NMR Crystallography

4-6 September 2024 | Birmingham, UK

Faraday Discussions

Wednesday 4 September 2024 (all timings are BST)

12:00	Registration and lunch
12:45	**Welcome and introductions** John Griffin *Lancaster University, UK* and Andrew Morris *University of Birmingham, UK* (*Co-Chairs of Scientific Committee*)
12:55	**Outline of Discussion format** Names, *Royal Society of Chemistry Publishing Editors*
13:00	**Introductory lecture – Spiers Memorial lecture** (Session chair: Andrew Morris) Lyndon Emsley *Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland*
	Session 1: Big data and simulations in NMR crystallography (Session chair: Andrew Morris)
14:00	**A machine learning approach for dynamical modelling of Al distributions in zeolites via ^{23}Na/^{27}Al solid-state NMR** Carlos Bornes *Charles University, Czech Republic*
14:05	**High Throughput calculations and machine learning modeling of 17O NMR in non-magnetic oxides** Zhiyuan Li *TU Darmstadt, Germany*
14:10	**Characterization of Ephedrine HCl and Pseudoephedrine HCl Using Quadrupolar NMR Crystallography Guided Crystal Structure Prediction** Carl Fleischer *Florida State University, USA*
14:15	Discussion
15:30	Refreshments
	(Session chair: Martin Dračínský**)**
16:00	**The interplay of density functional selection and crystal structure for accurate NMR chemical shift predictions** Greg Beran *University of California, Riverside, USA*
16:05	**Crystal structure determination of Verinurad via proton-detected ultra-fast MAS NMR and machine learning** Daria Torodii *EPFL, Switzerland*
16:10	Discussion
17:00	Lightning presentations (by invitation of the Scientific Committee) (Session chair: Andrew Morris)
17:30	Poster session and wine reception
18:30	Close of sessions

Thursday 5 September 2024 (all timings are BST)

09:30	Refreshments
	Session 2: Challenges and opportunities for NMR calculations (Session chair: Martin Dračínský)
10:00	**Accurate predictions of chemical shifts with the rSCAN and r^{2}SCAN mGGA exchange–correlation functionals** Jonathan Yates *University of Oxford, UK*
10:05	**Uniform Chi-Squared Model Probabilities in NMR Crystallography** Len Mueller *University of California, Riverside, USA*
10:10	**Organic NMR Crystallography: Enabling Progress for Applications to Pharmaceuticals and Plant Cell Walls** Steven P. Brown *University of Warwick, UK*
10:15	Discussion
11:30	Refreshments
	(Session chair: Sally Price)
12:00	**A Combined ^{7}Li NMR, Density Functional Theory and Operando Synchrotron X-Ray Powder Diffraction to Investigate a Structural Evolution of Cathode Material $LiFeV_2O_7$** Gillian Goward *McMaster University, Canada*
12:05	**The EFG Rosetta Stone: Translating between DFT calculations and solid state NMR experiments** Simone Koecher *IEK-9 Forschungszentrum Jülich, Germany*
12:10	Discussion
13:00	Lunch
	Session 3: Generating models that describe complex disorder (Session chair:)
14:00	**When can we trust structural models derived from pair distribution function measurements?** Andrew Goodwin *University of Oxford, UK*
14:05	**The essential synergy of MD simulation and NMR in understanding amorphous drug forms** Paul Hodgkinson *Durham University, UK*
14:10	**Atomic-level structure of the amorphous drug Atuliflapon by NMR crystallography** Jacob Holmes *EPFL, Switzerland*
14:15	Discussion
15:30	Refreshments
	(Session chair: John Griffin)
16:00	**Investigating the effect of particle size distribution and complex exchange dynamics on NMR spectra of ions diffusing in disordered porous carbons through a mesoscopic model** Celine Merlet *Toulouse-Paul Sabatier, France*
16:05	**First-principles NMR of oxide glasses boosted by machine learning** Thibault Charpentier *CEA Paris-Saclay, France*
16:10	Discussion
17:00	Close of sessions
18:00	Conference dinner

Friday 6 September 2024 (all timings are BST)

08:30	Refreshments
	Session 4: Understanding dynamics and mechanisms (Session chair: Danielle Laurencin)
09:00	**Tracking Li atoms in real-time with ultra-fast NMR simulations** Angela Harper *Fritz Haber Institute of the Max Planck Society, Germany*
09:05	**Metastable Layered Lithium-rich Niobium and Tantalum Oxides via Nearly Instantaneous Cation Exchange** Kent Griffith *University of California San Diego, USA*
09:10	**Temperature-induced mobility in Octacalcium Phosphate impacts crystal symmetry: water dynamics studied by NMR crystallography** Christel Gervais *Sorbonne Université, France*
09:15	Discussion
10:30	Refreshments
	(Session chair: Sally Price)
11:00	**Exploring the crystallisation of aspirin in a confined porous material using solid-state nuclear magnetic resonance** Pierre Thureau *AIx-Marseille University, France*
11:05	**Probing assembly/disassembly of ordered molecular hydrogels** Yaroslav Khimyak *University of East Anglia, UK*
11:10	**NMR Crystallization: In-Situ NMR Strategies for Monitoring the Evolution of Crystallization Processes** Kenneth Harris *Cardiff University, UK*
11:15	Discussion
12:30	**Concluding remarks lecture** (Session chair: John Griffin) Sharon Ashbrook *University of St Andrews, UK*
13:00	**Acknowledgements**
13:15	**Close of meeting and lunch**