



## PROGRAM

### MONDAY 12 SEPTEMBER 2022

14h00-16h30 Arrival, registration

#### 16h30-18h30 Session 1 : Materials Science I

16h30-16h40 Introduction

16h40-17h15	<b>Garlatti</b>	<b>Elena</b>	Investigating the role of phonons in magnetic relaxation of molecular nanomagnets with inelastic neutron scattering
17h15-17h40	<b>Meijer</b>	<b>Bernet</b>	Effects of orientational disorder on the dynamics of barocaloric adamantane
17h40-18h05	<b>Walker</b>	<b>Helen</b>	Exploring the entropy change in barocaloric ammonium sulfate using QENS and INS
18h05- 18h30	<b>Fogh</b>	<b>Ellen</b>	Tuning magnetoelectricity in a mixed-anisotropy antiferromagnet
19h00	Welcome buffet		

### TUESDAY 13 SEPTEMBER 2022

#### 9h00-12h00 Session 2 : Catalysis & Porous materials I

9h00-9h45	<b>Lennon</b>	<b>David</b>	The application of inelastic neutron scattering and quasielastic neutron scattering to investigate the methanol-to-hydrocarbons reaction over a ZSM-5 zeolite catalyst
9h45-10h20	<b>Glatzel</b>	<b>Jan Pieter</b>	Photon-in/photon-out spectroscopy in materials
10h20-10h45	Coffee break		
10h45-11h10	<b>Vottero</b>	<b>Eleonora</b>	Dynamics of a Pt/Al <sub>2</sub> O <sub>3</sub> catalyst in the presence of H <sub>2</sub> : complementary results from INS, FT-IR and DFT
11h10-11h35	<b>E Silva De Almeida</b>	<b>Gabrielli</b>	Investigation of C <sub>2</sub> H <sub>4</sub> and Ag exchanged Zeolites interaction by Inelastic Neutron Scattering and DFT calculations
11h35-12h00	<b>Fouquet</b>	<b>Peter</b>	Hydrogen mobility and reactivity in MoS <sub>2</sub> catalyst et First results from the wide angle spin echo spectrometer WASP
12h00-13h30	Lunch		

#### 13h30-18h30 Session 3 : Simulation session

13h30-14h05	<b>Genovese</b>	<b>Luigi</b>	Big DFT
14h05-14h30	<b>Aouane</b>	<b>Mohamed</b>	Dynamics in Confinement: a study of CH <sub>4</sub> @C60
14h30-17h30	Social activity		
17h30-18h30	Poster session		
19h00	Diner		

### WEDNESDAY 14 SEPTEMBER 2021

#### 9h00-13h00 Session 4 : Batteries & ionic conductors

9h00-9h45	<b>Famprakis</b>	<b>Theo</b>	Ion dynamics in solid electrolytes for batteries
9h45-10h20	<b>Goff</b>	<b>Jon</b>	Diffusion mechanisms in sodium-ion battery materials using polarized neutrons
10h20-10h45	<b>Shen</b>	<b>Xingchen</b>	Full Phonon Softening and Fast Ag Diffusive Dynamics in Liquid-like Argyrodites Ag <sub>8</sub> GeSe <sub>6</sub>
10h45-11h15	Coffee break		
11h15-12h00	<b>Karlsson</b>	<b>Maths</b>	Dynamics in functional oxide ion conductors studied with INS and QENS
12h00-12h35	<b>Zanotti</b>	<b>Jean-Marc</b>	Ionic Liquids: bulk vs 1D CNT confinement. Towards
12h35-13h00	<b>Schwaighofer</b>	<b>Bettina</b>	A Combined Experimental and Computational Study of Oxide Ion Conductors
13h00-14h30	Lunch		

**15h00-18h00****Session 5 : Catalysis & Porous materials II**

15h00-15h35	<b>Blasco</b>	<b>Teresa</b>	Solid state NMR spectroscopy: a tool for the investigation of zeolites as catalysts and adsorbents
15h35-16h10	<b>Terry</b>	<b>Lui</b>	Nanoconfining H <sub>2</sub> - manipulation of the phase diagram and consequences of reduced freedom
16h10-16h45	Coffee break		
16h45-17h10	<b>Abdel Sater</b>	<b>Mohammad</b>	Hydrogen Storage and Dynamics in Clay Materials
17h10-17h35	<b>Fernandez Blanco</b>	<b>Angel</b>	Probing the binding mechanism of toxic gases in Hofmann-clathrates: a combined neutron scattering and DFT study
17h35-18h00	<b>Guimpier</b>	<b>Charlene</b>	Clay sediments, a multiscale playground for hydrate principle lattice dynamics
19h00	Conférence diner		

**THURSDAY 15 SEPTEMBER 2022****9h00-10h10****Session 6 : Material Science II**

9h00-9h45	<b>De Boissieux</b>	<b>Marc</b>	Thermal conductivity and lattice dynamics in structurally complex materials
9h45-10h10	<b>Krzystynlak</b>	<b>Matthew</b>	Local structure and dynamics of tungsten oxide-based glasses: insights from concurrent neutron diffraction and Compton scattering
10h10-10h45	Coffee break		
10h45-11h10	<b>Druzicki</b>	<b>Kacper</b>	Cation Dynamics as a Probe of Local Structure in 3D Hybrid Perovskites: Insights from High-resolution Inelastic Neutron Scattering
11h10-11h35	<b>Kimura</b>	<b>Koji</b>	Phonon Dispersions of Ca-doped BaTiO <sub>3</sub> Studied by Inelastic X-ray and Neutron Scatterings
11h35-12h00	<b>Kulda</b>	<b>Jiri</b>	From molecular dynamics simulations to diffuse scattering maps
12h00-12h30	Closing		
12h30	Lunch and departure		