

Disordered Materials User Group Meeting
Cosener's House, Abingdon

Tuesday 14th June 2022

11:00 Registration Opens

12:30 Lunch @ Cosener's

Facility / Group Update (Chair: Daniel Bowron)

13:30 Opening Remarks *Dr Daniel Bowron (ISIS)* (5 mins)

13:35 ISIS Facility Update *Prof Roger Eccleston (Director of ISIS)* (10 mins)

13:45 Disordered Materials Group Update *Dr Daniel Bowron (ISIS)* (15 mins)

14:00 Deuteration Facility Update *Dr Sarah Youngs (ISIS)* (20 mins)

14:20 ISIS Impact Team Update *Dr Rosie de Laune (ISIS)* (10 mins)

14:30 Dissolve - Capability Update *Dr Tristan Youngs (ISIS)* (10 mins)

Session 1 (Chair: Oliver Alderman)

14:40 Exploiting proteins as biomaterial building blocks: current capabilities, future opportunities and the challenges ahead

(20 mins) *Prof Lorna Dougan (Leeds University) Remote, BST*

15:00 Atomic Structure of Amorphous Calcium Carbonate

(15 mins) *Prof Simon Clark (Macquarie University)*

15:15 In operando study of the atomic structure evolution of liquid metals and amorphous metals

(15 mins) *Prof Jiawei Mi (University of Hull)*

15:30 TBA

(15 mins) *Ms Elly Bathke (University of Bath)*

15:45 Coffee

Session 2 (Chair: Terri-Louise Hughes)

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) *Dr Helen Playford (ISIS)*

16:35 Electrochemical Redox Couples: A Combined XAS and Modulation Excitation study

(20 mins) *Mr Armando Ibraliu (University of Manchester)*

16:55 Exploiting Neutrons to Unveil Star Formation: Exploring Dynamical Amorphous Ice Systems

(20 mins) *Mr Zachary Amato (Open University)*

17:10 Short- range order in liquid Gallium-Indium alloys

(15 mins) *Dr Alfred Amon (University College London) Remote, BST-8*

17:25 Under Pressure: The Structure of Water in Compressed Aqueous Trimethylamine N-Oxide

(15 mins) *Dr Harrison Laurent (University of Leeds) Remote, BST*

17:40 Day 1 Close / Free Time

18:30 Pre-Dinner Drinks

19:00 UGM Dinner @ Cosener's House

Wednesday 15th June 2022

Session 3 (Chair: Daniel Bowron)

09:15 Structural Analysis of Potassium Borate Solutions
(20 mins) *Dr Zhu Fayan (Qinghai Institute of Salt Lakes) Remote, BST+8*

09:35 TBA
(20 mins) *Dr Natasha Rhys (Kings College London)*

09:55 Neutron scattering calculation for coarse grain models
(20 mins) *Dr Bindu Kolli (ISIS)*

10:15 TBA
(20 mins) *Prof John Holbrey (Queen's University Belfast)*

10:35 Field-induced spin ice in disordered pyrochlore Dy₂Zr₂O₇
(15 mins) *Ms Sheetal Devi (Indian Institute of Technology) Remote, BST+4.5*

10:50 Coffee

Session 4 (Chair: Tom Headen)

11:30 Hydrating hydrophobic molecules: Matrix-isolation of C₆₀ and adamantane in amorphous ice
(15 mins) *Prof Christoph Salzmann (University College London)*

11:45 Detailed characterization of the microscopic hydration of adamantane
(15 mins) *Dr Luis Carlos Pardo Soto (Universitat Politècnica de Catalunya)*

12:00 TBA
(20 mins) *Dr Kathi Edkins (University of Manchester)*

12:15 Study of magnesium aluminosilicate glasses with neutron diffraction with isotopic substitution
(15 mins) *Mr Hesameddin Mohammadi (University of Bath)*

12:25 GudPy - Enhanced GUI for Gudrun
(15 mins) *Mr Jared Swift (ISIS)*

12:40 Lunch @ Cosener's

Session 5 (Chair: Alex Hannon)

13:40 EPSR and X-ray total scattering studies of local 3D atomic structure evolution in the semi-solid state of Aluminum-based alloys
(15 mins) *Mr Huang Shi (University of Hull)*

13:55 Recreating JournalViewer
(15 mins) *Mr Ethan Devlin (ISIS)*

14:10 When is a bond not a bond?: Tellurite glasses and the question of coordination number
(15 mins) *Dr Emma Barney (University of Nottingham)*

14:25 Something Old, Something New, Something Borrowed (But Nothing Blue)
(15 mins) *Dr Andrew Seel (ISIS)*

14:40 Local structure and dynamics of tungsten oxide-based glasses: insights from concurrent neutron diffraction and Compton scattering
(15 mins) *Dr Matthew Krzystyniak (ISIS)*

14:55 Unfolding field induced ferroelectric phase transition in advanced piezoelectric ceramics
(15 mins) *Miss Zimeng Hu (Queen Mary University of London)*

15:10 Coffee

Session 6 (Chair: Oliver Alderman)

15:50 Phosphate-based glasses for biomedical applications

(15 mins)

Dr Daniela Carta (University of Surrey) Remote, BST

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 From Newtons to Neutrons: Complementary Insight from Surface Force Analysis and Total Scattering

(15 mins)

Dr James Hallett (University of Reading)

17:40 Day 2 Close / End of Science Meeting

18:30 Dinner @ Cosener's House

Thursday 16th June 2022

Data Analysis Workshop (EPSR and Dissolve parallel sessions)

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

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

10:10 Dissolve Overview
(15 mins) *Dr Tom Headen (STFC)*

10:30 Coffee

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 @ ?

Friday 17th June 2022

Data Analysis Workshop (EPSR and Dissolve parallel sessions)

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