

DYNAFUN DYNAmics of FUNctional materials

Report of Contributions

Contribution ID: 1

Type: **Oral**

DYNAFUN introduction

Monday, 12 September 2022 16:30 (10 minutes)

Functional materials are those possessing desirable tuned properties for applications such as, but not limited to, energy harvesting, storage, memory and communication devices. Functional materials can be any type of specially designed material with a determined function: semiconductors, polymers, porous media, molecular crystals or nanoparticles are good examples of them. Their special physico-chemical properties make functional materials so special.

With this workshop, we invite you to share and listen the latest achievements in the understanding of the fundamental origin of these functional properties at the atomic level. The investigation of the dynamics of such materials, and in particular ion dynamics, represents the preferential way to gather information on these functional properties. For this reason, this event emphasize on the use of neutron spectroscopy technique, but welcome any important highlight using complementary spectroscopic techniques and computational methods.

The program will leave time for informal but lively discussions of specific topics, like sample environment developments and modelling infrastructures and software, aiming to receive input from the community in order to define future needs.

The workshop will take place in the holiday centre Le Pré du Lac at Saint-Jorioz, on Annecy lakeshore (France), with accommodation on-site, leaving plenty of space for discussions in the relaxing atmosphere of the Annecy lakeshore.

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Session Classification: Session 1 : Materials Science 1

Contribution ID: 2

Type: Oral

The application of inelastic neutron scattering and quasielastic neutron scattering to investigate the methanol-to-hydrocarbons reaction over a ZSM-5 zeolite catalyst

Tuesday, 13 September 2022 09:00 (45 minutes)

Methanol holds an important role in the chemical manufacturing industry. Not only is it an important commodity on its own but, additionally, it can fulfil a role as a chemical vector and/or an energy vector. An example of methanol being actively used as a chemical vector is the methanol-to-hydrocarbon (MTH) reaction over zeolite catalysts. Methanol is readily available as a feedstock via traditional C1 chemistry routes, whilst the MTH reaction provides access to gasoline grade hydrocarbons for use in transportation fuels. The material that makes the MTH reaction work is the zeolite ZSM-5 [1,2]. Its functionality is exceptional, however not all fundamental physico-chemical aspects of that functionality are well understood. Working towards the development of sustainable chemical process operations, this presentation will outline how neutron scattering techniques can be used to provide a fresh perspective on the operational phase of a working MTH catalyst [1-3].

The concept of a 'hydrocarbon pool' (HCP) is commonly used to describe MTH chemistry over ZSM-5, with the dynamical process accounting for the formation of short chain olefins and methylated aromatics [1,2]. Although understood at a contextual level, details of what constitutes the HCP over the lifetime of a catalyst is not so well defined. This includes its variability with respect to different operational conditions such as temperature.

The presentation will describe a two-pronged approach to investigate aspects of HCP formation over a commercial grade ZSM-5 catalyst active for the MTH reaction [2]. In the first instance inelastic neutron scattering (INS) is used to define the form and nature of the HCP. Three regimes are explored: (i) a catalyst conditioning stage, (ii) steady-state operation and (iii) a catalyst deactivation phase. The resulting spectra indicate the complexity of the HCP but, with referral to suitable reference spectra [4], molecular descriptors for the form of the HCP under the various regimes examined are deduced [5]. Secondly, quasielastic neutron scattering measurements on the post-reaction catalyst samples are used to interrogate how the differing degrees of hydrocarbon retention within the zeolite perturb diffusion within the intricate pore network of the ZSM-5 catalyst.

References

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Session Classification: Session 2 : Catalysis & Porous materials I

Contribution ID: 3

Type: Oral

Investigation of C₂H₄ and Ag exchanged Zeolites interaction by Inelastic Neutron Scattering and DFT calculations

Tuesday, 13 September 2022 11:10 (25 minutes)

The production of ethylene exceeds 200 million tons per year, consolidating this molecule as a critical feedstock material for petrochemical industry. A fundamental step for the application of this alkene in derivatives is its separation/ purification from ethane after being obtained by naphta or ethane steam cracking. The state of art method for such task is cryogenic distillation, one of the most energy consuming industrial processes nowadays.

