis acidic zeolites have gained much interest recently, owing to their ability to efficiently catalyse several important reactions. Tin-BETA (Sn-β) is a tin-containing zeolite of the BEA-type framework, which shows remarkable activity and selectivity for numerous catalytic reactions, such as the Baeyer-Villiger oxidation (BVO), the Meerwein-Ponndorf-Verley reductions (MPV reduction), and other important reactions in the development of green and sustainable technology, such as the conversion of biomass into renewable fuels. [1][2][3] Conventional methods of zeolite synthesis, such as hydrothermal methods, pose a problem as the procedure requires strong acids, along with high temperatures and pressures, which are environmental harmful and industrially inappropriate, hindering the wide-spread uptake of Sn-β as a catalyst for the production of renewable fuels. Alternative methods of synthesis are therefore desirable, allowing for the industrial uptake of this catalytic technology. New promising methods of synthesis, such as solid-state incorporation (SSI) [4], have successfully inserted Sn into the BEA framework from a tin(II) acetate precursor, without impairing the catalytic activity. Though there have been several experimental studies, the exact mechanism of SSI remains elusive. Therefore, computational investigations into the formation of these tin sites within the BEA framework is necessary in elucidating the formation of the catalytic active site, which is the focus of our research, extending on work conducted by experimental collaborators [5]. We employ periodic Density Functional Theory (DFT), along with cluster embedded quantum mechanics/ molecular mechanics (QM/MM) hybrid techniques, and other contemporary modelling methods to study the transformation of tin-containing precursors into the active site of Sn-β. To date we have identified three main steps in the SSI procedure, namely, tin-coordination, acetate formation, and oxidation, where furthering our understanding of tin insertion can lead to an optimisation of the synthetic procedure, and the catalytic performance, potentially leading to successful industrial applications.

References:

[1] A. Corma et al. Nature 2001, 412, 423–426
[2] A. Corma et al. J. Am. Chem. Soc. 2002, 124, 13, 3195-5
[3] Davis et al PNAS, 107, 6164 – 6168, (2010).
[4] Hammond, C, et al., Angew. Chem. Int., (2012)
[5] Hammond C, et al., ChemCatChem (2015) 7, 3322-3331 [6]

Multiscale Modeling of lithium diffusion and NMR properties solid state electrolytes

Presenter: Mahmoud ATTIA
Co-author: Thibault CHARPENTIER; Jean-Paul CROCOMBETTE
French Atomic Energy and Alternative Energies Commission

Delegate talk 7

Designing solid-state batteries (SSBs) requires the design of new highly efficient solid electrolytes (SSEs) that exhibit high ionic conduction properties. Though they have numerous drawbacks, liquid organic-based electrolytes are the ones most commonly used in current battery technologies. They are not only dangerous and less efficient but also degrade faster which decreases their lifetime for long-term applications. Hence the necessity for a safer and longer-lived alternative for batteries is a must. To this end, SSEs are now at the forefront of all the materials studied, as they combine factors of safety (non-flammable), efficiency, lower cost, and ease of fabrication. Among them, Doped-LLZO (Lithium lanthanum zirconium oxide) $Li_7La_3Zr_2O_{12}$ is considered to be one of the most promising materials serving this purpose. Our project aims at modelling Li diffusion and spectroscopic data (NMR and Electrochemical Impedance Spectroscopy (EIS)) with Molecular Dynamics (MD) simulations by harnessing both (i) short time and length scales (from DFT and ab-initio Molecular Dynamics (AIMD)) and (ii) long time and length scales (from classical MD and KMC (Kinetic Monte Carlo)) to define a multi-scale methodology for understanding the impact of doping on Li mobility in the solid electrolytes materials (e.g. LLZO) by linking the simulations data to the microscopic diffusion measurements techniques (high- resolution NMR) and EIS. Our aim is to develop a Kinetic Monte Carlo Model, parameterized with inputs from MD simulations (both classical and ab-initio) capable of predicting NMR properties such as 7Li NMR lineshapes and nuclear relaxation times. Density-based clustering approaches are employed to analyze Li-trajectories. In addition, standard DFT-GIPAW calculations are performed for predictions of Al MAS NMR spectra in Al-doped LLZO (LLAZO).

On the formation of C_2H_4O isomers on dust surfaces in the ISM

Presenter: Reetu, Reetu
Co-author: Prof. A. J. H. M. Meijer
University of Sheffield Delegate talk 8

The most abundant elements in the ISM are H and He with small contribution of biogenic elements such as O, C, and N. The combination of these elements leads to the formation of small, large and complex organic molecules. Formation of CO, CH^+, C_2H_2, C_2H_4 and other small organic molecules has been reported in the cold dense clouds. Accumulations of these atoms and molecules may lead to the formation of species such as CH_3OH, H_2CCHOH, CH_3CHO, and C_2H_4 isomers by their reactions on dust surfaces. Detection of these species has attracted special attention because they play an important role in astrobiology. In particular, acetaldehyde and ethylene oxide are key raw materials for the formation of amino acids, which are key for life. However, the abundance of these molecules depends upon the physical and chemical environment of the ISM. Therefore, it is important to investigate how the environment affects their formation pathways. In the past, the formation pathways of three isomers of C_2H_4O from O(3P) and $H_2C{=}CH_2$ (acetaldehyde CH_3CHO, ethylene oxide (CH_2OCH_2), and vinyl alcohol CH_2CHOH) in the gas phase have been reported. 2-4 However, the formation pathways of these isomers on dust surfaces is still unclear. Herein, we have performed Density functional theory (DFT) calculations to understand the formation of different isomers by the reaction of oxygen atom with ethylene in the gas phase as well as on a model dust surface (bi-layer graphite surface). The dust surface induced lower formation energy barrier and promoted the formation of C_2H_4O. In additional, some additional routes for the transformation of one isomer to other on the surface in comparison to the gas phase reactions will also be reported.

References:
1 T. W. Hartquist and D. A. Williams, The molecular astrophysics of stars and galaxies, Oxford University Press, 1998, vol. 4.
2 B. Fu, Y.-C. Han, J. M. Bowman, F. Leonori, N. Balucani, L. Angelucci, A. Occhiogrosso, R. Petrucci and P. Casavecchia, JCP, 2012, 137, 22A532.
3 F. Talotta, S. Morisset, N. Rougeau, D. Lauvergnat and F. Agostini, JPC A, 2021, 125, 6075–6088.
4 B. J. Smith, M. T. Nguyen, W. J. Bouma and L. Radom, JACS, 1991, 113, 6452–6458.

Simulation as a tool in materials Chemistry and Physics

Presenter: Prof. Richard Catlow
Department of Chemistry, University College London; School of Chemistry, Cardiff University. Invited talk 5

Over the lifetime of CCP5, simulation has developed into a set of tools that are used, widely and often routinely in materials chemistry and physics. This talk will briefly review some of the current capabilities in four key areas: *structure prediction, surface science, defect properties, and reactivity and catalysis.* In each case we contrast the current state-of-the-art with that in the early days of the CCP5 project. We will conclude with speculation as to the future developments in the field.

Optimisation of sustainable plastics by tuning the filler-polymer interface

Presenter: Dr. Karen Johnston
Co-author: Dominic Wadkin-Snaith; David McKechnie; Paul Mulheran,
University of Strathclyde

Invited talk 6

Plastics are used in a wide range of applications from functional plastics used in high-end electronics to commodity plastics used in packaging, and have thus become ubiquitous in modern society. However, plastic pollution is now a major global environmental problem, and has become a societal challenge to reduce reliance on plastics, particularly on fossil fuel-based polymers. In addition to reducing and recycling plastic, there is a focus on moving to sustainable polymers. However, to transition to sustainable polymers, it is necessary to optimize their properties to make them competitive with traditional polymers.

A common approach to improve polymer properties is to mix in additives, such as filler particles, to form a composite. Filler particles are known to alter the glass transition temperature of the polymer [1] and promote polymer crystallisation [2,3], both of which strongly affect the composite properties. While there are numerous experimental studies on a wide range of polymer composites, there is a lack of understanding of how the filler surface influences the composite properties. Simulations provide molecular level insight into the structure and dynamics of the filler-polymer interface, which is extremely challenging to measure or observe experimentally.

I will present simulation results on the influence of a surface on polymer structure and dynamics, and explore how the surface properties can be used to control the glass transition, crystal nucleation, and degree of crystallisation. This insight will help to enable the design of new plastic materials, and accelerate the transition to sustainable plastics.

References:

[1] D. McKechnie *et al*. Polymer **195**, 122433 (2020)
[2] K. Majerczak et al. Polymer International, in press (2022)
[3] Wadkin-Snaith et al, in preparation

Modelling Organic-Inorganic Interfaces of Urinary Calculi

Presenter: Rhiannon Morris
Co-author: Helen Chappell; Andrew Scott; Antonia Borissova; James Smith
University of Leeds

Delegate talk 9

Urinary calculi (kidney stones) is a common ailment effecting around 10% of the world's population and resulting in more than 97,000 finished consultant episodes (FEC) each year in the UK alone [1]. The key chemical interactions relating to stone crystallisation and aggregation are not fully understood. Urinary calculi are solid clusters of small stones, composed of crystals that have precipitated from urine, built up on the luminal surface of the epithelial cell surfaces of the microtubule in the kidney. Kidney stones are often found complexed to organic matrices, such as proteins and amino acids. This research uses first principles modelling (CASTEP) to help elucidate the crystallisation phenomena and unravel the chemistry behind stone composition. Urine analysis of kidney stone patients has previously revealed that their urine contains higher amounts of phospholipids in comparison to healthy patients [2]. The fundamental chemistry underlying its interaction with kidney stones is unknown. In order to begin to understand the nucleation process, we have constructed surface models of calcium oxalate monohydrate and calcium oxalate dihydrate and modelled stone growth, simulating further calcium oxalate adsorption onto these surfaces. The interactions between urinary macromolecules and crystal surfaces at an atomic level are unexplained, we performed ab initio molecular dynamics of phosphocholine adsorption on calcium oxalate surfaces and have shown that the phosphocholine head groups become entrapped within the growing crystal. The lowest energy structures are those where the calcium oxalate dihydrate surfaces change their crystallographic structure. The crystallographic waters are implicit in driving the encapsulation of the phosphocholine head group.

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Interfacial Free Energies from MD Simulations: Application to $CaSO_4{\cdot}xH_2O$

Presenter: Stephen Yeandel
Co-author: Colin Freeman; John Harding
University of Sheffield

Delegate talk 10

The calculation of solid/liquid surface enthalpies using Molecular Dynamics simulations is now routine. But these calculations exclude entropic contributions, which can be an important factor in systems where the solid surface can impose strong ordering in the liquid. What is required is a method for calculating Interfacial Free Energies (IFEs) which include enthalpic and entropic contributions. Such methods do exist [1] but tend to be developed for simple systems and are difficult to transfer to more complex systems. We present a general method for calculating IFEs which can easily deal with complex materials and surfaces, which may also contain miscible species. Our method relies on transforming the solid component of the interface into bulk material via an Einstein Crystal; avoiding the need to define an explicit real-space pathway for the transformation. Furthermore, the method is very efficient as many values may be computed once and re-used for multiple different interfaces. Our method has been applied to the calculation of IFE of different members of the $CaSO_4{\bullet}xH_2O$ group of materials with water. This is a particularly challenging system to study due to strong binding between the Ca^{2+} ion and water [2], the inclusion of miscible water molecules which formally belong to the bulk material but may behave as liquids at the interface, and the presence of surface dipoles for the hemihydrate phase (Bassanite, $CaSO_4{\bullet}0.5H_2O$). Our results indicate that entropy accounts for between 55-85% of the IFE in $CaSO_4{\bullet}xH_2O$ systems, in contrast to the NaCl/water interface where entropy accounts for approximately only 20%. We also find that in general the IFEs of Bassanite interfaces ($CaSO_4{\bullet}0.5H_2O$) are lower than that of Gypsum ($CaSO_4{\bullet}2H_2O$), indicating a possible reason why Bassanite is often observed first during crystallisation from solution [3]. Predicted equilibrium morphologies also show good agreement with previous studies.

