

PROGRAMME DMM-II

FRIDAY 5th July

11:00	REGISTRATION	
12:00	LUNCH	
13:45	INTRODUCTION - Professor Stephen Clark , Head of the School of Chemistry of the University of Glasgow	
title	CATALYSIS & ENERGY MATERILAS	01:30
14:00	Parker* -The use of direct geometry spectrometers for catalysis and molecular spectroscopy	
14:40	Warringham - Vibrational Analysis of an Industrial Fe-based Fischer-Tropsch Catalyst Employing Inelastic Neutron Scattering	
15:00	Fultz* - Polaron Dynamics in LiFePO4	
15:30	TEA	
title	ENERGY MATERIALS - 1	01:00
16:00	Queen* -Physical aspects of gas adsorption in microporous crystalline frameworks	
16:30	Borgschulte* -Neutron scattering of hydrogen storage materials: from anharmonic vibrations to thermodynamics	
title	INSTRUMENTS & DISCUSSION	01:00
17:00	Ivanov - Lagrange	
17:20	Mole - Pelican: A cold neutron TOF spectrometer with polarisation analysis.	
17:40	Larese - Vision	
18:00	Rudić - Recent and future developments on TOSCA	
	DINNER & BEER	

SATURDAY 6th July

title	QUANTUM	01:30
09:00	Horsewill* - Quantum Translator-Rotator Dynamics: INS investigations of the spin-isomers of H2 and H2O molecules trapped inside fullerene cages	
09:30	Ulivi - Quantum dynamics of hydrogen molecules in simple and binary clathrate-hydrates: measurements and computation	
09:50	Natkaniec - IINS and DFT studies of vibrational spectra of water retained in graphene oxide	
10:10	Edge -Inelastic Neutron Scattering of H2 adsorbed in Laponite	
10:30	COFFEE	
title	ENERGY MATERIALS - 2	01:45
11:00	Grothe* -Inelastic Neutron Scattering and Neutron Diffraction of Nitric Acid Hydrates	
11:30	Yang* - Inelastic neutron scattering study on functional energy materials	
12:00	Callear -The structure and dynamics of hydrogen absorption in a metal alloy	
12:20	Larese - Inelastic Neutron Scattering(INS) Studies of Hydrogen Spillover on Pure and Pd decorated Metal Oxides	
12:45	LUNCH	
title	MOLECULAR CRYSTALS & POLYMERS	01:30
14:00	Duyker* - Unique vibrational mechanisms for negative thermal expansion in a series of metal-cyanide framework materials	
14:30	Spencer - Insights into the stability of γ -Al2O3 nanoparticles from Inelastic Neutron Scattering	
14:50	Mukhopadhyay -Investigation on Soft Vibrational Modes of Croconic Acid using Inelastic Neutron Scattering	
15:10	Chudoba - Vibrational spectroscopy of selected molecular crystals studied by means of density functional perturbation theory	
15:30	TEA	
title	BIOLOGY & POLYMERS	01:20
16:00	Tsapatsaris - Polymorphism, Drugs and Neutrons: Is making more stable phases really that simple?	
16:20	Rubio - Polymer Chain Dynamics of Thermosensitive Microgels	
16:40	Appel -Neutron spectroscopy of ferrocene and ferrocene containing polymers	
17:00	Barroso Bujans - Exploring vibrational modes of poly(ethylene oxide) confined in 2D and 3D with TOSCA spectrometer	
17:20	DISCUSSION & CONCLUSION	
	DINNER & MORE BEER	

POSTERS

Kelvin GOH - Nuclear spin conversion of H₂O@C₆₀

Romantsova - Thermal properties of unusual glass-like solids: crystalline clathrate hydrates

Sharapova - The isomeric effect in the thermal conductivity of solid butyl alcohol at low temperatures

Meinzel - Crystal structure, inter-molecular interactions and vibrational spectroscopy of di- and tri-halogeno-trimethylbenzenes

Holderna-Natkaniec - Dynamics of methyl groups of isomers of dimethylpyridine studied by INS and computational methods

Rudic - Inelastic neutron scattering and theoretical investigation of L-aspartic and L-glutamic acid, and their derivatives

Kibble - ISIS Glasgow Catalyst Panel

Morrison - Giant spin fluctuations and their effect on the first order magnetic transition in the itinerant ferromagnet, LaFe_{13-x}Si₆

Rols - Hydrogen on graphene investigated by inelastic neutron scattering

Ivanov - Lagrange

Natkaniec - Parameters of the NERA spectrometer for cold and thermal moderators of the IBR-2M pulsed reactor

Morisse - Characterisation of hydrocarbonaceous overlayers important in metal-catalysed selective hydrogenation reactions