Porous solids adsorbents have been addressed as a highly promising alternative solution for this matter, being represented by Metal Organic Frameworks (MOFs) and zeolites. While some MOFs may present a rather poor stability, zeolites have been standing the roughness of industrial applications since the 1950's. Another great advantage of zeolites is their tunability in terms of pore size, shape and surface functionality, allowing specific selective adsorption processes even at ambient temperatures. Due to the small differences of ethylene and ethane kinetic diameters and their nearly identical physical properties, molecular sieving effect by itself is not effective for their separation. Thus, this process must rely also on a Lewis acid-base interaction between the alkene and a transition metal cation, specially Cu(I) and Ag(I), allocated in the adsorbent. Nevertheless, the exact adsorption mechanism of ethylene on Ag(I) exchanged CHA, for example, is not completely understood yet.

In this work, we characterized this interaction between ethylene and silver aluminosilicate CHA at a microscopic level using a multidisciplinary approach involving Inelastic Neutron Scattering (INS), Nuclear Magnetic Resonance (NMR), UV-vis, Infrared (IR) and Density Functional Theory (DFT) calculations parting from a real system. From UV-vis analysis, it was seen that the system under investigation contains not just cations but also 3 atoms charged Ag clusters. Both species interact with the ethylene, as confirmed by the comparison between the experimental INS spectrum and the DFT calculated INS spectra obtained for a cationic and a cluster models. ¹³C-Solid State NMR showed an upfield shift from 123 ppm to 110 ppm, suggesting a stronger proton shielding and electron transfer between the adsorbant/adsorbent. This fact was corroborated by DFT electron density difference calculations, proving the nature of this interaction, known as π -complexation. Finally, by analyzing the red shift of C-C stretching modes and C-C bond lengthening with information provided by IR, INS and DFT, we could not just have a further confirmation of its nature, but could also evaluate the extension of the interaction for each model, attesting the higher preference of ethylene to cationic Ag species in such a complex system.

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Session Classification: Session 2 : Catalysis & Porous materials I

Contribution ID: 4

Type: **Poster**

Quantification of Dynamic Structural Disorders in Energy Conversion Materials

Tuesday, 13 September 2022 17:45 (15 minutes)

Defects and structural disorders are well recognized as crucial for the energy conversion process. However, the precise description of the types and concentrations of defects is an intriguing and complex challenge, requesting the combination of various advanced experimental in situ and post mortem methods such as laboratory- and synchrotron-based X-ray diffraction, neutron diffraction, X-ray photoelectron spectroscopy, and electrical transport properties as well as theoretical modeling and simulation techniques. In particular, the changes of the defects and disorder happen in most energy conversion processes affected by environmental factors such as temperature changes or light excitation. Four types of materials are currently in the focus of our research where the defect structure and dynamics are to be understood in detail: i) the change in the occupation of the ideally empty structural site in thermoelectric half-Heusler materials leading to disorder and intrinsic doping effects by the creation of in-gap states in the band structure[1,2], ii) the transport of oxygen ions via (disordered) oxygen vacancies and electrons in oxygen transport membrane materials for the plasma-assisted CO₂ conversion[3,4], iii) perovskite-type oxynitrides for solar water splitting containing Ta⁴⁺ or Ta⁵⁺ on the B-site showing presence or absence of O/N ordering depending on the investigated length scale[5,6], and finally iv) the role of defects on optical properties of perovskite-type halides for photovoltaics[7,8].

Basically, the dynamics of the defects and disorder are expected to play a crucial role for the efficiency and lifetime of an energy conversion material. Except for photovoltaic and other photo-induced converters, such dynamic effects are studied relatively seldom[9]. In addition to the methods mentioned above, time-resolved measurements, e.g., by neutron spectroscopic methods are necessary to get experimental access to the ongoing changes in a material during energy conversion. An extended understanding of the dynamic phenomena is needed in order to enable a conceptual implementation into future material design. Accordingly, this will allow a longer lifetime of the material in a specific energy conversion process helping also to reduce the demand for material resources.