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Interfacial Free Energies of Calcium Carbonate with Water from Atomistic Simulations

Presenter: Emma Armstrong
Co-author: Stephen Yeandel; Colin Freeman; John Harding
University of Sheffield Delegate talk 11

Calcite and aragonite are two of the most commonly found forms of crystalline calcium carbonate. Despite only a small difference in thermodynamic stability, calcite is observed precipitating far more often than aragonite [1]. Although some methods are known to induce aragonite production over calcite (inclusion of Mg^{2+} ions or high temperatures [2]), the control over polymorph selection in calcium carbonate is still of significant concern [3]. In particular, the reasoning and understanding of the environmental influence on polymorph selection in these systems. By calculating the interfacial free energies of a variety of calcium carbonate surfaces, we can determine the expected morphologies of the polymorphs as well as obtain a greater thermodynamic understanding of the formation of calcite and aragonite. In this work we have used a novel method [4], taking the Einstein crystal as the reference state in thermodynamic integration, to calculate the interfacial energies of calcite and aragonite surfaces with water. Previous methods have calculated interfacial energies and morphologies based on enthalpy alone, however the current technique also includes the entropic contribution. Our results indicate that the {104} faces significantly dominate the hydrated calcite structure and have a much lower free energy than any other calcite face. For aragonite, there is far less difference in energy between the surfaces, supporting the variety of structures observed experimentally. The entropic contribution varied greatly for the aragonite surfaces, indicating its importance when calculating free energies and its potential part in the polymorph selection of calcium carbonate.

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Atomistic Modelling of Interfaces

Presenter: Prof. Steve Parker
University of Bath Invited talk 7

CCP5 has continued to provide support for all engaged in developing and exploiting computer simulation methods for condensed matter systems. One of the distinctive features of CCP5 over its 40 years of activity, thanks largely to the efforts of the team at Daresbury, is its successful strategy of developing and disseminating new codes and methods. In the early 1990s I routinely used codes such as CASCADE, THBREL and THBPHON. However, in this presentation I want to highlight the continued relevance of this contribution by briefly describing work in 4 current projects which depend on the continued support of the CCP5 codes, DL_FIELD, DL_POLY and DL_MONTE. The first project involves the investigation of interfacial properties of cellulose. Cellulose is the most abundant biopolymer in the biosphere. However, it is difficult to dissolve in conventional aqueous and organic solvents which limits its use as a feedstock, and hence understanding the role of the cellulose-liquid interface is central to understanding the molecular processes behind dissolution. Here, I will describe recent work on applying DL_FIELD and DL_POLY to these interfaces. In the second example, also considering an important biopolymer, I will show how the application of DL_POLY and DL_MONTE when combined can give a mechanistic insight towards understanding the factors controlling the barrier properties of Polyethylene Furanoate to molecular oxygen. The final two examples, both consider the important oxide material, cerium dioxide, which finds use in three-way catalysts, solid oxide fuel cells, and biomedicine. These include the application of lattice switch Monte Carlo in DL_MONTE for evaluating surface energies, and hence allows for the inclusion of explicit anharmonicity. The final example uses the semi-grand ensemble to investigate the structure and stability of zirconium doping as a function of dopant concentrations and temperature. In both cases the goal is move beyond just considering the energetics and model the free energy contributions. Thus the CCP5 codes provide an excellent suite of tools that are both highly stable and reliable, and with bespoke support can allow the community to tackle yet more challenging and interesting problems.

A DFT study on the stability and vibrational fingerprint of phosphate species on the surfaces of Ceria

Presenter: Minh Khoa Ta
Co-author: Samuel Moxon; Roger M. Phillips; David J. Cooke; Marco Molinari
University of Huddersfield Delegate talk 12

Ceria nanoparticles (CeNPs) are nanozymes with enzyme mimicking properties (superoxide dismutase, catalase, phosphatase, etc.). When used in vivo, however, the activities of CeNPs are hampered by the adsorption of bodily electrolytes onto their surface. As phosphate ions are present as electrolytes in the cellular environment, we have studied the adsorption of phosphate ions on CeNPs. The interaction strength between different phosphate ion adsorption configurations is determined using density functional theory (DFT). We found that the order of stability for phosphate adsorption on ceria surfaces follows the order {100} > {110} > {111}. An adsorbed 5-fold coordinated phosphate species is also observed and calculated to be a stable intermediate, implying that this species is responsible for the early stages of ceria surface scavenging, a known experimental process that results in the transformation of ceria into cerium phosphate. The IR and Raman spectra are generated using Phonopy-Spectroscopy code and so vibrational modes characteristic of phosphate species adsorbed onto {111}, {110}, {100} surfaces are reported. This vibrational fingerprint provides an insight on the interactions between phosphate species and nanoceria facets as well as the unique avenue to define phosphate adsorption on ceria surfaces.

How does lattice thermal conductivity "work"? Insight from first-principles calculations

Presenter: Jonathan Skelton
Co-author: J. Cen; J. M. Filtcroft; M. Molinari; S. Moxon; I. Pallikara; J. Tang; J. Tse; B. Wei
University of Manchester Delegate talk 13

The lattice thermal conductivity (k_{latt}) is typically the dominant mechanism of heat transport in semiconductors and insulators. As such it is an important factor in a number of applications including, for example, in the performance of thermoelectric materials, the carrier recombination in solar-cell absorber materials, and the safety profile of nuclear fuels. k_{latt} can be accurately calculated by performing structural-dynamics calculations to model the lattice vibrations (phonons) within the harmonic approximation and applying a third-order perturbation to model the phonon lifetimes. At present the most widely-used "workhorse" method is the single-mode relaxation-time approximation (RTA), which provides a closed solution to the phonon Boltzmann transport equations. The RTA determines the macroscopic k_{latt} as a sum of microscopic contributions from individual phonon modes, and as such provides an unprecedented level of detail into the underlying transport processes. However, leveraging this data to make useful comparisons between materials can be somewhat challenging. In this talk, we will discuss various approaches to analysing k_{latt} calculations within the RTA to obtain a simple set of metrics for comparing between systems. The constant relaxation-time approximation (CRTA) approach casts the k_{latt} into the product of a harmonic term and a weighted-average phonon lifetime, allowing differences in thermal conductivity to be straightforwardly attributed to differences in group velocities (chemical bonding) and phonon lifetimes. An approximate model for the phonon linewidths, with a fitted constant phonon-phonon interaction strength, further allows differences in the lifetimes to be attributed to the strength of the three-phonon scattering processes and the conservation of energy and crystal momentum dictated by the shape of the phonon spectrum. The application of these techniques will be illustrated by comparing the k_{latt} of a variety of materials including current high-performance thermoelectrics, and we will also show how they lead to approximate models for the thermal conductivity that enable the study of more complex systems for which computing the third-order force constants is not practical.

Exploring the phase behaviour of Hard-Sphere Dimers

Presenter: Omar-Farouk Adesida
Co-author: David Quigley; Livia Bartok-Partay
University of Warwick Delegate talk 14

Hard sphere potentials are of particular interest due to their ability to express complex behaviour while being relatively cheap. We employ the nested sampling algorithm in order to explore the phase behaviour of hard-sphere dimers using their separation as a parameter which express three characteristic solid phases.

Determining the Phase Diagram of a Machine-Learned Carbon Potential *via* Nested Sampling

Presenter: George Marchant
Co-author: Dr. Livia Bartók-Pártay
University of Warwick Delegate talk 15

We detail how the many-body potential energy landscape of a machine-learned (ML) interatomic potential for carbon [1] can be explored by utilising the nested sampling algorithm,[2] allowing for the determination of carbon's phase diagram up to high pressures. The ML potential in question is the GAP-20 model, which was developed in recent years using the gaussian approximation potential methodology to describe the properties of bulk crystalline and amorphous carbon phases with the accuracy of electronic structure methods. With the nested sampling algorithm the 3N-dimensional potential energy surface of the GAP-20 potential can be automatically (and efficiently) sampled at constant pressure, providing a set of configurations with which to test the potential's thermodynamic capabilities. As a point of comparison the phase diagrams of other interatomic potentials - including the ReaxFF, EDIP and Tersoff potentials - are also studied. Despite having been trained on optimised structures at only zero pressure, GAP-20 provides an accurate description of carbon's macroscopic properties up to approximately 200 GPa. Our results also highlight areas for future improvement of the potential.

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Nested sampling: what can we learn about an interatomic potential?

Presenter: Dr Livia Bartok-Partay
Co-author: George Marchant; Noam Bernstein; Gábor Csányi
University of Warwick Invited talk 8

In recent years we have been working on adapting the Bayesian statistical approach, nested sampling, for studying atomistic systems. Nested sampling automatically generates all the relevant atomic configurations, unhindered by high barriers, and one of its most appealing advantages is that the global partition function can be calculated very easily, thus thermodynamic properties, such as the heat capacity or compressibility becomes accessible. Nested sampling is a top-down sampling technique, in the materials application this means starting from the high energy region of the potential energy landscape (gas phase configurations) and progressing towards the ground state structure (crystalline solid) through a series of nested energy levels, estimating the corresponding phase space volume of each. This way the method samples the different basins proportional to their volume, and instead of providing an exhaustive list of the local minima, it identifies the thermodynamically most relevant states without any prior knowledge of the structures or phase transitions. The use and advantages of the nested sampling method has been demonstrated in sampling the potential energy landscape of several model systems, allowing us to calculate the complete pressure-temperature phase diagram of the system. These often result in the discovery of previously unknown thermodynamically stable solid phases, highlighting that the macroscopic properties of interatomic potential models can be very different than expected or intended.

The history of CCP5

Presenter: Prof. Bill Smith
Co-author:
CCP5 - UKRI STFC Daresbury Laboratory Invited talk 9

This talk will describe the background to the creation of CCP5 and the people who were key to its creation and subsequent success as a communal project. It will also describe how the organisational structure of the project evolved and its relevance to CCP5's long term survival. The origin and purpose of CCP5's activities will be discussed and their impact on the simulation community in the UK and elsewhere. Lastly, where did it succeed and where did it fail?

Using molecular dynamics simulation to predict the aggregation propensity of mAb formulations & accelerate development

Presenter: Yuhan Wang
Co-author: Hywel D Williams; Paul DalbyHywel D Williams; Paul Dalby
University College London Delegate talk 16

Protein aggregation is one of the biggest challenges in the pharmaceutical manufacturing area, for it largely affects the efficiency of antibody drugs and causes financial loss. Aggregation is increasingly thought to occur through the partial unfolding of protein structure to expose sites that are more prone to self-interaction. The self-association of proteins happens due to both extrinsic and intrinsic factors. To name a few, temperature, pH, and protein concentration are extrinsic causes, while aggregate prone regions (APRs) within the protein is an intrinsic one. Hence, the aim of this project will be to develop a workflow of molecular dynamics (MD) simulation approaches and artificial intelligence (AI) that can provide molecular-level insights into the aggregation behaviour of mAbs observed experimentally in a range of conditions, including variation in pH, temperature, freeze/thaw or other stressors, and the presence or absence of stabilising excipients. This will also validate the computational approaches and build confidence in their use for predictive purposes. First of all, all-atom molecular dynamics simulations under different environmental parameter settings (temperature, pH, ionic strength) will be implemented on a Fab domain, which will then be followed by coarse-grained simulations on full antibodies with at least two copies introduced into the system. The data from MD simulations such as RMSD, RMSF, along with the protein sequence and structure information, will serve as the input for the subsequent machine learning process. The combination of MD and AI will offer an opportunity to predict protein stability without additional laboratory work that has been proved to be time-consuming and uneconomical.

