

Tuesday, 12 December

from **12:15** Registration (Ground floor, Calman Learning Centre) and buffet lunch (Top floor). Poster presenters to put posters up at arrival.

Session 1

Chair: David Quigley (Univ. Warwick)

13:30 Welcome

13:35 **Andrew Goodwin** (Univ. Oxford)

Session Introduction + *Title TBC*

14:15 **Samuli Ollila** (VTT Technical Research Centre of Finland)

NMRlipids project delivers quality evaluated membrane simulations for data-driven applications

14:45 **Elena Patyukova** (Univ. Liverpool)

Structural disorder in inorganic crystalline materials: a comprehensive analysis

15:15 Refreshments and Poster Session 1 (Top floor)

Session 2

Chair: Paul Hodgkinson (Univ. Durham)

16:15 **Ricardo Grau-Crespo** (Univ. Reading)

Session Introduction + *Modelling the NMR spectra of solid solutions: canonical and grand-canonical ensembles, DFT and machine learning*

16:55 **Martin Wilkening** (Univ. Graz)

Li ion diffusion in disordered materials as seen by NMR

17:25 **Manuel Cordova** (EPFL)

Atomic-level structure determination of amorphous molecular solids by NMR

19:30 Conference dinner. Hatfield College dining room.

Wednesday, 13 December

Session 3:

Chair: Frédéric Blanc (Univ. Liverpool)

9:00 **Thibault Charpentier** (Univ. Paris-Saclay)
Session Introduction + Boosting NMR-Driven Reverse Monte Carlo Simulations of Glasses with Machine Learning

9:40 **Nicholas Hine** (Univ. Warwick)
Calculation of Absorption and Emission Spectra in Explicit Solvent using Large-Scale DFT and Machine Learned Interatomic Potentials

10:10 **Andrew Morris** (Univ. Birmingham)
Combining ss-NMR with XAS and first principles calculations to build and verify finite temperature amorphous models

10:40 Refreshments and Poster Session 2 (Top floor)

Session 4

Chair: Vasily Oganessian (Univ. East Anglia)

11:40 **Kim Jelfs** (Imperial College, London)
Session Introduction + Computational Modelling of Amorphous Microporous Materials

12:20 **Yaroslav Khimyak** (Univ. East Anglia)
Understanding phase transitions and nature of disorder in pharmaceutical materials: polymorphs, co-crystals and nano-confined systems

12:50 **Karen Johnston** (Univ. Durham)
Probing Structural Subtleties in Anti-Perovskite Solid Electrolytes

13:20 Meeting close followed by buffet lunch. Posters to be removed.