References

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Session Classification: Poster session

Contribution ID: 5

Type: **Oral**

Exploring the entropy change in barocaloric ammonium sulfate using QENS and INS

Monday, 12 September 2022 17:40 (25 minutes)

Ammonium sulfate, a common garden fertiliser, displays a ferroelectric phase transition with a large entropy change whose origins have proved controversial. Understanding this will provide an important insight into its barocaloric properties, and how these might be developed into future environmentally friendly cooling applications. Here we approach this question using quasielastic, inelastic, and total neutron scattering, as functions of both temperature and pressure, and DFT simulation.

Our QENS results reveal a geometry of hydrogen motion that is inconsistent with the usual simple order-disorder model of configurational entropy. In addition, pressure is unusually found to decrease the barrier to rotation in the low temperature phase, due to the stiff hydrogen bond network being destabilised, increasing the possibility for hydrogen atoms to buckle sideways, which relates to the observed inverse barocaloric effect. Conversely, in the high temperature phase, pressure has little effect, as the denser hydrogen bond network prevents the buckling.

Instead our INS and DFT results indicate that the entropy arises from large-amplitude, anharmonic librations in the high temperature phase. In the low temperature phase the ammonium librational modes, partially identified by their negative mode Grüneisen parameters, are separate from the other low frequency collective modes, suggesting that the hydrogen bonding holds these ions relatively firmly in place. In addition the librational ammonium motions are able to drag the neighbouring sulfate ions along with them causing the lattice to contract with temperature, giving rise to a region of negative thermal expansion. In the high temperature phase the ammonium ions sit on a new mirror-plane and are more loosely held in place, leading to lower vibrational frequencies that exert less influence over the shape and size of the lattice.

Our combined study suggests that, in the search for molecular materials with large entropy changes, vibrational entropy arising from broad, anharmonic energy minima is likely to be just as important as configurational entropy arising from crystallographic disorder.

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Session Classification: Session 1 : Materials Science 1

Contribution ID: 6

Type: **Oral**

Investigating the role of phonons in magnetic relaxation of molecular nanomagnets with inelastic neutron scattering

Monday, 12 September 2022 16:40 (35 minutes)

In the quest for quantum technologies, Molecular Magnetism is offering a variety of promising systems. Indeed, Molecular NanoMagnets (MNM)s can either be exploited as classical bits in high-density magnetic memories or as qubits for quantum information processing. One of the most important goals in the current research in this field is to reach a deep understanding of magnetic relaxation and decoherence in MNMs, being this aspect of paramount importance in the design of new systems acting as classical or quantum bits. Despite their crucial role in relaxation dynamics, very limited experimental investigations on phonons in MNMs were performed so far. This motivated a series of Inelastic Neutron Scattering (INS) experiments that we performed with the aim to measure, for the first time, phonon dispersions and density of states (DOS) in MNMs.

In an innovative and challenging experiment we exploited 4-dimensional INS to directly investigate phonon dispersions in a molecular qubit [1]. 4D-INS is a very powerful technique to study phonons, since it enables a direct and immediate access to phonon dispersions by measuring the four-dimensional scattering function in large portions of the reciprocal space. We detected both acoustic and optical branches along different symmetry directions and we compared the results with DFT calculations of phonon energies and polarisation vectors. Both these quantities are in fact necessary for a quantitative evaluation of spin-phonon coupling coefficients, which contain information on the main contributions to relaxation dynamics. We also exploited INS to measure the DOS of Dy-based SMMs with high-energy anisotropy barrier but very different relaxation dynamics. We then combined the so-obtained vibrational properties with relaxation measurements to test a new theoretical approach for the relaxation dynamics of SMMs, able to give more physical insight than phenomenological models, but not as demanding as fully ab-initio calculations.