The role of surface ionisation and topology in the hydration-induced swelling of Graphene Oxide (GO) membranes

Presenter: Mohd Rafie Bin Shaharudin
Co-author: CD. Williams, P. Carbone
University of Manchester
Delegate talk 17

Graphene oxide (GO) membranes are hydrophilic materials that swell in the presence of water either in a humid environment or when in contact with liquid water and the magnitude and mechanism of the swelling is dependent on the degree of ionisation of the functional groups present on the surface of the GO flakes. In this work, using Grand Canonical Monte Carlo and Molecular Dynamics simulations we investigate the effect that the surface charge, resulting from the ionisation process, has on both the amount of water adsorbed in the membranes at various humidity conditions and the swelling of the membranes in contact with liquid water. We show that by incorporating ionised functional groups, the onset of adsorption is shifted to a lower chemical potential and the internal membrane pressure increases due to the repulsive interactions between the graphene flakes. Our simulations also show that the presence of ions in the channels reduced the swelling due to screening effect but also increases the amount of water adsorbed when the membrane is immersed in liquid water. At low chemical potential, instead, the amount of water adsorbed is determined by the number of ionised groups and the topology of the membrane. The charged model is able to qualitatively reproduce experimental data showcasing the importance of including surface charge in GO model to predict hydration and swelling mechanism. We also included the complex topology of GO membrane by modelling a disordered GO membrane to understand the contribution of both surface charge and topology on adsorption and swelling. The disordered models give a good estimation to experimental results at low humidity while the idealised model gives a good estimation to experimental results at high humidity. Our results suggest that the surface charge and topology of GO membrane changes with humidity during the swelling phenomenon and the state of the swelling should be considered while modelling the membrane at different conditions. These findings are crucial in underpinning the future development of GO membranes in simulation and experimental study for aqueous separations since hydration induced swelling is widely known to lead to significant deterioration in performances.

Topological network analysis of thin ionomer membranes

Presenter: James Elliott
Co-author: Kazuto Akagi, Peter Vanya
University of Cambridge
Delegate talk 18

An improved understanding of how the structure of nanometre-thin, substrate-supported layers of polymer electrolyte membranes (PEMs) such as Nafion differ from the bulk polymer is crucial in order to enhance their permeability and performance in fuel cell catalyst layers. Despite several studies demonstrating the existence of layered structures close to the substrate interface, it is difficult to obtain direct experimental information due to the small size and complexity of these structures. In this work, we apply a recently developed coarse-grained modelling technique, known as Many-Body Dissipative Particle Dynamics (MDPD), with novel topological data analysis method based on topological data analysis (TDA) to describe multidimensional structures within the polymer and water networks in bulk and substrate. We will see how such complex structure of Nafion systems can be characterized by TDA and related to the anisotropic behaviour of water diffusion.

Towards High-throughput simulations of polymers plasticizers

Presenter: Lois Smith
University of Manchester, Continental AG Delegate talk 19

Plasticizers are small molecules that are mixed with the polymer matrix to modify the polymer mechanical properties and viscosity. Here we develop a fully automated high throughput simulation procedure to potentially screen thousands of molecules using geometrical and thermodynamic descriptors to categorise the molecules based on their geometry and internal flexibility. We then use such descriptors to perform an initial screening of their potential miscibility

Composites made of Polyaniline and $SrTiO_3$: Thermoelectric Abilities

Presenter: Nathan Wood
Co-author: Joshua S. Tse; Jonathan M. Skelton; David J. Cooke; Lisa J. Gillie; Marco Molinari
University of Huddersfield Delegate talk 20

The promising thermoelectric oxide $SrTiO_3$ is limited in its thermoelectric (TE) ability by an intrinsically high thermal conductivity (9–12 $Wm^{-1}K^{-1}$) at room temperature (RT), resulting in applications exclusive to high temperatures. A thermoelectric (TE) device allows for the recovery of waste heat in both domestic and industrial settings by converting a temperature gradient created between two ends of the device directly into electricity. TE devices consist two semi-conductive materials, n-type and p-type. To gauge the performance of these materials, the figure of merit can be used ($ZT=S^2 \sigma T/\kappa$) where S is Seebeck coefficient, σ is the electrical conductivity and κ is the thermal conductivity. Limiting κ is a key focus of TE research and can be achieved via several routes: nanostructuring, doping and nanocompositing. However, nanostructuring in $SrTiO_3$ has been shown to be less effective compared to other TE materials, while doping has led to improvements in σ and κ. Recent research has concentrated on nanocomposites, which combine $SrTiO_3$ with dissimilar materials like graphene or conductive polymers. These produce an interface at which the phonons' mean free path can be disrupted and whilst also inducing quantum effects that may improve the TE properties. In fact, research by Lin et al. has demonstrated that adding graphene to La doped $SrTiO_3$ lowers the operating temperature and results in an increase in ZT of about 280% (ZT = 0.42) at RT in comparison to pristine $SrTiO_3$. Therefore, it is anticipated that the addition of other organic species, in this case polyaniline (PANI), will produce results that are comparable. Indeed, PANI alone expresses p-type TE properties, with a typical ZT = 10^{-4} in the range and an inherently low κ = ~0.3 - 0.4 at RT. Using DFT+U methodology and energy minimization techniques, our research aims to examine the structural and TE characteristics of the interface between a {100} $SrTiO_3$ surface and polyaniline in its various oxidation states.

Machine Learning Force Fields for Multicomponent Organic Liquids: Applications for Battery Electrolytes

Presenter: Ioan-Bogdan Magdau
Co-author: Daniel Jose Arismendi; Kersti Hermansson; Gabor Csanyi
University of Cambridge

Delegate talk 21

ML methods have been successfully employed to model organic molecules in vacuum, as well as inorganic liquids and solids. The molecular condensed phase presents unique challenges due to the large separation of scales between intra- and inter-molecular interactions. Typical loss functions minimise total energies and forces, and since inter-molecular interactions are significantly weaker, ML models get good intra- and poor inter- relative accuracy. Previous attempts to model molecular liquids have employed several strategies to tackle this imbalance. One approach is to fit separate force fields for the molecules and the liquid. This solves the problem of scale separation; however, it prevents the modelling of reactions. We demonstrate that by crafting sufficiently diverse training data through iterative training and by carefully testing the accuracy of our models on the relevant inter-molecular scale, we can fit a general purpose potential which describes the EC:EMC binary liquid solvent with ab initio accuracy.

Molecular Fluid Dynamics

Presenter: Edward Smith
Co-author: David Heyes; Daniele Dini; Billy Todd; Peter Daivis; Carlos Braga; Alessio Lavino; Omar Matar; Tamer Zaki
Brunel University London

Delegate talk 22

In this talk, I will present an overview of our work using molecular dynamics to study engineering fluid flow. This includes a mathematics framework for the control volume, a vital tool in fluid dynamics, applied to molecular systems, and a way to get the pressure tensor in a discrete system. This framework can provide new insights and ways to measure quantities like viscosity, heat flux and surface tension. I will finish with several applications, including the liquid-vapour interface, bubble nucleation and turbulent flow.

New understanding of liquid thermodynamics, viscosity and its lower bounds

Presenter: Prof. Kostya Trachenko
Queen Mary University of London Invited talk 10

Understanding most basic thermodynamic properties of the liquid state such as energy and heat capacity turned out to be a long-standing problem in physics [1]. Landau&Lifshitz textbook states that no general formulas can be derived for liquid thermodynamic functions because the interactions are both strong and system-specific. Phrased differently, liquids have no small parameter. Recent theoretical results open a new way to understand liquid thermodynamics on the basis of collective excitations (phonons) as is done in the solid-state theory. Differently from solids, the phase space for these excitations reduces with temperature [1,2], explaining the universal decrease of liquid constant-volume specific heat. I will discuss the implication of the above theory for fundamental understanding of liquids. I will also explain how this picture extends above the critical point where the Frenkel line separates two physically distinct states on the supercritical phase diagram [3]. I will subsequently describe how this leads to the theory of minimal quantum viscosity in terms of fundamental physical constants [4]. This answers the long-standing question discussed by Purcell and Weisskopf of why viscosity never drops below a certain value [5]. This also means that water and life and well attuned to the degree of quantumness of the physical world [5]. I will finally note that the kinematic viscosity of the quark-gluon plasma is surprisingly close to the kinematic viscosity of liquids at their minimum [6].

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Diffusion in Oxides and Halides – Insights and Surprises from Simulations

Presenter: Prof. Neil Allan
Co-author: C.E. Mohn (University of Oslo)
University of Bristol Invited talk 11

Ab initio simulation techniques are increasingly able to provide new insights into diffusion processes in condensed phases. In this presentation: (i) Links between local structure and ionic migration are explored by examining the energy landscapes, calculated ab initio, of fast-ion conductors. Examples include: (a) fast-ion oxygen-deficient perovskites where oxygen transport involves transitions between basins in the energy landscape corresponding to different local minima; (b) the high-temperature disordered phase of δ-Bi_2O_3 where a very different picture from the conventional emerges. Only the mean structure is cubic - transitions between energetically accessible minima, with structures similar to low symmetry motifs in the low temperature ordered phases are responsible for the high oxide mobility. We compare δ-Bi_2O_3 and BIMEVOX. (ii) We discuss recent ab initio molecular dynamics simulations for fluoride ion transport in PbF_2 and hydride ion conduction in Ba_2ScHO_3, a recently synthesized oxyhydride with an unusual anion ordering. (iii) We discuss the diffusion of noble gases in MgO, which as periclase is an important component of the Earth’s mantle, at ambient and high pressures.

A first-principles study of the impact of Frenkel and Schottky defects on the thermal properties of ceria

Presenter: Thomas Smith
Co-author: Samuel Moxon; Joshua S. Tse; Jonathan Skelton; David J. Cooke; Lisa J. Gillie; Marco Molinari
University of Huddersfield

Delegate talk 23

For decades cerium dioxide (CeO_2 or ceria) has been widely studied for its applications in green technologies. Ceria is commonly used as a simulant material for PuO_2 in mixed oxide (MO_X) fuels as both species share the fluorite structure and similar thermal conductivities in addition to Ce and Pu both occupying the 3+ and 4+ oxidation states. The advantage of ceria as a surrogate is that plutonia is toxic and radioactive which CeO_2 is not. Ceria also requires less computational resources when utilising modelling techniques such as density functional theory as spin-orbit coupling and non-collinear magnetic do not need to be employed. The high temperatures nuclear fuels experience during their operation result in the formation intrinsic Frenkel and Schottky defects. These defects impact the redox cycle, oxygen storage capacity and thermal properties, for example the thermal conductivity of the defect models of ThO_2 reduced by 90% compared to the pristine model. We used DFT to study the structural dynamics and thermal properties of the Frenkel and Schottky defect models of ceria finding the defects broaden the main branches in the phonon dispersions, have characteristic features in the IR spectrums and significantly reduce the thermal conductivity compared to the pristine structure. This methodology can be applied to any nuclear materials to model thermal properties.

High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation

Presenter: Ioanna Pallikara
Co-author: Jonathan M. Skelton; Joseph M. Flitcroft
University of Manchester

Delegate talk 24

Major technological advancement is largely driven by materials discovery and is key to overcoming some of our most pressing social challenges, such as climate change and future energy supply. The predictive power of Density Functional Theory (DFT) has made it possible to use high-throughput materials modelling to screen for candidate materials with particular properties. The Materials Project is a core program of the Materials Genome Initiative and offers a database of the DFT-calculated properties of all known inorganic compounds. Despite its versatility, standard modelling with DFT works from frozen snapshots of the atomic structure and fails to account for the effects of thermal motion, leading to a gap between theory and experiment. To bridge this gap, the theory of Lattice Dynamics models the phonons in solids to incorporate both temperature and pressure effects into theoretical models. In this work, we use Lattice Dynamics within the Quasi-Harmonic Approximation (QHA) for the high-throughput prediction of materials finite-temperature properties. We start by selecting an exchange-correlation functional suitable for large-scale QHA calculations. In particular, we perform a comparative study on the accuracy of five exchange-correlation functionals, spanning the local density approximation (LDA), generalised gradient approximation (GGA) and meta-GGA levels of theory, for predicting the properties of ten binary oxides of Group 1, 2 and 12 metals. Then, we present an automated workflow for these large-scale calculations and test it on approximately 150 materials using PBEsol. The resulting dataset is used for both explorative data analysis and for the search of new structure-property relationships. Our findings show that the predictions are bounded by the LDA, which tends to underestimate lattice parameters and cell volumes relative to experiments but yields the most accurate results for bulk moduli, expansion coefficients and Grüneisen parameters, and the PBE GGA, which shows the opposite behaviour. PBEsol gives the best overall predictions of the lattice parameters and constant-pressure heat-capacities whilst also giving relatively reliable results for other properties. The dataset generated through the automated workflow is verified by comparison to experiments where available. Further analysis reveals some systematic trends and some high correlations between several properties. Interestingly, the latter allows us to explore the possibility of using only athermal (DFT) properties to generate all other materials properties at finite temperatures and pressures. More specifically, we introduce mathematical expressions where DFT-computed properties such as the bulk moduli, lattice energies and volumes can be substituted to generate predictions for the quasi-harmonic properties.

