

Disordered Materials User Group Meeting  
Cosener's House, Abingdon

Tuesday 16 <sup>th</sup> April	
<b>11:00</b>	<b>Registration Opens</b>
<b>12:30</b>	<b>Lunch @ Cosener's</b>
<b>Facility / Group Update</b>	
13:30	Opening Remarks
(5 mins)	<i>Dr Daniel Bowron (ISIS)</i>
13:35	ISIS Facility Update
(20 mins)	<i>Prof Sean Langridge</i>
13:55	Disordered Materials Group Update
(20 mins)	<i>Dr Daniel Bowron (ISIS)</i>
14:15	Communications team Update
(5 mins)	<i>Dr Rosie de Laune (ISIS)</i>
<b>Session 1 (Chair: Daniel Bowron)</b>	
14:20	Shining a light on "NMR-invisible" biocidal borate glasses
(20 mins)	<i>Dr Courtney Calahoo (University of Alberta)</i>
14:40	Using the New and Improved I15-1 Beamline to Examine Disordered Materials with X-rays
(20 mins)	<i>Dr Daniel Irving (Diamond Light Source)</i>
15:00	Exploiting Neutrons to Unveil Star-Formation: Exploring Dynamical Amorphous Ice Systems
(20 mins)	<i>Mr Zachary Armato (The Open University/ISIS)</i>
15:20	Neutron total scattering studies of hard carbon electrodes for batteries
(20 mins)	<i>Miss Rebecca Shutt (University College London)</i>
<b>15:40</b>	<b>Coffee</b>
<b>Session 2 (Chair: Tom Headen)</b>	
16:20	Neutrons as probes for structural investigation of uranium compounds in solution
(20 mins)	<i>Dr Robert Baker (Trinity College Dublin)</i>
16:40	Evolving GudPy for the Masses
(20 mins)	<i>Miss Noella Spitz (ISIS)</i>
17:00	Disordered materials in battery applications.
(20 mins)	<i>Dr Pheobe Allan (University of Birmingham)</i>
17:20	Total scattering studies of amorphous metal-organic frameworks and MOF-glass composite materials
(20 mins)	<i>Dr David Keen (ISIS)</i>
17:40	Long-range structure in Water-in-Salt Electrolytes
(15 mins)	<i>Dr James Hallet (University of Reading)</i>
<b>18:00</b>	<b>Day 1 Close / Free Time</b>
<b>19:00</b>	<b>UGM Dinner @ Cosener's House</b>

Wednesday 17<sup>th</sup> April

Session 3 (Chair: Terri-Louise Hughes)

09:30 Solvent and Counter-ion Behaviour at a Charged, Nanoscale Interface  
(20 mins) *Dr Camilla Di Mino (University College London)*

09:50 A Cation Disordered LiNiO<sub>2</sub> as Cathode for Li-ion batteries  
(15 mins) *Dr Javier Castells Gil (University of Birmingham)*

10:05 Metal ion dissolution in deep eutectic solvents  
(20 mins) *Dr Oliver Hammond (Aarhus University)*

10:25 Total scattering measurements for hydrogen storage systems  
(20 mins) *Mrs Anastasiia Kuznetsova (Helmholtz-Zentrum Hereon (WPN))*

10:45 Coffee

Session 4 (Chair: Oliver Alderman)

11:25 Structure-Property Relationships in Water-Ionic Liquid Mixtures  
(20 mins) *Dr Shurui Miao (University of Oxford)*

11:45 Dissolve-ing polymers - an update  
(15 mins) *Dr Alison Paul*

12:00 A comparison of different Fourier transform procedures for analysis of diffraction data from simple fluids  
(20 min) *Dr John Proctor (University of Salford)*

12:20 Visualization of Self-Assembly and Hydration of a  $\beta$ -Hairpin through Integrated Small and Wide-Angle Neutron Scattering  
(15 mins) *Dr Harrison Laurent (University of Leeds)*

12:35 2024 DMUGM Group Photograph

12:40 Lunch @ Cosener's

Session 5 (Chair: Tristan Youngs)