The results of these studies provided new hints for the design of new and better-performing systems for quantum information processing applications. In particular, we highlighted the role of low-energy non-dispersive phonon modes, which undermine coherence times in molecular qubits due to acoustic-optical phonons anti-crossings and make Raman mechanisms more efficient in SMMs. Our latest results also involve the study of phonons with INS in applied hydrostatic pressure and the exploitation of complementary techniques like Inelastic X-ray Scattering.

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Session Classification: Session 1 : Materials Science 1

Contribution ID: 7

Type: **Poster**

Solid state NMR studies of ethylene/Ag-zeolites systems

Tuesday, 13 September 2022 18:00 (15 minutes)

Ethylene is an important raw material for the production of wide variety of polymers. However, this gas usually appears mixed with other components, as for instance ethane and purification to a single component is required. Nevertheless, the separation of these gases, which have similar properties, sizes and molecular structures is still challenging. In the case of ethylene, its separation using Ag-zeolites is possible due to the selective interaction between ethylene and silver located in zeolite structure (π -complexation). In fact, high stability of the π -complex prevents the participation of ethylene in aromatization reaction on Ag-containing zeolites at high temperatures. [1-3]

The aim of this work is the characterization of the silver species formed in chabazite zeolite (CHA), depending on the degree of hydration and after adsorption of ethylene.

CHA zeolite with a Si/Al =5 molar ratio was synthesized by hydrothermal method and then, Ag-CHA was prepared by ion exchange using a 0.3M AgNO₃ solution obtaining a silver content 11 wt%. Ethylene adsorbed on the sample degassed at 400°C during in an amount equivalent to one molecule of ethylene per unit cell.

UV-Vis analysis of as-prepared sample presents a main signal at 211 nm corresponding to dispersed Ag⁺, while the evacuated material shows signals at 283 and 317 nm indicating that most silver is forming clusters (Ag_m δ^+). One more signal is also noted at 404 nm, corresponding to metallic silver nanoparticles. The 109Ag solid state NMR spectrum shows a signal at 30 ppm in the as-prepared sample, assigned to Ag⁺. In contrast, the spectrum of dehydrated sample presents a peak at 5256 ppm, corresponding to Ag⁰. A priori the cationic silver signal is not observed, as indicated by UV-Vis, so the possibility of paramagnetic silver species is an idea to consider because the presence of these species may affect the relaxation time of the nucleus under study. After that, the presence of paramagnetic species is confirmed by Electron Paramagnetic Resonance (EPR) with high intensity signal with $g = 2.003$.

In addition, the ¹³C NMR spectrum recorded after the adsorption of ethylene shows a broad signal at 110 ppm, while ethylene gas appears at 120 ppm. In the case of ¹⁰⁹Ag NMR spectrum, a signal at 5284 ppm is observed. These changes in the chemical shift of signals at both ¹³C and ¹⁰⁹Ag NMR proves the ethylene-silver interaction.

In conclusion, the interaction between silver and ethylene is observable by solid-state NMR spectroscopy. The presence of paramagnetic silver clusters in the dehydrated sample is demonstrated by UV-Vis and EPR studies.

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Session Classification: Poster session

Contribution ID: 8

Type: **Oral**

Full Phonon Softening and Fast Ag Diffusive Dynamics in Liquid-like Argyrodites Ag₈GeSe₆

Wednesday, 14 September 2022 10:20 (25 minutes)

Argyrodites exhibit weak temperature dependence and low magnitude lattice thermal conductivity (κ_L) along with decent electrical performances at the high-temperature cubic superionic phase in the virtue of the partially occupied mobile Ag-sublattice interpenetrating a rigid network of (Si, Ge, Sn)₄ tetrahedra. However, the fundamental understanding of the interesting κ_L in terms of temporal-spatial lattice dynamics and atomic diffusion in the superionic phase of Argyrodites remains unexplored. Herein, we report the inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS) investigations of the lattice dynamics and atomic diffusion on Ag₈GeSe₆ complemented by synchrotron x-ray diffraction (SYXRD) and Ab initio molecular dynamics simulation (AIMD). We observe a full phonon softening and increasing QENS signal across the superionic phase transition temperature $T_c \sim 350$ K. We identify a fast Ag diffusion process with a short residence time (τ) of ~ 0.68 ps and reveal the Ag diffusion mechanism. The results emanated from this study will provide a coherent multi-scale understanding of the lattice dynamics and atomic diffusion mechanism, and enrich our knowledge of the heat conduction of Argyrodites.