Alkali metal nitrates: a new model for crystallisation

Presenter: Vittoria Fantauzzo
University of Sheffield Delegate talk 25

Alkali metal nitrates are both of industrial and scientific interest. $NaNO_3$ and KNO_3 have extensive use as fertilizers but nitrate-based salts also are used as heat transfer fluids in solar power. The nitrate anion has a similar structure to carbonate and nitrates have a similar rich polymorphic behaviour, particularly $NaNO_3$, KNO_3 and $RbNO_3$. Nevertheless, the solution behaviour is simpler since there is no equivalent to the bicarbonate anion. Also, since nitrates are much more soluble in water than carbonates, it is easier to perform experiments at concentrations where simulations are possible. Previous work used AMBER-type potentials to calculate activity coefficients for $LiNO_3$, $NaNO_3$ and KNO_3 but free energies of formation for dimers and clusters have not been calculated. Limited tests have been performed to demonstrate that these forcefields can reproduce basic solid state and solution data. We present a new rigid-ion force-field for the alkali metal nitrates that is suitable for simulating solution chemistry, crystallisation and polymorphism. We show that it gives a good representation of the crystal structures, lattice energies, elastic and dielectric properties of these compounds over a wide range of temperatures. Since all the alkali metal nitrates are fitted together using a common model for the nitrate anion, the forcefield is also suitable for simulating solid solutions. We utilise our model by exploring KNO_3 behaviour in a range of systems. These include calculating the free energies of formation of alkali metal nitrates clusters growing on a stable surface of their own kind of molecules from various concentration solution, starting with KNO_3. We add a constant chemical potential methods (CμMD) to our model to determine growth mechanisms and rates. We compare these to the behaviour of supersaturated KNO_3 solutions in bulk and at the surface of self-assembled monolayers to examine the clustering and nucleation of the system.

Epoxy coatings: lessons learned from molecular simulations

Presenter: Prof. Flor Siperstein
University of Manchester Invited talk 12

Epoxy coatings are used in a wide range of applications, from sealers to paints. They are complex formulations, but they essentially have an epoxy resin and a curing agent in addition to other ingredients to provide specific functionalities or desirable physical properties. The phenomena observed at the interface between an epoxy coating and a solid substrate can provide valuable insights into the behaviour and performance of a coating. In this talk, some of the lessons learned from molecular simulations on adsorption of epoxy resins on metal oxide surfaces will be presented, where the importance of the metal oxide structure and local environment, such as the presence of water or the curing agent, are highlighted.

Materials Modelling Activities at CHPC: Collaboration with CCP5

Presenter: Happy Sithole
Co-author: Krishna Govender; Nkwe Monama; Anton Lopis
CHPC-South Africa Delegate talk 26

The talk intends to give a background of the Material Science Community Projects in South Africa that benefited from the collaboration with CCP5.

Wettability of graphite under 2D confinement

Co-author: Mara Chiricotto , Joshua D. Elliott, Fausto Martelli, Paola Carbone
Presenter: Zixuan Wei

University of Manchester Delegate talk 27

The thermodynamics of solid/liquid interfaces under nanoconfinement has tremendous implications for liquid transport properties. Here using molecular dynamics, we investigate graphite nanoslits and study how the water/graphite interfacial tension changes with the degree of confinement. We found that, for nanochannel heights between 0.7 nm and 2.6 nm, graphite becomes more hydrophobic than in bulk, and that the value of the surface tension oscillates before eventually converging towards a constant value for larger slits. The value of the surface tension is correlated with the slip length of the fluid and explained in terms of the effective and interfacial density, hydration pressure and friction coefficient. The study clearly indicates that there is a critical channel height of 0.9 nm (achievable experimentally [2]) at which the surface tension reaches its highest value, but the water diffusion across the channel is at its minimum. The structural analysis shows that for this pore size a transition between a 2D and 3D hydrogen bond network is accompanied by an abrupt increase in configurational entropy. Our results show that the wettability of solid surfaces can change under nanoconfinement and the data can be used to interpret the experimental permeability data.

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Ethylenediamine series as additives to control the morphology of magnetite

Presenter: David Cooke
Co-author: Norfolk, Laura; Kapusta, Klaudia; Staniland, Sarah
University of Huddersfield Delegate talk 28

Magnetite nanoparticles play a key role in the nano-industry, with crucial importance in the developing nanomedicine sector. Such particles must be homogeneous, with a consistent shape and size, due to the growing need to tailor particles to more defined faceted morphologies. Molecular dynamics simulations have been used to study interface between the low index surfaces of magnetite and the ethylenediamine series (H_2N-(–CH_2CH_2N–)nH_2, n = 2 (DETA), 3 (TETA), 4 (TEPA), and 5 (PEHA)). Binding to the octahedral (111) face is calculated to be preferred for all additives with binding to the (100) face unfavourable for TETA, TEPA and PEHA, showing a preference to bind and direct an octahedral morphology for these 3 additives. This is further explained by the increased numbers of interactions of the longer additives with the (111) surface through O and Fe in the magnetite surface bonding to H and N in the additive which is better able to lie flat on the (111) surface.

The influence of water, carbon dioxide and hydrogen peroxide on the morphology of cerium oxide nanoparticle

Presenter: Molinari, Marco[§]
Co-author: Samuel Moxon[§]; Stephen C. Parker[¥]; David J. Cooke[§]; Marco Molinari[§]
[§] University of Huddersfield
[¥] University of Bath

Delegate talk 29

Cerium oxide is an important material in many applications including water gas shift reactions, three-way catalysis, soot oxidation, and enzyme mimetic activity. Control of size and morphology of CeNPs is key for the design of energy and catalytic materials as it significantly affects the surface composition, reactivity and selectivity, and thus the performance of the material. Our modelling is aimed at identifying strategies to enhance the expression of catalytically active surfaces and to prevent their disappearance over many catalytic cycles. We used density functional theory to predict the surface composition and energetics of the most stable {111}, {110} and {100} surfaces of the material in the presence of water, carbon dioxide and hydrogen peroxide. We found that there is a strong chemical adsorption of all species. Whereas water and hydrogen peroxide display dissociative adsorption, carbon dioxide forms surface carbonates. The strength of the adsorption is surface dependent. Using a thermodynamic strategy, we then calculate the surface free energy of adsorbed surfaces as a function of external conditions. This allows us to predict changes in the equilibrium CeNP morphology as a function of temperature, water and oxygen partial pressure.

Poster abstracts

Exploring the phase behaviour of Hard-Sphere Dimers using Nested Sampling
Presenter: Omar-Farouk Adesida
Co-author: David Quigley, Livia Bartok-Partay
Univerisity of Warwick Poster

Hard sphere potentials are of particular interest due to their ability to express complex behaviour while being relatively cheap. We employ the nested sampling algorithm in order to explore the phase behaviour of hard-sphere dimers using their separation as a parameter which express 3 characteristic solid phases.

Interfacial Free Energies of Calcium Carbonate with Water from Atomistic Simulations
Presenter: Emma Armstrong
Co-author: Stephen Yeandel, Colin Freeman, John Harding
University of Sheffield Poster

Calcite and aragonite are two of the most commonly found forms of crystalline calcium carbonate. Despite only a small difference in thermodynamic stability, calcite is observed precipitating far more often than aragonite [1]. Although some methods are known to induce aragonite production over calcite (inclusion of Mg^{2+} ions or high temperatures [2]), the control over polymorph selection in calcium carbonate is still of significant concern [3]. In particular, the reasoning and understanding of the environmental influence on polymorph selection in these systems. By calculating the interfacial free energies of a variety of calcium carbonate surfaces, we can determine the expected morphologies of the polymorphs as well as obtain a greater thermodynamic understanding of the formation of calcite and aragonite. In this work we have used a novel method [4], taking the Einstein crystal as the reference state in thermodynamic integration, to calculate the interfacial energies of calcite and aragonite surfaces with water. Previous methods have calculated interfacial energies and morphologies based on enthalpy alone, however the current technique also includes the entropic contribution. Our results indicate that the {104} faces significantly dominate the hydrated calcite structure and have a much lower free energy than any other calcite face. For aragonite, there is far less difference in energy between the surfaces, supporting the variety of structures observed experimentally. The entropic contribution varied greatly for the aragonite surfaces, indicating its importance when calculating free energies and its potential part in the polymorph selection of calcium carbonate.

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Alkali metal nitrates: a new model for crystallisation
Presenter: Vittoria Fantauzzo
Co-author: Stephen Yeandel, Colin Freeman, Aaron Finney, Matteo Salvalaglio, John Harding
University of Sheffield Poster

Alkali metal nitrates are both of industrial and scientific interest. $NaNO_3$ and KNO_3 have extensive use as fertilizers but nitrate-based salts also are used as heat transfer fluids in solar power. The nitrate anion has a similar structure to carbonate and nitrates have a similar rich polymorphic behaviour, particularly $NaNO_3$, KNO_3 and $RbNO_3$. Nevertheless, the solution behaviour is simpler since there is no equivalent to the bicarbonate anion. Also, since nitrates are much more soluble in water than carbonates, it is easier to perform experiments at concentrations where simulations are possible. Previous work used AMBER-type potentials to calculate activity coefficients for $LiNO_3$, $NaNO_3$ and KNO_3 but free energies of formation for dimers and clusters have not been calculated. Limited tests have been performed to demonstrate that these forcefields can reproduce basic solid state and solution data. We present a new rigid-ion force-field for the alkali metal nitrates that is suitable for simulating solution chemistry, crystallisation and polymorphism. We show that it gives a good representation of the crystal structures, lattice energies, elastic and dielectric properties of these compounds over a wide range of temperatures. Since all the alkali metal nitrates are fitted together using a common model for the nitrate anion, the forcefield is also suitable for simulating solid solutions. We utilise our model by exploring KNO_3 behaviour in a range of systems. These include calculating the free energies of formation of alkali metal nitrates clusters growing on a stable surface of their own kind of molecules from various concentration solution, starting with KNO_3. We add a constant chemical potential methods (CμMD) to our model to determine growth mechanisms and rates. We compare these to the behaviour of supersaturated KNO_3 solutions in bulk and at the surface of self-assembled monolayers to examine the clustering and nucleation of the system.

QM/MM Boundary Workflow for Ionic Solids - An MgO(100)/TiO_2(110) Case Study

Presenter: Gabriel Bramley
Co-author: Andrew Logsdail & Harry Jenkins
Cardiff University
Poster

TiO_2 and MgO have been touted as effective, inexpensive supports and photocatalysts for green chemistry applications. Periodic simulations of these surfaces are feasible with DFT, but, which produce large errors (>1 eV) for properties such as the band gap. QM/MM methods, by reducing the number of atoms considered in the DFT segment of the energy evaluation, enable the use of higher quality hybrid DFT functionals for extended surfaces. This is especially important for spectroscopic features such as the band gap and reaction energies, where GGA functionals produce considerably larger errors compared to their HF exchange counterparts. However, the correct representation of the QM/MM boundary remains a challenge, where force fields must be constructed for the MM atoms to minimise strain between the QM and MM regions. Furthermore, the QM region should be designed such that features such as the frontier orbitals are consistent with periodic simulations. In this work, we present a workflow for production QM/MM calculations of ionic solids, comparing structural and electronic energy values to counterpart periodic simulations. Furthermore, we will compare adsorption characteristics for small molecules such as CO_2, which are precursors to organic compounds in photocatalytic reactions.

