

Disordered Materials User Group Meeting
Cosener's House, Abingdon

Tuesday 14 th June 2022		
11:00	Registration Opens	
12:30	Lunch @ Cosener's	
Facility / Group Update (Chair: Daniel Bowron)		<i>Hybrid in-person + online</i>
13:30	Opening Remarks	<i>Dr Daniel Bowron (ISIS) (5 mins)</i>
13:35	ISIS Facility Update	<i>Prof Roger Eccleston (Director of ISIS) (15 mins)</i>
13:50	Disordered Materials Group Update	<i>Dr Daniel Bowron (ISIS) (15 mins)</i>
14:05	Deuteration Facility Update	<i>Dr Sarah Youngs (ISIS) (15 mins)</i>
14:20	ISIS Impact Team Update	<i>Dr Rosie de Laune (ISIS) (10 mins)</i>
14:30	Dissolve - Capability Update	<i>Dr Tristan Youngs (ISIS) (10 mins)</i>
Session 1 (Chair: Oliver Alderman)		<i>Hybrid in-person + online</i>
14:40	Exploiting proteins as biomaterial building blocks: current capabilities, future opportunities and the challenges ahead	
(20 mins)	<i>Prof Lorna Dougan (Leeds University) Remote, BST</i>	
15:00	Atomic Structure of Amorphous Calcium Carbonate	
(15 mins)	<i>Prof Simon Clark (Macquarie University)</i>	
15:15	In operando study of the atomic structure evolution of liquid metals and amorphous metals	
(15 mins)	<i>Prof Jiawei Mi (University of Hull)</i>	
15:30	The structure of tartaric acid based chiral DES	
(15 mins)	<i>Ms Elly Bathke (University of Bath)</i>	
15:45	Coffee	
Session 2 (Chair: Terri-Louise Hughes)		<i>Hybrid in-person + online</i>
16:20	How fast can we go? Total scattering measurements on the Polaris diffractometer and the effect of noisy data on reverse Monte Carlo refinements	
(15 mins)	<i>Dr Helen Playford (ISIS)</i>	
16:35	Electrochemical Redox Couples: A Combined XAS and Modulation Excitation study	
(20 mins)	<i>Mr Armando Ibraliu (University of Manchester)</i>	
16:55	Exploiting Neutrons to Unveil Star Formation: Exploring Dynamical Amorphous Ice Systems	
(20 mins)	<i>Mr Zachary Amato (Open University)</i>	
17:15	Short- range order in liquid Gallium-Indium alloys	
(15 mins)	<i>Dr Alfred Amon (University College London) Remote, BST-8</i>	
17:30	Under Pressure: The Structure of Water in Compressed Aqueous Trimethylamine N-Oxide	
(15 mins)	<i>Dr Harrison Laurent (University of Leeds) Remote, BST</i>	
17:45	Day 1 Close / Free Time	
18:30	Cosener's Bar Open – Pre-Dinner Socializing	
19:00	UGM Dinner @ Cosener's House	