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Session Classification: Session 4 : Batteries & ionic conductors

Contribution ID: 9

Type: **Oral**

Phonon Dispersions of Ca-doped BaTiO₃ Studied by Inelastic X-ray and Neutron Scatterings

Thursday, 15 September 2022 11:10 (25 minutes)

Recently, BaTiO₃(BT)-based compounds have received much attention as Pb-free piezo-electric materials. It has been reported that Ca-doping is effective in enhancing the piezo-electric performance of BT, which was confirmed in several compounds such as (Ba, Ca)(Zr, Ti)O₃, (Ba, Ca)(Sn, Ti)O₃, and (Ba, Ca)(Hf, Ti)O₃ [1]. Therefore, it is important to investigate the effect of Ca-doping on the atomic dynamics of BT in order to understand the origin of their high piezo-electricities at the atomic level.

In this study, we performed inelastic x-ray and neutron scattering (IXS and INS) experiments on (Ba,Ca)TiO₃ (BCT) to elucidate the effect of Ca-doping on the phonon dispersion of BT. The IXS and INS experiments were performed at BL35XU in SPring-8 and BL01 in J-PARC in Japan. Ba–O optical modes in BT and BCT were clearly observed by both IXS and INS experiment. Furthermore, Ti–O soft modes in these compounds were detected by INS, which is sensitive to lighter elements. In the presentation, effects of Ca-doping on these modes will be discussed in relation to the piezo-electricity.

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Session Classification: Session 6 : Material Science II

Contribution ID: 10

Type: Oral

Effects of orientational disorder on the dynamics of barocaloric adamantane

Monday, 12 September 2022 17:15 (25 minutes)

Weak van der Waals interactions that bind together organic molecules in the solid state lie at the heart of many highly relevant scientific problems, from soot formation in the atmosphere to polymorphism in pharmaceutical compounds. Nonetheless, the effects of these forces on the structure and (especially) dynamics of molecular materials are not yet fully understood.

Another application of van der Waals solids that has drawn recent attention is in environmentally-friendly solid-state cooling. These materials often undergo orientational order-disorder transitions with temperature and pressure, which can form the basis of a barocaloric cooling cycle. To optimise the cooling efficiency by crystal engineering, it is necessary to understand the atomic basis of these materials' functional behaviour.

Two recent developments – respectively in experiment and simulation – have finally allowed us to do this. Together, they provide an unrivalled insight into the atomic dynamics of these materials under working conditions. In this talk, I will highlight the impact of both these developments with the case study of adamantane, a paradigmatic close-packed van der Waals (or 'plastic') crystal.

First, the atomic dynamics under working conditions – that is, under pressures similar to those that would be needed in a working refrigerator – can now be studied in detail with neutron spectroscopy, due to the recent development of low-background, high-pressure gas cells. Pressure QENS and single-crystal INS experiments combine to provide a complete view of the pressure-induced phase transition in adamantane. Further insight can be drawn from calculation; however, the presence of disorder in adamantane's high-temperature phase complicates the calculation of vibrational modes. This brings us to the second development: a new theoretical framework for studying phonons in disordered systems, by mapping the vibrational modes of representative supercells onto the Brillouin zone of the disordered crystal. This reveals the disorder-induced broadening in different parts of the Brillouin zone, and a significant shift in the distribution of librational/translational modes between the two phases. Hence, combining experiment and modelling has allowed us to characterise in new detail the molecular dynamics of this orientationally disordered, barocaloric van der Waals material.