Computational Study of Anharmonic Effects in Zeolite Sn-BEA

Presenter: Owain Beynon
Co-author: Alun Owens, Andrew J. Logsdail
Cardiff University
Poster

Lewis acidic zeolites have gained much interest recently, owing to their ability to efficiently catalyse several important reactions. Tin-BETA (Sn-β) is a tin-containing zeolite of the BEA-type framework, which shows remarkable activity and selectivity for numerous catalytic reactions, such as the Baeyer-Villiger oxidation (BVO), the Meerwein-Ponndorf-Verley reductions (MPV reduction), and other important reactions in the development of green and sustainable technology, such as the conversion of biomass into renewable fuels. [1][2][3] Conventional methods of zeolite synthesis, such as hydrothermal methods, pose a problem as the procedure requires strong acids, along with high temperatures and pressures, which are environmental harmful and industrially inappropriate, hindering the wide-spread uptake of Sn-β as a catalyst for the production of renewable fuels. Alternative methods of synthesis are therefore desirable, allowing for the industrial uptake of this catalytic technology. New promising methods of synthesis, such as solid-state incorporation (SSI) [4], have successfully inserted Sn into the BEA framework from a tin(II) acetate precursor, without impairing the catalytic activity. Though there have been several experimental studies, the exact mechanism of SSI remains elusive. Therefore, computational investigations into the formation of these tin sites within the BEA framework is necessary in elucidating the formation of the catalytic active site, which is the focus of our research, extending on work conducted by experimental collaborators [5]. We employ periodic Density Functional Theory (DFT), along with cluster embedded quantum mechanics/ molecular mechanics (QM/MM) hybrid techniques, and other contemporary modelling methods to study the transformation of tin-containing precursors into the active site of Sn-β. To date we have identified three main steps in the SSI procedure, namely, tin-coordination, acetate formation, and oxidation, where furthering our understanding of tin insertion can lead to an optimisation of the synthetic procedure, and the catalytic performance, potentially leading to successful industrial applications. Through collaborations with the Fritz-Haber Institute in Berlin, we have sought to study the effects of anharmonicity within the zeolite framework and its consequence on simulated vibrational spectra. The finite-difference harmonic approximation used to describe molecular vibrations thus far is a straightforward and computationally affordable method, making it widely popular in the literature. The assumption, however, that the potential energy landscape around any given atom is harmonic in nature does not hold for complex materials, such as zeolites, where anharmonic effects are observed. For instance, exothermic catalytic processes within bulk materials for zeolites, can lead to local increases in temperature that dissipate via anharmonic effects. Recently, significant advancements have been made to model anharmonic effects within materials, deriving measures to quantify anharmonicity, whilst aiming to capture and understand more complex behavior and properties. [9] Computational techniques afford a high throughput way of classifying materials based on anharmonic contributions, whilst rationalizing macroscopic properties. Therefore, through developing our understanding of anharmonic effects within Sn-β, we strive to understand fundamental properties of the material and better bridge spectroscopic data and simulation by moving away from the harmonic approximation. Early results from this work indicate the strong harmonic nature of BEA compared to other zeolitic and silicious systems. Using a measure for anharmonicity it is apparent that the vibrational modes of BEA have strong anharmonic contributions, especially when compared to sodalite and quartz. This suggests that the harmonic approach as employed by the finite-difference method of simulating vibrational spectra is not sufficient for system where anharmonicity dominates such as BEA. Therefore, for valid and accurate comparison between simulated and experimentally obtained vibrational spectra, which is essential in uncovering the mechanism of SSI, an anharmonic treatment for the vibrational modes of BEA is needed.

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Construction of a Gaussian Process Regression Model of Formamide for Use in Molecular Simulations

Presenter: Matthew Brown
Co-author: Jonathan Skelton, Paul L. A. Popelier
University of Manchester Poster

Traditional force fields are a necessary tool in many projects due to their computationally expensive way of simulating large systems for longer timescales than methods such as ab initio molecular dynamics can feasibly provide. However, the accuracy of these simulations is often limited by approximations in bonding potentials and the use of point charges to represent electrostatic interactions. FFLUX [1-3] is a novel force field that utilises Gaussian process regression (GPR) machine learning models trained on atomic energies and multipole moments up to the hexadecapole obtained from quantum chemical topology (QCT) calculations. Specifically the interacting quantum atoms (IQA) scheme [4] is used, which unambiguously partitions the wavefunction energy into atomic contributions. The models are used to predict atomic energies and atomic multipole moments on-the-fly in molecular dynamics simulations of fully flexible molecules. The use of the GPR model replaces the need for parameterised bonded terms, and as such that the intramolecular potential energy surface in FFLUX closely resembles that of the quantum-mechanical method used for training. This work will present recent results from FFLUX simulations on formamide which we have chosen as an example to validate the FFLUX methodology due to its size and relative rigidity making it relatively easy candidate for accurate modelling. A monomeric formamide GPR model has been constructed at the B3LYP/aug-cc-pVTZ level of theory and has been tested in molecular dynamics simulations of formamide dimers, giving results consistent with the level of theory used in training. In the near future, these preliminary models will be extended to cover more complex simulations of crystal structures and liquids. References:

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The theory and simulation of the effects of three-body terms on the phase behaviour of a simple model

Presenter: Wenziyi Chen
Co-author: Andrew Masters
University of Manchester Poster

As one of the simplest models, the penetrable sphere model (PSM), in which the overlap of spheres is penalized by a finite constant energy, became popular as a prototype for the interaction between micelles in a solvent. A modified PSM, incorporating a three-body potential, is applied to investigate the many-body potential effect on the PSM properties at high temperature over a wide range of density. Reasonable agreement between theory and Monte Carlo simulation results is found in the fluid phase. Surprisingly, simulation shows that the solid has a body-centred cubic (BCC) structure at low pressure before transforming to a close-packed face-centred cubic (FCC) structure at higher pressures.

Time Series Decomposition of Spontaneous Bladder Activity: connecting statistical mechanics with thermodynamics.

Presenter: Arun Chind
Co-author:
Proshen Health & Risk Consulting Ltd. Poster

The walls of hollow viscera such as the gall bladder and urinary bladder are a composite of several structures including elastic elements (such as elastin and collagen) and smooth muscle. The smooth muscle component is recognised to be necessary for the active contraction of the viscera, allowing expulsion of content. The value of spontaneous contractions for the function of hollow viscera are not known. Recent advances in statistical mechanics have recognised smooth muscle as a form of active matter. In order to characterise the spontaneous smooth muscle activity using time series statistics, archival recordings of spontaneous activity of the rabbit urinary bladder were converted to digital form for statistical analysis. The time series were tested for stationarity, cyclicality, trend, autocorrelation and partial autocorrelation to allow model selection and fitting. Investigations have revealed that the spontaneous contractions form a stationary autocorrelated time series with downward trend, seasonality and cyclicality. The Unobserved Components Model (UCM) with seasonality 15 and cyclicity 2 was found to provide the best fit for this data. The features of the spontaneous activity time series provide evidence of fluctuation-dissipation phenomena in the rabbit urinary bladder. The spontaneous activity (wall fluctuations) is hypothesised to assist in the exchange and dissipation of energy in the wall of the urinary bladder in the storage phase of the micturition cycle. These findings help to harmonise the dynamics of active soft matter with classical statistical mechanics including gas dynamics. This study of time series decomposition of spontaneous bladder activity helps make the link between statistical mechanics and thermodynamics. The findings in this work offer the promise of generalisation of the theoretical framework to spontaneous activity in other contractile-propulsive soft tissue structures and active matter.

Ethylenediamine series as additives to control the morphology of magnetite

Presenter: David Cooke
Co-author: Laura Norfolk, Klaudia Kapusta and Sarah Staniland
University of Huddersfield Poster

Magnetite nanoparticles play a key role in the nano-industry, with crucial importance in the developing nanomedicine sector. Such particles must be homogeneous, with a consistent shape and size, due to the growing need to tailor particles to more defined faceted morphologies. Molecular dynamics simulations have been used to study interface between the low index surfaces of magnetite and the ethylenediamine series ($H_2N\text{-}(–CH_2CH_2N–)nH_2$, n = 2 (DETA), 3 (TETA), 4 (TEPA), and 5 (PEHA)). Binding to the octahedral (111) face is calculated to be preferred for all additives with binding to the (100) face unfavourable for TETA, TEPA and PEHA, showing a preference to bind and direct an octahedral morphology for these 3 additives. This is further explained by the increased numbers of interactions of the longer additives with the (111) surface through O and Fe in the magnetite surface bonding to H and N in the additive which is better able to lie flat on the (111) surface.

Thermoelectric Properties of Rocksalt and Pnma Structured SnS/SnSe

Presenter: Joseph Flitcroft
Co-author: I. Pallikara, J.M. Skelton
University of Manchester Poster

In order to combat climate change a wide range of approaches are required. Using thermoelectric power generators to recover electrical energy from waste heat represents one such avenue for increasing the efficiency of energy-intensive processes and thus reducing greenhouse gas emissions. Thermoelectric materials convert waste heat directly to electrical power and are scalable to applications ranging from wireless sensors, to car engines, to industrial equipment. The tin chalcogenides SnS and SnSe are promising candidate thermoelectrics, with orthorhombic SnSe showing some of the highest figures of merit ZT reported to date. Other notable Group IV chalcogenide thermoelectrics, including PbS, PbSe and PbTe, form rocksalt phases, and these phases are predicted to be accessible to SnS and SnSe under certain conditions. However, the thermoelectric properties of these phases remain largely unexplored. We have applied a fully ab initio modelling protocol to compare the ZT of the orthorhombic and rocksalt phases of SnS and SnSe. Electronic structures calculated using hybrid density-functional theory were used to predict the Seebeck coefficient, electrical conductivity and electronic thermal conductivity, including approximate models for the electron relaxation times. Lattice dynamics calculations were performed to model the phonon spectra and lattice thermal conductivities. We obtained good estimates of the ZT of the well-studied orthorhombic phases. The rocksalt phases were predicted to show larger electrical conductivities and similar Seebeck coefficients to the orthorhombic phases, resulting in higher thermoelectric power factors, but these were offset by larger thermal conductivities. Given that the large thermal conductivities are primarily due to the symmetric structure, this strongly motivates further investigation of the thermoelectric properties of the recently discovered π-cubic phases, which are based on a distorted rocksalt structure and are expected to show much lower thermal conductivity.

Expanding the boundaries of developing atomic interaction models

Presenter: Sebastian Havens
Co-author:
University of Warwick Poster

Here, we present our work on developing a strategy for making iterative improvements to interatomic potential models, in order to improve their reliability in reproducing macroscopic properties. Our test systems are embedded atom models of copper and lithium, and we use the nested sampling technique to sample the potential energy surface of the models, locating phase transitions and identifying stable solid structures in an automated way. These information are utilised within a cost function to evaluate the performance of the model, then the Nelder-Mead optimisation algorithm uses this cost function to make iterative modifications to the functions within the embedded atom model.

Machine Learning Force Fields for Multicomponent Organic Liquids: Applications for Battery Electrolytes.

Presenter: Ioan-Bogdan Magdau
Co-author: Ioan-Bogdan Magdău, Daniel Jose Arismendi, Kersti Hermansson and Gabor Csanyi
University of Cambridge Poster

ML methods have been successfully employed to model organic molecules in vacuum, as well as inorganic liquids and solids. The molecular condensed phase presents unique challenges due to the large separation of scales between intra- and inter-molecular interactions. Typical loss functions minimise total energies and forces, and since inter-molecular interactions are significantly weaker, ML models get good intra- and poor inter- relative accuracy. Previous attempts to model molecular liquids have employed several strategies to tackle this imbalance. One approach is to fit separate force fields for the molecules and the liquid. This solves the problem of scale separation; however, it prevents the modelling of reactions. We demonstrate that by crafting sufficiently diverse training data through iterative training and by carefully testing the accuracy of our models on the relevant inter-molecular scale, we can fit a general purpose potential which describes the EC:EMC binary liquid solvent with ab initio accuracy.