13:35 Water and Counterion Structuring around Cyclic Anionic Surfactants in Solution  
(20 mins) *Miss Laura Deeming (Lund University)*

13:55 Disproportionation of species in silicate glasses  
(15 mins) *Dr Alex Hannon (ISIS)*

14:10 One Potential Set to Rule Them All: Multi-Compositional EPSR of Phosphate Glasses  
(20 mins) *Mr Daniel Bradley (University of Nottingham)*

14:30 Trimethylamine-N-oxide depletes urea in a peptide solvation shell  
(20 mins) *Mr Mazin Nasralla (University of Leeds)*

14:50 Investigating preferential adsorption of N<sub>2</sub> from the air in Zeolite 13X using total neutron scattering  
(20 mins) *Dr Marta Falkowska (University of Manchester)*

15:05 Structure of Liquid Thiophene - Derived with Dissolve  
(15 mins) *Dr Adam Clancy (University College London)*

15:20 Coffee

Session 6 (Chair: Alex Hannon)

16:00	Elucidation of Adsorption-Induced Structural Transitions in Zeolitic Imidazolate Frameworks at High Pressures
(20 mins)	<i>Dr Thokozile Kathyola (Diamond Light Source)</i>
16:20	Enhancing the sensitivity of neutron scattering experiments for chemically active sample components: Modulation Excitation with Phase Sensitive Detection (ME-PSD)
(15 mins)	<i>Dr Daniel Bowron (ISIS)</i>
16:35	Calcium local environment in casting powders with various Ca/Si and fluorine content
(15 mins)	<i>Dr Riccardo Bono (University of Milano)</i>
16:55	Ethylene Glycol-Water Mixtures: Structure, Properties, & Catalysis
(20 mins)	<i>Mr Luke Roebuck (University of Manchester)</i>
17:15	Surface Forces and Bulk Structure in Model Cytosol Solutions
(15 mins)	<i>Mr Keiran Agg (University of Oxford)</i>
17:30	Highly performance manganese oxide cathode material enabled by Grotthuss topochemistry for aqueous zinc ion batteries
(15 mins)	<i>Mr Fangjia Zhao</i>
18:00	<b>Day 2 Close / End of Science Meeting</b>
18:30	<b>Dinner @ Cosener's House</b>

**Disordered Materials User Group Meeting**  
**Cosener's House, Abingdon**

**16<sup>th</sup> – 19<sup>th</sup> April 2024**

**Thursday 18<sup>th</sup> April**

**Data Analysis Workshop (EPSR and Dissolve parallel sessions)**

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

10:15 Dissolve Overview  
(15 mins) *Dr Tristan Youngs (STFC)*

**10:30 Coffee**

**11:00 Workshop Session 1**

Groups 1 & 2 – EPSR – Garden Room  
Group 3 – Dissolve – Quiet Room  
Group 4 – Dissolve – Thames Room

**12:30 Lunch @ Cosener's**

**13:30 Workshop Session 2**

Groups 1 & 2 – EPSR – Garden Room  
Group 3 – Dissolve – Quiet Room  
Group 4 – Dissolve – Thames Room

**15:00 Coffee**

**15:30 Workshop Session 3**

Groups 1 & 2 – EPSR – Garden Room  
Group 3 – Dissolve – Quiet Room  
Group 4 – Dissolve – Thames Room

**17:30 End of Workshop Day 1**

**18:30 Workshop Dinner**

**Friday 19th April**

**Data Analysis Workshop (EPSR and Dissolve parallel sessions)**

09:30 MuSSic Overview  
(30mins)  
*Dr Bindu Kolli (STFC)*

10:00 EPSR extended use  
(30 mins)  
*Dr Marta Falkowska (STFC)*

**10:30 Coffee**

**11:00 Workshop Session 1**

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Group 4 – Dissolve – Thames Room

**12:30 Lunch @ Cosener's**

**13:30 Workshop Session 2**

Groups 1 & 2 – EPSR – Garden Room  
Group 3 – Dissolve – Quiet Room  
Group 4 – Dissolve – Thames Room

**15:00 Coffee**

**15:30 End of Workshop Day 2**