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Session Classification: Session 1 : Materials Science 1

Contribution ID: 11

Type: Oral

Dynamics of a Pt/Al₂O₃ catalyst in the presence of H₂: complementary results from INS, FT-IR and DFT

Tuesday, 13 September 2022 10:45 (25 minutes)

Supported platinum nanoparticles are largely employed in industrial hydrogenation processes thanks to their great catalytic activity which, in turn, derives from their ability to activate and split the H₂ molecules at the metal surface to form reactive hydride species. Albeit these systems were among the very first heterogeneous catalyst to be discovered and employed, many details about their behaviour under reaction conditions are still matter of debate and subject of extensive research effort.

The sample we have been focusing on is characterized by a very large dispersion of the Pt nanoparticles (1.4 ± 0.4 nm), which are supported on a high surface area transition alumina. The sample was prepared in the laboratories of the industrial company Chimet S.p.A. and subjected to an extensive characterization work, aimed to better understand its behaviour under hydrogenation conditions. Among the employed techniques, Inelastic Neutron Scattering (INS) spectroscopy had been fundamental, thanks to its great sensitivity towards the vibrational modes of all H-containing species. The INS spectra of the sample were measured under a high and low H₂-pressure on the IN1-Lagrange instrument at the ILL, resulting in significantly different spectral profiles [1]. The spectra were interpreted on the basis of an extensive DFT simulation work comprehensive of 26 different Pt_xHy/γAl₂O₃ models, performed in collaboration with IFPEN. The comparison clearly indicated that under high H₂-pressure conditions the Pt nanoparticles mostly reconstructed into cuboctahedric morphologies in weak interaction with the support, while the spectral profile collected at low H₂-pressure is compatible with less symmetric morphologies where the nanoparticle is in stronger interaction with the support. In the latter case, the spillover of some H onto the support and the following formation of surface -OH groups was also observed. Complementary information was obtained by means of FT-IR experiment performed in operando conditions, allowing to follow the evolution of the system upon the progressive decrease of the H₂ concentration. In this latter case, the spectral evolution clearly indicated the conversion of multi-folded Pt-H species into linear ones upon their removal [2]. Both these findings are in good agreement with previous AIMD simulations, predicting the reconstruction of Pt₁₃ nanoparticles supported on γ-Al₂O₃ as a function of the temperature and the H₂ equilibrium pressure [3].

Overall, this study provided important new complementary information on the dynamic behaviour of Pt/Al₂O₃ catalyst under hydrogenation reaction conditions, representing a new important step in the understanding of their real nature.

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Session Classification: Session 2 : Catalysis & Porous materials I

Contribution ID: 12

Type: Oral

Tuning magnetoelectricity in a mixed-anisotropy antiferromagnet

Monday, 12 September 2022 18:05 (25 minutes)

The ability to control magnetic and electric properties is attractive for tailoring materials for devices, data storage and sensor technology. In magnetoelectric materials, these two degrees of freedom are closely linked and this makes them particularly interesting [1]. Here we study one such system, $\text{LiNi}_{1-x}\text{Fe}_x\text{PO}_4$, using magnetometry, polarized neutron diffraction, pyrocurrent measurements and Monte Carlo simulations. The parent compounds of this mixed system, LiNiPO_4 and LiFePO_4 , possess mismatched magnetic anisotropies and we demonstrate that by random magnetic anisotropy mixing it is possible to tune the magnetic and magnetoelectric properties. Interestingly, the ordered moment in the ground state is rotated off the plane spanned by the easy axes of the parent compounds. Such behavior was previously theoretically predicted and our study provides the first clear experimental evidence for such phase. Most remarkably, as a consequence of the lower magnetic symmetry, additional magnetoelectric couplings are unlocked and enhanced in the system. Hence, our study shows that mixed-anisotropy magnetoelectric antiferromagnets represent a promising route with general applicability towards control of magnetoelectric properties, relying only on chemical randomness.