Modelling the effects of oxygen on the electronic properties of graphene

Presenter: Nikki Mansouriboroujeni
Co-author: Natalia Martsinovich
The University of Sheffield Poster

It has been almost two decades since graphene was discovered, and the research so far has uncovered the incredible properties of graphene which make this material suitable for a wide variety of applications. [1] Currently, some of the key directions in materials research is centred on chemical functionalisation, characterization, and real-life applications of graphene-based thin carbon films. This study focuses on the effects that oxygen groups have on graphene, comparing the properties of pure and oxygenated graphene and aerosol gel graphene. This research is a part of an international project aiming to develop a low-cost graphene-based sensor for real time measurement of phosphate content within soils. This work used density-functional theory (DFT) to investigate the structures and electronic properties of pure graphene, curved graphene (a model for aerosol gel graphene) and graphene oxide (GO) - graphene with various oxygen functional groups (epoxide, hydroxyl and substitutional oxygen) in different arrangements and concentrations. The optical absorption properties of graphene, aerosol gel graphene and graphene oxide (GO) derivatives were computed. The impacts of oxygen on the electronic structure of graphene and graphene derivatives were also investigated using projected density of states (DOS). Results show that oxygen atoms have a significant effect of the optical properties of graphene: when compared to graphene they have lower absorbance, and extra peaks in absorption appear when an oxygen group is present in the system. The projected DOS of the carbon atoms that are surrounding the oxygen atom were examined; the results suggest that all carbon atoms in the system were influenced by the presence of oxygen. As expected, the most strongly affected are the carbons that were directly bonded to the epoxide or hydroxyl. Moreover, none of the carbons in oxygenated graphene systems exhibited the DOS exactly as in pure graphene; this shows that the effect of O extends over a long range and is observed even at very low oxygen concentrations.

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Determining the Phase Diagram of a Machine-Learned Carbon Potential via Nested Sampling

Presenter: George Marchant
Co-author: Livia Bartók-Pártay
University of Warwick Poster

We detail how the many-body potential energy landscape of a machine-learned (ML) interatomic potential for carbon [1] can be explored by utilising the nested sampling algorithm,[2] allowing for the determination of carbon's phase diagram up to high pressures. The ML potential in question is the GAP-20 model, which was developed in recent years using the gaussian approximation potential methodology to describe the properties of bulk crystalline and amorphous carbon phases with the accuracy of electronic structure methods. With the nested sampling algorithm the 3N-dimensional potential energy surface of the GAP-20 potential can be automatically (and efficiently) sampled at constant pressure, providing a set of configurations with which to test the potential's thermodynamic capabilities. As a point of comparison the phase diagrams of other interatomic potentials - including the ReaxFF, EDIP and Tersoff potentials - are also studied. Despite having been trained on optimised structures at only zero pressure, GAP-20 provides an accurate description of carbon's macroscopic properties up to approximately 200 GPa. Our results also highlight areas for future improvement of the potential.

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Significance of atomic-scale defects in flexible surfaces on local solvent and ion behaviour

Presenter: Veselina Marinova
Co-author: Colin L. Freeman, John H. Harding
University of Sheffield Poster

Many factors can affect the course of heterogeneous nucleation, such as surface chemistry, flexibility and topology, substrate concentration and solubility. Atomic-scale defects are rarely investigated in detail and are often considered to be unimportant surface features. In this work, we set out to investigate the significance of atomic-scale defects in a flexible self-assembled monolayer surface for the behaviour of clusters of Ca^{2+} and CO_3^{2-} ions in water. To this end, we use molecular dynamics simulations to estimate the diffusion coefficients of ion clusters at different topological surface features and obtain ionic radial distribution functions around features of interest. Well-tempered metadynamics is used to gain insight into the free energy of ions around selected surface defects. We find that certain defects, which we refer to as active defects, can impair ionic surface diffusion, as well as affect the diffusion of ions in close proximity to the surface feature in question. Our findings suggest that this effect can result in an ability of such topological features to promote ion clustering and increase local ionic concentration at specific surface sites. The work reported here shows how the presence of small atomic-scale defects can affect the role of a surface in the process of heterogeneous nucleation and contributes towards a rational definition of surfaces as effective nucleating agents.

Modelling mineral-organic interactions: Adsorption of organic molecules and biomolecules on the alpha-Al_2O_3 (0001) surface

Presenter: Natalia Martsinovich

Co-author:
University of Sheffield Poster

Binding of organic molecules on oxide mineral surfaces is a key process in soil preservation due to its ability to protect soil organic carbon from microbial degradation. To understand the nature and strength of sorption of organic carbon in soil, we investigated the binding of small organic molecules and larger polysaccharide biomolecules (typical building blocks of soil organic carbon) on alpha-Al_2O_3, a common soil mineral which is known to strongly bind organic matter. The calculations of adsorption on the alpha-Al_2O_3 (0001) surface were carried out using density functional theory with empirical dispersion correction. First, adsorption of small organic molecules containing of a variety of functional groups was investigated and compared to the binding of water. Amine, amide and carboxylic acid functional groups were found to bind to this surface more strongly than water. Alcohol, ether, thiol and ester groups had binding energies very similar to that of water, while hydrocarbons were found to bind less strongly. Carboxylic acids were the strongest bound adsorbates in this study. Dissociated adsorption configurations were usually more favourable than molecular adsorption; hydrogen bonding was also found to make a significant contribution to the strength of adsorption. Thus, a number of organic functional groups were identified, such as amine, amide and carboxylic acids, which are able to bind to the alpha-Al_2O_3 (0001) surface more strongly than water and are likely to adsorb on this mineral surface under ambient conditions. Informed by these insights into adsorption of small molecules, we modelled adsorption of biomolecules, fragments of polysaccharides which naturally occur in soil: cellulose, chitin, chitosan and pectin. Pectin, which contains hydroxyl and carboxylic groups, and chitosan, which contains hydroxyl, amine and amide groups, were found to bind strongly, consistent with the strong binding of the functional groups present in these molecules. Cellulose, which contains only ether and hydroxyl groups, showed the least strong adsorption among the biomolecules studied. Our results show that biomolecules containing acid, amine and amide groups, such as pectin and chitosan, bind strongly to soil minerals and therefore are likely to be stable in soil.

Modelling Organic-Inorganic Interfaces of Urinary Calculi

Presenter: Rhiannon Morris
Co-author: Helen Chappell, Andrew Scott, Antonia Borissova and James Smith
University of Leeds Poster

Urinary calculi (kidney stones) is a common ailment effecting around 10% of the world's population and resulting in more than 97,000 finished consultant episodes (FEC) each year in the UK alone[1]. The key chemical interactions relating to stone crystallisation and aggregation are not fully understood. Urinary calculi are solid clusters of small stones, composed of crystals that have precipitated from urine, built up on the luminal surface of the epithelial cell surfaces of the microtubule in the kidney. Kidney stones are often found complexed to organic matrices, such as proteins and amino acids. This research uses first principles modelling (CASTEP) to help elucidate the crystallisation phenomena and unravel the chemistry behind stone composition. Urine analysis of kidney stone patients has previously revealed that their urine contains higher amounts of phospholipids in comparison to healthy patients[2]. The fundamental chemistry underlying its interaction with kidney stones is unknown. In order to begin to understand the nucleation process, we have constructed surface models of calcium oxalate monohydrate and calcium oxalate dihydrate and modelled stone growth, simulating further calcium oxalate adsorption onto these surfaces. The interactions between urinary macromolecules and crystal surfaces at an atomic level are unexplained, we performed ab initio molecular dynamics of phosphocholine adsorption on calcium oxalate surfaces and have shown that the phosphocholine head groups become entrapped within the growing crystal. The lowest energy structures are those where the calcium oxalate dihydrate surfaces change their crystallographic structure. The crystallographic waters are implicit in driving the encapsulation of the phosphocholine head group.

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Straining Ceria Surfaces: a Density Functional Theory Study

Presenter: Sidra Munir
Co-author: Sidra Munir, Minh Khoa Ta, Thomas Smith , Marco Molinari
University of Huddersfield Poster

Nanoparticles of cerium oxide (CNPs) exhibit significant catalytic properties owing to its surface redox capacity induced by the coexistence of Ce^{3+} and Ce^{4+}. CNPs may be grown as core@shell structures in conjunction with other materials for biomedical applications. Strain will arise at the interface between the core and the shell materials. Such strain will have an effect on the redox activity of ceria and as such control has to be gained. The aim of our preliminary study is to strain stoichiometric and reduced CeO_2 {111}, {110} and {100} surfaces and define its reducibility as a function of strain. The {111} surface appears to remain the most stable under tensile and compressing strain. Additionally, we investigate the surface speciation of strained ceria surfaces as a function of water coverage. Finally, we have calculated the temperature of desorption of water as a function of water partial pressure and applied strain.

Theory and simulation of the structural, interfacial and thermodynamic properties of equation of state based potentials

Presenter: James O'Connor
Co-authors: Joanne L. Cook, Ian P. Stott, Andrew J. Masters, Carlos Avendaño
University of Manchester Poster

Equations of state have been shown to reproduce the thermodynamic properties of homogenous systems with great success, however they are difficult to apply to inhomogeneous systems found in soft matter, such as surfactant and polymer solutions as they form aggregates such as micelles. Simulations however, are readily able to simulate inhomogeneous systems, but the techniques used to simulate the length and timescales demanded by mesoscopic systems commonly possess unphysical thermodynamics. In this poster, we investigate a mesoscopic potential, the many body DPD potential (MDPD) which is designed to reproduce the bulk thermodynamics of an equation of state of choice. We apply this potential to the van der Waals equation of state to reproduce vapour-liquid equilibria. We also investigate a simple DFT that can reproduce the interfacial and structural properties of the potential. We now seek to apply this potential to a high-quality equation of state to investigate aggregating systems such as surfactant micelles.

High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation

Presenter: Ioanna Pallikara
Co-authors: Jonathan M. Skelton and Joseph M. Flitcroft
University of Manchester Poster

Major technological advancement is largely driven by materials discovery and is key to overcoming some of our most pressing social challenges, such as climate change and future energy supply. The predictive power of Density Functional Theory has made it possible to use high-throughput materials modelling to screen for candidate materials with particular properties. The Materials Project is a core program of the Materials Genome Initiative and offers a database of the DFT-calculated properties of all known inorganic compounds. Despite its versatility, standard modelling with DFT works from frozen snapshots of the atomic structure and fails to account for the effects of thermal motion, leading to a gap between theory and experiment. To bridge this gap, the theory of Lattice Dynamics models the phonons in solids to incorporate both temperature and pressure effects into theoretical models. In this work, we use Lattice Dynamics within the Quasi-Harmonic Approximation (QHA) for the high-throughput prediction of materials finite-temperature properties. We start by selecting an exchange-correlation functional suitable for large-scale QHA calculations. In particular, we perform a comparative study on the accuracy of five exchange-correlation functionals, spanning the local density approximation, generalised gradient approximation and meta-GGA levels of theory, for predicting the properties of ten binary oxides of Group 1, 2 and 12 metals. Then, we present an automated workflow for these large-scale calculations and test it on approximately 150 materials using PBEsol. The resulting dataset is used for both explorative data analysis and for the search of new structure-property relationships. Our findings show that the predictions are bounded by the LDA, which tends to underestimate lattice parameters and cell volumes relative to experiments but yields the most accurate results for bulk moduli, expansion coefficients and Grüneisen parameters, and the PBE GGA, which shows the opposite behaviour. PBEsol gives the best overall predictions of the lattice parameters and constant-pressure heat-capacities whilst also giving relatively reliable results for other properties. The dataset generated through the automated workflow is verified by comparison to experiments where available. Further analysis reveals some systematic trends and some high correlations between several properties. The latter allows us to explore the possibility of using only athermal properties to generate all other materials properties at finite temperatures and pressures. More specifically, we introduce mathematical expressions where DFT-computed properties such as the bulk moduli, lattice energies and volumes can be substituted to generate predictions for the quasi-harmonic properties.