Wednesday 15 th June 2022	
Session 3 (Chair: Daniel Bowron) <i>Hybrid in-person + online</i>	
09:15 (20 mins)	Structural Analysis of Potassium Borate Solutions <i>Dr Zhu Fayan (Qinghai Institute of Salt Lakes) Remote, BST+8</i>
09:35 (15 mins)	From Newtons to Neutrons: Complementary Insight from Surface Force Analysis and Total Scattering <i>Dr James Hallett (University of Reading)</i>
09:50 (20 mins)	Neutron scattering calculation for coarse grain models <i>Dr Bindu Kolli (ISIS)</i>
10:10 (20 mins)	Sodium acetate trihydrate/urea - a convergence of molten salt hydrates, deep eutectics and ionic liquids? <i>Prof John Holbrey (Queen's University Belfast)</i>
10:30 (15 mins)	Field-induced spin ice in disordered pyrochlore Dy ₂ Zr ₂ O ₇ <i>Ms Sheetal Devi (Indian Institute of Technology) Remote, BST+4.5</i>
10:45	Group Photo
11:00	Coffee
Session 4 (Chair: Tom Headen) <i>Hybrid in-person + online</i>	
11:30 (15 mins)	Hydrating hydrophobic molecules: Matrix-isolation of C ₆₀ and adamantane in amorphous ice <i>Prof Christoph Salzmann (University College London)</i>
11:45 (15 mins)	Detailed characterization of the microscopic hydration of adamantane <i>Dr Luis Carlos Pardo Soto (Universitat Politècnica de Catalunya)</i>
12:00 (20 mins)	Take drugs with water – solution structure of cimetidine influencing crystal hydrate formation <i>Dr Kathi Edkins (University of Manchester)</i>
12:20 (15 mins)	Study of magnesium aluminosilicate glasses with neutron diffraction with isotopic substitution <i>Mr Hesameddin Mohammadi (University of Bath)</i>
12:35 (15 mins)	GudPy - Enhanced GUI for Gudrun <i>Mr Jared Swift (ISIS)</i>
12:50	Lunch @ Cosener's
Session 5 (Chair: Oliver Alderman) <i>Hybrid in-person + online</i>	
13:50 (15 mins)	EPSR and X-ray total scattering studies of local 3D atomic structure evolution in the semi-solid state of Aluminum-based alloys <i>Mr Huang Shi (University of Hull)</i>
14:05 (15 mins)	Recreating JournalViewer <i>Mr Ethan Devlin (ISIS)</i>
14:20 (15 mins)	When is a bond not a bond?: Tellurite glasses and the question of coordination number <i>Dr Emma Barney (University of Nottingham)</i>
14:35 (15 mins)	Something Old, Something New, Something Borrowed (But Nothing Blue) <i>Dr Andrew Seel (ISIS)</i>
14:50 (15 mins)	Local structure and dynamics of tungsten oxide-based glasses: insights from concurrent neutron diffraction and Compton scattering <i>Dr Matthew Krzystyniak (ISIS)</i>
15:05 (15 mins)	SANS Investigations of N ₂ and CO ₂ Adsorption in Soft Templating Porous Carbon <i>Ms Evangelin Hutamaningtyas (Queen Mary University of London)</i>

15:20 Coffee

Session 6 (Chair: Alex Hannon)

Hybrid in-person + online

15:50 Phosphate-based glasses for biomedical applications

(15 mins)

Dr Daniela Carta (University of Surrey)

16:05 Fluids within porous materials – studies by total neutron scattering

(15 mins)

Dr Marta Falkowska (The University of Manchester)

16:20 Structure and dynamics of water in ordinary Portland and low CO₂ cements

(15 mins)

Dr Zhanar Zhakiyeva (ILL) Remote, BST-5

16:35 Effective Defective Cathodes for Lithium Ion Batteries

(15 mins)

Dr Thomas Ashton (University College London)

16:50 Metal-organic Frameworks-Glass Composites

(20 mins)

Dr Celia Castillo-Blas (University of Cambridge)

17:10 Octahedral oxide glass networks at ambient pressure: Structure of neodymium titanate glass

(15 mins)

Dr Stephen Wilke (Materials Development, Inc.) Remote, BST-6

17:25 Day 2 Close / End of Science Meeting

18:30 Dinner @ Cosener's House

Thursday 16th June 2022

Data Analysis Workshop (Introductory Lectures)

Hybrid in-person + online

09:30 Introduction to Disordered Materials Data Analysis
(20 mins) *Dr Tom Headen (STFC)*

09:50 EPSR26 Overview
(20 mins) *Dr Daniel Bowron (STFC)*

10:10 Dissolve Overview
(20 mins) *Dr Tristan Youngs (STFC)*

10:30 Workshop Group Photo

10:40 Coffee

Data Analysis Workshop (EPSR and Dissolve parallel sessions)

In-person only

11:00 Workshop Session 1

Dissolve – Garden Room
EPSR26 – Hamilton Room/Quiet Room

12:30 Lunch @ Cosener's

13:30 Workshop Session 2

Dissolve – Garden Room
EPSR26 – Hamilton Room/Quiet Room

15:00 Coffee

15:30 Workshop Session 3

Dissolve – Garden Room
EPSR26 – Hamilton Room/Quiet Room

17:30 End of Workshop Day 1

18:30 Workshop Dinner @ Abingdon Spice

Friday 17th June 2022

Data Analysis Workshop (EPSR and Dissolve parallel sessions)

In-person only

09:30 Workshop Session 4

Dissolve – Garden Room

EPSR26 – Hamilton Room/Quiet Room

10:30 Coffee

11:00 Workshop Session 5

Dissolve – Garden Room

EPSR26 – Hamilton Room/Quiet Room

12:30 Lunch @ Cosener's

13:30 Workshop Session 6

Dissolve – Garden Room

EPSR26 – Hamilton Room/Quiet Room

15:00 Coffee