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Session Classification: Session 1 : Materials Science 1

Contribution ID: 13

Type: **Oral**

Hydrogen Storage and Dynamics in Clay materials

Wednesday, 14 September 2022 16:45 (25 minutes)

Hydrogen storage technologies play an important and crucial role in the so-called “hydrogen economy”. However, clay minerals have poorly been studied for this purpose, while they possess valuable properties (stability, low cost, green material) to be exploited in this domain.

We have recently studied H₂ adsorption on synthetic smectite, specifically laponite and its gel (before hydrothermal treatment) where nickel ions are inserted into the structure (Fig.1(a)). Obtained X-ray scattering (Fig. 1(b)), the local structure of the gel, noted gel-Ni-laponite, is shown to be similar to that of Ni-laponite, while long-distance order is significantly reduced. The adsorption isotherms (Fig.1(c)) reveal a higher sorption of gel than that of laponite.

Figure 1. Link: <https://ibb.co/DLg2F12>

Inelastic neutron scattering (INS) is extremely useful at probing locally the direct vicinity of adsorbed molecular H₂. The INS spectrum of a free H₂ molecule is characterized at low temperature by a sharp and well-defined rotational feature at an energy of 14.7 meV corresponding to the transition of H₂ from a para- (molecular spin $S = 0$, angular momentum $J = 0$) state to an ortho- ($S = 1$, $J = 1$) state. The para-to-ortho transition line J01 has a three-fold degeneracy which is lifted as a function of the local symmetry of the adsorption site, with

line-shifts that are dependent on the interaction between the H₂ molecule and the host surface. We will present here the results obtained on the gel precursor using the spectrometer PANTHER at the ILL (fig. 1(d)). At 41K, well above the solidification temperature of bulk H₂, the J01 peak exhibits a fine structure which can be fitted by two gaussian lines with an intensity ratio of 2:1 (low energy component: high energy component, fig. 1(d)). The splitting is in line with 1D hindering (H₂ axis lying parallel to a surface). Upon further cooling, other lines appear until bulk-like hydrogen signal becomes progressively visible.

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Session Classification: Session 5 : Catalysis & Poursous materials II

Contribution ID: 14

Type: **not specified**

Clay sediments, a multiscale playground for hydrate formation.

Wednesday, 14 September 2022 17:35 (25 minutes)

Gas hydrates are crystalline structures consisting of cages resulting from the hydrogen bonding of water molecules (host) enclosing relatively small gas molecules (guest), such as hydrogen, methane and other small hydrocarbons [1]. Gas hydrates occur naturally on continental margins and in the permafrost region where the pressure and temperature conditions are favorable for hydrate formation and stability [2,3]. Methane hydrates represent the largest natural reservoir of methane on Earth (with estimates ranging between 600-10000 GT). However, large uncertainties remain about the amount of methane trapped and the mechanisms governing methane fate, limiting conclusions about climate implications [4,5]. The Romanian sector of Black Sea is known to host a large amount of hydrates, and samples have been collected at around 700m water depth (70bars), where the seafloor temperature is close to 282K. Furthermore, the scientific cruises Ghass (2015) and Ghass2 (2021) conducted by Ifremer, revealed that the hydrates are formed in a clay-rich sediment. In the context of the study of the Black Sea hydrate deposit, the influence of the complex clay/sand matrix on the methane hydrate formation is studied using Raman spectroscopy, Inelastic Neutron Scattering and Neutron diffraction. Methane hydrate structural properties, spatial distribution in sediments and formation kinetics are investigated in presence of both natural and synthetic sedimentary environment and NaCl. These physical-chemistry results provide new insights on the formation mechanism, including original findings on the impact of clay structure and salinity on hydrate kinetics with investigations ranging from minutes to several months.