The role of surface ionisation in the induced swelling of graphene oxide membranes

Presenter: Mohd Rafie Bin Shaharudin
Co-authors: Paola Carbone, Christopher D. Williams
University of Manchester Poster

Graphene oxide (GO) membranes are hydrophilic materials that swell in the presence of water either in a humid environment or when in contact with liquid water and the magnitude and mechanism of the swelling is dependent on the degree of ionisation of the functional groups present on the surface of the GO flakes. In this work, using Grand Canonical Monte Carlo and Molecular Dynamics simulations we investigate the effect that the surface charge, resulting from the ionisation process, has on both the amount of water adsorbed in the membranes at various humidity conditions and the swelling of the membranes in contact with liquid water. Three models with increasing surface charge from -63 mC/m^2 to -177 mC/m^2 and a neutral one are used. We show that by incorporating ionised functional groups, the onset of adsorption is shifted to a lower chemical potential and the internal membrane pressure increases due to the repulsive interactions between the graphene flakes. We suggest that for a fairly ordered membrane as the ones modelled here a surface charge of -120 mC/m^2 is the upper limit before membrane delaminate. Our simulations also show that the presence of ions in the channels reduced the swelling due to screening effect but also increases the amount of water adsorbed when the membrane is immersed in liquid water. At low chemical potential, instead, the amount of water adsorbed is determined by the number of ionised groups. The charged model is able to qualitatively reproduce experimental data showcasing the importance of including surface charge in GO model to predict hydration and swelling mechanism. These findings are crucial in underpinning the future development of GO membranes in simulation and experimental study for aqueous separations since hydration-induced swelling is widely known to lead to significant deterioration in performances.

Materials Science activities at CHPC

Presenter: Happy Sithole
Co-author: Nkwe Monana, Krishna Govender and Anton Lopis
CHPC-South Africa Poster

South Africa has a long standing collaboration with CCP5 activities since the mid-90s. This collaboration has seen a lot of developments in materials science studies and increased demand on applications software such as DL_POLY. This talk will show case these areas of collaborations, and propose future collaboration that can further strengthen the work between two groups.

The magnetic properties of cubic PuH_2 and PuH_3: a first-principles investigation

Presenter: Thomas Smith
Co-authors: Samuel Moxon, David J. Cooke, Robert M. Harker, Mark T. Storr and Marco Molinari
University of Huddersfield Poster

Plutonium (Pu) undergoes corrosion via oxygen and hydrogen forming PuO_2 and PuH_x, respectively. The pyrophoric nature of PuH_x and its ability to catalyse the oxidation reaction of Pu leads to a subsequent volume increase placing the storage vessel under mechanical strain potentially leading to containment failure, make it species of interest. A discrepancy on the magnetic order of PuH_2 is present in the experimental literature with both antiferromagnetic (AFM) and ferromagnetic (FM) order reported. Experimental studies are hindered by the radioactivity and toxicity of Pu therefore experimental publications on PuH_x are scarce. Computational studies, based on density functional theory (DFT), offer valuable into hazardous and challenging materials. The dispute on the magnetic order of PuH_2 is also stated DFT studies with only a very small difference in energy (10^{-2} eV) present between AFM and FM orders. We employ DFT at two levels of theory, PBEsol+U+SOC and HSE06sol+SOC, utilising spin-orbit coupling, on-site Coulombic correction and noncollinear magnetism. To determine the magnetic nature of both cubic PuH_2 and PuH_3 we imposed FM, longitudinal AFM and transverse AFM orders in the <111>, <110> and <100> directions. Using PBEsol+U+SOC, we sampled the Hubbard correction U between 0 – 7 eV finding the magnetic order of both cubic PuH_2 and PuH_3 dependant on the value of U with a swap in magnetic order predicted in both structures. When employing HSE06sol+SOC, the most stable magnetic orders for PuH_2 and PuH_3 were FM in the <110> and <111> directions respectively, the energy difference between FM and AFM orders is tiny (10^{-2} - 10^{-3} eV) in agreement with the literature.

Predicting thermodynamic properties of adsorption monolayers with lattice models

Presenter: Pavel Stishenko
Co-author: Andrew Logsdail, Amit Chaudhari
Cardiff University Poster

Lattice models of adsorption monolayers are a powerful tool for prediction of adsorbate species arrangements, adlayer phase stability and interpretation of experimental data. Solid theoretical background and efficient algorithms enable highly accurate computations of adlayer's configurational entropy and phase's discovery. Recent advances in automation of lattice model's building and parametrization pave the way to routine usage of this technique. Here we provide a review of contemporary modelling methods and a few interesting models of adsorption monolayers: metal-organic networks, terminating hydrogen layer on MXene's, chlorine on anatase surface.

Phosphate Adsorption on Cerium Oxide Surfaces

Presenter: Minh Khoa Ta
Co-authors: Samuel Moxon, Roger M. Phillips, David J. Cooke, Marco Molinari
University of Huddersfield Poster

Cerium oxide nanoparticles (CeNPs) are promising candidates as nanozymes. CeNPs mimic enzymatic activities such as superoxide dismutase, catalase, phosphatase etc. However, the enzyme mimetic activities of CNPs are highly variable with many reactions able to occur simultaneously. It is therefore imperative that we investigate how to control such activities, especially for use in biomedicine. Surface composition and charge (e.g. CeIV/CeIII ratio) appear to be a key factor to control reactivity, in addition to shape and size. Whilst phosphates interact strongly with CeNPs, phosphate bearing molecules interact selectively. CeNPs may also be scavenged by phosphates and convert to cerium phosphate. The strength of interaction between phosphates and the {111}, {110}, and {100} surfaces of CeNPs is investigated using Density Functional Theory. It is found that the {100} surface forms strong bonds with phosphate species that can even displace surface atoms. The surface free energy is calculated as a function of phosphate concentration and temperature. This allow us to map the surface composition of CeNPs surfaces. Our results may indicate that CeNPs with an octahedral shape are better suited in protecting the nanoparticle shape, whereas CeNPs with a cuboidal shape are scavenged despite having higher catalytic activity.

Atomistic simulations of structure and stability of coincidence site lattice grain boundaries in CeO_2

Presenter: Susanna Vigorito
Co-authors: David J. Cooke and Marco Molinari
University of Huddersfield Poster

A key challenge to determine the role of microstructure on the properties of materials is to identify their structures and distinguish their individual behaviours. Grain boundaries are common structural features in oxide energy materials and many are coincidence site lattice (CSL) grain boundaries, where there is a relatively well-ordered grain boundary plane. For example, the space charge effect is common in grain boundaries of fluorite structured materials, which ultimately hinders ionic conductivity through the boundary. Cerium dioxide, CeO_2, is an important electrolyte in solid oxide fuel cells and a catalyst in homogeneous and heterogeneous systems and as such the effect of grain boundaries on its properties has drawn great interest. Using atomistic simulations based on classical energy minimization, we investigated a large range of grain boundary structures in CeO_2 arising from mirroring surfaces with Miller indices {hkl} where h, k, and l = 0-9. We have mapped the minima and maxima of the potential energy surface of the resulting 160 symmetry independent grain boundaries arising from the mirroring of the surfaces. We demonstrate that our search for grain boundary structures yields quantitative comparison with known experimental CSL structures. We have calculated the formation and cleavage energies for the lowest energies grain boundary configurations and identified trends between these quantities and the so-called sigma value specific to each structure.

Emerging mutations in SARS-CoV-2 NSP10 and their effects on the stability and functionality

Presenter: Huan Wang
Co-author: Danni Dong, Frank Kozielski and Shozeb Haider
University College London Poster

The novel coronavirus SARS-CoV-2 represents one of the major outbreaks of this century. Although immediate actions were taken to discover potential therapies and develop vaccination, the devastating impacts of COVID-19 are still ongoing. There is an urgent need to find alternative therapies that are independent of the current vaccines. There is a growing body of research that focuses on the molecular mechanisms that guide the replication of this virus. Recent works have established that the non-structural protein 10 (NSP10) acts as a cofactor for two enzymes, NSP16 (2'- O-methyltransferase) and NSP14 (proofreading exoribonuclease and N7 methyltransferase), that are essential for the replication of the viral genome as well as evading the innate immunity. Details of how these small proteins regulate the activity of larger viral enzymes remain unclear. In this study we carried out a comprehensive analysis of the globally collected whole-genome sequences (WGS) of SARS-CoV-2, submitted to the Global Initiative Sharing All Influenza Data (GISAID). These 7,070,539 sequences were aligned to the reference genome Wuhan/WIV04/2019 to identify the most common mutations in NSP10. The three most frequent NSP10 mutations are T12I, T102I and A104V. The stabilising and destabilising effects of NSP10 mutations were predicted from the free energy change using the program DynaMut2. MutaBind2 was also applied to examine the effects of these specific mutations on the binding affinity and stability of both NSP14-NSP10 and NSP16-NSP10 complexes. These effects may reflect the roles they play in SARS-COV-2 and the relationship between the structure and function. We also expressed, purified, and characterised the three most frequent NSP10 mutations and compared these to native NSP10 to discover functional changes induced by mutational evolution of the virus genome.

Using molecular dynamics simulation to predict the aggregation propensity of mAb formulations & accelerate development

Presenter: Yuhan Wang
Co-authors: Hywel D Williams; Paul Dalby
University College London Poster

Protein aggregation is one of the biggest challenges in the pharmaceutical manufacturing area, for it largely affects the efficiency of antibody drugs and causes financial loss. Aggregation is increasingly thought to occur through the partial unfolding of protein structure to expose sites that are more prone to self-interaction. The self-association of proteins happens due to both extrinsic and intrinsic factors. To name a few, temperature, pH, and protein concentration are extrinsic causes, while aggregate prone regions (APRs) within the protein is an intrinsic one. Hence, the aim of this project will be to develop a workflow of molecular dynamics (MD) simulation approaches and artificial intelligence (AI) that can provide molecular-level insights into the aggregation behaviour of mAbs observed experimentally in a range of conditions, including variation in pH, temperature, freeze/thaw or other stressors, and the presence or absence of stabilising excipients. This will also validate the computational approaches and build confidence in their use for predictive purposes. First of all, all-atom molecular dynamics simulations under different environmental parameter settings (temperature, pH, ionic strength) will be implemented on a Fab domain, which will then be followed by coarse-grained simulations on full antibodies with at least two copies introduced into the system. The data from MD simulations such as RMSD, RMSF, along with the protein sequence and structure information, will serve as the input for the subsequent machine learning process. The combination of MD and AI will offer an opportunity to predict protein stability without additional laboratory work that has been proved to be time-consuming and uneconomical.

Wettability of graphite under 2D confinement

Presenter: Zixuan Wei
Co-authors: Mara Chiricotto , Joshua D. Elliott, Fausto Martelli, Paola Carbone
The University of Manchester Poster

The thermodynamics of solid/liquid interfaces under nanoconfinement has tremendous implications for liquid transport properties. Here using molecular dynamics, we investigate graphite nanoslits and study how the water/graphite interfacial tension changes with the degree of confinement. We found that, for nanochannel heights between 0.7nm and 2.6nm, where the number of water layers is dramatically reduced, graphite becomes more hydrophobic than in bulk, and that the value of the surface tension oscillates before eventually converging towards a constant value for larger slits. The value of the surface tension is correlated with the slip length of the fluid and explained in terms of the effective and interfacial density, hydration pressure and friction coefficient. The study clearly indicates that there is a critical channel height of 0.9nm (achievable experimentally 1 at which the surface tension reaches its highest value, but the water diffusion across the channel is at its minimum. The structural analysis shows that for this pore size a transition between a 2D and 3D hydrogen bond network is accompanied by an abrupt increase in conformational entropy. Our results show that the wettability of solid surfaces can change under nanoconfinement and can be used to interpret the experimental permeability data.

A rigid-ion potential model for mixing $SrTiO_3$ with PANI

Presenter: Nathan Wood
Co-authors: Joshua S. Tse, David J. Cooke, Lisa J. Gillie and Marco Molinari
University of Huddersfield Poster

Whilst the physical and chemical properties arising from the interactions between organic molecules and small-to-moderately sized inorganic systems can be investigated with relative ease using ab initio simulation methods such as density-functional theory, problems with cost, time and resources begin to arise when modelling large (> 10^3 atoms) and macroscale systems. The use of classical methods such as those based on potential models can be used to model large systems using far less computational power whilst also allowing for a significant reduction in cost and time, often without sacrificing much of accuracy that DFT provides. We present the use of an empirical rigid-ion potential model to define the interaction between $SrTiO_3$ and polyaniline (PANI). The derivation of this potential set hopes to see applicability for modelling large scale inorganic-organic systems for thermoelectric applications. This will allow for estimation of physical properties of the composite, such as the thermal conductivity, a vital parameter in the performance of thermoelectric composite materials.

DL_FIELD – a software workflow and infrastructure tool for force field models.

Presenter: Chin Yong
Co-authors:
MCC, STFC, Daresbury Laboratory Poster

DL_FIELD software is a support application tool for DL_POLY in setting up force field (FF) models for molecular systems. DL_FIELD contained a unified FF framework that enable smooth data transformation among a wide range of FF schemes that are implemented within DL_FIELD: CHARMM, AMBER, OPLS, PCFF, CVFF, and their variants. Within the similar framework, DL_FIELD also contained inorganic force fields for a wide range of materials such as zeolites, glass, and minerals. The software tool allows users to easily switch FFs, via a single-step process, and to construct complex mixed FF models, including those of bio-inorganic systems. DL_FIELD program has three main functions: (i)Force field model convertor. Conversion of a user's atomic configuration into force field (FF) files that are readily run in DL_POLY. (ii)Force field editor: Allows users to edit or modify a particular FF scheme to produce a customised scheme that is specific to a particular molecular model. (iii)Force field model repertoire: DL_FIELD has a consistent file structure format for all FF schemes and molecular structure definitions. (iv)Chemical-sensitive atom typing and identification, by making use of the DL_F Notation [1], to facilitate chemistry-based atomic interactions analysis. DL_FIELD is designed to handle a wide range of molecular system of varying complexity: from simple ionic compounds, small covalent molecules to systems with complex topologies such as biomolecules, carbohydrates, drug molecules and organic cages. In addition, the unification of file formats and data structures based on the DL_FIELD framework facilitates migration of one class of FF system model to another, with minimum learning curve. This encourages researchers to carry out new classes of molecular systems spanning across multidisciplinary fields, from material sciences to biological and pharmaceutical areas. Future directions in DL_FIELD development would harness DL_FIELD's capabilities and improve format interoperability and data transformation, to produce data files for other simulation packages such as Gromacs, LAAMPS, NAMD, etc. Such a unified infrastructure would significantly expand the user base to enjoy the benefits of setting up complex FF models, thus paving potential pathways for the research Community to explore research capabilities in new areas.

[1] C. W. Yong, J. Chem. Inf. Model. vol.56, pp 1405-1409 (2016)

Molecular Simulations of Novel Water-In-Salt Aqueous Redox Flow Batteries

Presenter: Hannah Wood
Co-author: Paola Carbone, Robert Dryfe
University of Manchester Poster

Redox flow batteries (RFBs) provide an alternative approach to traditional lithium ion batteries, comprising two half-cells which contain different electrolyte solutions, separated by a membrane to prevent mixing. Current RFB technology is limited by the use of rare metals such as vanadium, and expensive membranes based on the ion-conducting polymer, NafionTM. Aqueous biphasic systems (ABSs) – systems of two immiscible aqueous solutions in separate phases – may offer a solution. It was recently demonstrated that ABSs can be composed of two salts sharing the same cation (Li^+) but different anions (sulfonamides and halides). These "water-in-salt" electrolyte solutions have an electrochemical stability window of up to 4 V. Using ABS, new RFBs may be developed with no membrane between the cells. This work aims to build on the limited knowledge of ABS using a combination of Molecular Dynamics (MD), Quantum Mechanics (QM) and Machine Learning (ML) force fields, to study phase separation and the physisorption mechanism of ions at graphene electrodes.

Studying the phase behaviour of soft bounded attractive-repulsive potentials

Presenter: Michael Seaton
Co-author: Vlad Sokhan, Ilian Todorov
UKRI STFC Daresbury Laboratory Poster

We study a new pairwise interaction potential based on one commonly used for mesoscopic Dissipative Particle Dynamics (DPD). The new potential, described as nDPD, is a generalisation of the 'standard DPD' Groot-Warren model with a higher-order power term for repulsions and an additional attractive term, requiring no long-range corrections beyond a cutoff and providing finite values for zero separations. This interaction model is able to support liquid phases, including coexistence with vapour without requiring density-dependent many-body terms, and is a potential candidate for coarse-grained representations of complex condensed matter phenomena. We have been able to construct phase diagrams from DPD calculations using nDPD with three different repulsive powers and have observed some interesting phase behaviour, including an unusually broad range of temperatures for liquid phases, variation in concavity of the liquid coexistence branch with model parameters, and negative thermal expansion in the solid phase.

Molecular Dynamics Modelling of Polymeric Nanocomposites

Presenter: Jacob Earnshaw
Co-author: Doug Cleaver, Alex Hamilton
Sheffield Hallam University Poster

We present a molecular simulation study for a series of organically functionalised polyhedral oligomeric silsesquioxanes (POSS) systems and elucidate the thermomechanical capabilities of POSS-containing materials. POSS systems can exhibit a wide range of behaviours through variation of the geometry of their central inorganic cores. We systematically explore i) the range of ligands appended (uniformally or asymmetrically), ii) mixing ratios of various POSS forms and iii) their influence on polymer matrices. We identify the key molecular degree of freedom which freezes in at Tg, thereby providing insight for synthetic control of this property. We also present steps towards more ambitious systems of functionalised POSS cubes incorporated into polymeric melts.

List of Delegates

Name	Email	Institution/Company
Kostya Trachenko	k.trachenko@qmul.ac.uk	Queen Mary University of London
Paola Carbone	paola.carbone@manchester.ac.uk	The University of Manchester
Jeremy Winter	jerry.winter@unilever.com	Unilever
Richard Catlow	c.r.a.catlow@ucl.ac.uk	University College London Cardiff University
Steve Parker	s.c.parker@bath.ac.uk	University of Bath
Alison Walker	a.b.walker@bath.ac.uk	University of Bath
Neil Allan	neil.allan@bristol.ac.uk	University of Bristol
Bill Smith	-	UKRI STFC Daresbury Laboratory
David Cooke	d.j.cooke@hud.ac.uk	University of Huddersfield
Marco Molinari	m.molinari@hud.ac.uk	University of Huddersfield
John Harding	j.harding@sheffield.ac.uk	University of Sheffield
Karen Johnston	karen.johnston@strath.ac.uk	University of Strathclyde
Livia Bartok-Partay	Livia.Bartok-Partay@warwick.ac.uk	University of Warwick
Michael Allen	m.p.allen@bristol.ac.uk	University of Warwick University of Bristol
Ben Ellis	ben.ellis@awe.co.uk	AWE
Mark Storr	mark.storr@awe.co.uk	AWE
Joshua Tse	joshua.tse@awe.co.uk	AWE
Berk Onat	berk.onat@3ds.com	BIOVIA Scientific Software Engineering Manager
Edward Smith	edward.smith@brunel.ac.uk	Brunel University London
Owain Beynon	beynonot@cardiff.ac.uk	Cardiff University
Gabriel Bramley	BramleyG@cardiff.ac.uk	Cardiff University
Pavel Stishenko	stishenkop@cardiff.ac.uk	Cardiff University
Happy Sithole	hsithole@csir.co.za	CHPC-South Africa
Alin Elena	alin-marin.elena@stfc.ac.uk	Daresbury Laboratory
Mahmoud Attia	mah_most@mans.edu.eg	French Atomic Energy and Alternative Energies Commission
Arun Chind	arunpeter@yahoo.com	Proshen Health & Risk Consulting Ltd
Chin Yong	chin.yong@stfc.ac.uk	STFC, Daresbury Laboratory
Ilian Todorov	ilian.todorov@stfc.ac.uk	UKRI STFC
Omar-Farouk Adesida	o.adesida@warwick.ac.uk	University of Warwick
Yuhan Wang	ucbeywa@ucl.ac.uk	University College London
Huan Wang	ucnvhw0@ucl.ac.uk	University College London
Joe Crossley-Lewis	jc14269@bristol.ac.uk	University of Bristol
Harry Stroud	hs14458@bristol.ac.uk	University of Bristol
James Elliott	jae1001@cam.ac.uk	University of Cambridge
Ioan-Bogdan Magdau	i.b.magdau@gmail.com	University of Cambridge
Sidra Munir	sidra.munir@hud.ac.uk	University of Huddersfield
Thomas Smith	thomas.smith@hud.ac.uk	University of Huddersfield
Minh Khoa Ta	khoa.ta@hud.ac.uk	University of Huddersfield
Susanna Vigorito	susanna.vigorito@hud.ac.uk	University of Huddersfield
Nathan Wood	nathan.wood@hud.ac.uk	University of Huddersfield
Rhiannon Morris	fsrwm@leeds.ac.uk	University of Leeds
Flor Siperstein	flor.siperstein@manchester.ac.uk	University of Manchester
Mohd Rafie Bin Shaharudin	mohdrafiebin.shaharudin@manchester.ac.uk	University of Manchester
Zixuan Wei	zixuan.wei@manchester.ac.uk	University of Manchester
Guinan Zhao	guinan.zhao@postgrad.manchester.ac.uk	University of Manchester

Matthew Brown	matthew.brown-8@postgrad.manchester.ac.uk	University of Manchester
Joseph Flitcroft	joseph.flitcroft@manchester.ac.uk	University of Manchester
Kieran Harris	Kieran.harris@postgrad.manchester.ac.uk	University of Manchester
Andrew Masters	andrew.masters@manchester.ac.uk	University of Manchester
James O'Connor	james.oconnor-3@postgrad.manchester.ac.uk	University of Manchester
Ioanna Pallikara	ioanna.pallikara@postgrad.manchester.ac.uk	University of Manchester
Jonathan Skelton	jonathan.skelton@manchester.ac.uk	University of Manchester
Lois Smith	lois.smith-2@postgrad.manchester.ac.uk	University of Manchester
Nikki Mansouriboroujeni	nnmansouriboroujeni1@sheffield.ac.uk	University of Sheffield
Xue Yong	x.yong@sheffield.ac.uk	University of Sheffield
Wenziyi Chen	wenziyi.chen@postgrad.manchester.ac.uk	University of Sheffield
Nasiru Aminu Rano	narano1@sheffield.ac.uk	University of Sheffield
Emma Armstrong	earmstrong1@sheffield.ac.uk	University of Sheffield
Vittoria Fantauzzo	vfantauzzo1@sheffield.ac.uk	University of Sheffield
Veselina Marinova	v.marinova@sheffield.ac.uk	University of Sheffield
Natalia Martsinovich	n.martsinovich@sheffield.ac.uk	University of Sheffield
Reetu Reetu	rna3@sheffield.ac.uk	University of Sheffield
Stephen Yeandel	s.yeandel@sheffield.ac.uk	University of Sheffield
Nabeel Anwar	na5g20@soton.ac.uk	University of Southampton
Sebastian Havens	s.havens@warwick.ac.uk	University of Warwick
George Marchant	george.marchant@warwick.ac.uk	University of Warwick
Hannah Wood	hannah.wood-4@postgrad.manchester.ac.uk	University of Manchester
Michael Seaton	michael.seaton@stfc.ac.uk	UKRI STFC Daresbury Laboratory
Alveena Khan	alveena.khan@postgrad.manchester.ac.uk	University of Manchester
Sophie Guillemot	sophie.guillemot@manchester.ac.uk	University of Manchester
Colin Freeman	c.l.freeman@sheffield.ac.uk	University of Sheffield
Jacob Earnshaw	b5020117@my.shu.ac.uk	Sheffield Hallam University