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Session Classification: Session 5 : Catalysis & Poursous materials II

Contribution ID: 15

Type: **Oral**

Dynamics in Confinement: a study of CH₄@C₆₀

Tuesday, 13 September 2022 14:00 (30 minutes)

Endofullerenes are substances in which small molecules or atoms are encapsulated in highly symmetrical cages of carbon atoms. Each encapsulated atom or molecule behaves as a textbook example of a quantized particle-in-a-box. The newest and largest member of the endofullerene family tree, namely CH₄@C₆₀, is the first organic molecule trapped inside the cage and the main interest of this abstract. The use of various spectrometers at ILL, namely PANTHER, IN5 and IN1-LAGRANGE, have allowed us to probe a large energy window up from 1 to 100 meV. The goal from these experiments was to probe the rotational and translational states of the confined CH₄ molecule, and observe the coupling between said states due to the confinement. A novel result that we have observed in this endofullerene, was the effect of the I_h symmetry of the C₆₀ on the rotational states of the CH₄ using inelastic neutron scattering, an effect that was absent in previous endofullerene studies. We have also performed QENS measurements, using PANTHER, that have allowed us to observe slight differences in the rotational dynamics of both the C₆₀ and CH₄, confirming the stronger guest-host coupling that we observed in our INS measurements.

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Presenter: AOUANE, Mohamed

Session Classification: Session 3 : Simulation session

Contribution ID: 16

Type: **Oral**

A Combined Experimental and Computational Study of Oxide Ion Conductors

Wednesday, 14 September 2022 12:35 (25 minutes)

Solid oxide ion conductors are remarkable materials with significant market potential due to their importance in technological applications like oxygen sensors, fuel cells and separation membranes. A crucial factor for advancement of their applicability is the development of new oxide ion conductors with higher conductivities at lower temperatures. Detailed knowledge of the structural characteristics, resulting conduction pathways and dynamics in these materials is a key requirement for improving their properties. Quasi-elastic neutron scattering is an excellent method for studying solid state diffusion and allows the observation of oxygen dynamics on a microscopic timescale. Combined with ab-initio molecular dynamics simulations, it can provide a comprehensive insight into diffusion processes on the atomic scale. We used this combined approach to investigate and compare the different oxide ion dynamics in two isostructural materials: $\text{Bi}_{0.852}\text{V}_{0.148}\text{O}_{1.648}$ and $\text{Bi}_{0.852}\text{P}_{0.148}\text{O}_{1.648}$, and account for the superior performance of the vanadate. Using the backscattering spectrometer IN16b and the time-of-flight spectrometer IN5 at the ILL allowed direct observation of dynamics on the nanosecond and picosecond timescales, and analysis in conjunction with molecular dynamics simulations allowed us to elucidate the nature of the observed dynamics as well as the structural characteristics important for oxide ion conduction in these doped bismuth oxides.

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Presenter: SCHWAIGHOFER, Bettina

Session Classification: Session 4 : Batteries & ionic conductors

Contribution ID: 17

Type: **Oral**

From molecular dynamics simulations to diffuse scattering maps

Thursday, 15 September 2022 11:35 (25 minutes)

Modern materials often exhibit a considerable portion of structural disorder, playing a key role in their functionalities. In order to characterise local atomic arrangements and short-range correlations one has to study the shape of Bragg lines and the distribution of diffuse scattering below and between them.

To extract information from experimental data one has to compare model-based intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism. Alternatively, one may retrieve the displacement pattern without making assumptions on its origin by reverse Monte-Carlo (RMC) modelling

With this progress in place the bottleneck has shifted from producing supercell models to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue being the fact that scattering amplitudes from a distorted lattice cannot be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor $\exp(-i\mathbf{Q}\mathbf{R})$ being \mathbf{Q} -dependent. As a consequence, many efforts in recent years have been restricted to simple models on small supercells [1,2] or to more involved pair distribution function (PDF) analysis [3-5], where the summation problem is reduced to a single dimension.

To address this issue, we will present the results of a new approach [6], based on recent developments of the non-uniform fast Fourier transform algorithm [7], implemented in the MP_tools program suite [8]. Diffracted intensities from model supercells containing millions of atoms as well as dynamic scattering functions $S(\mathbf{Q},\omega)$ based on time sequences of thousands of frames can be addressed in an interactive manner.

Many motivating discussions with my colleagues Marek Pasciak, Petr Ondrejčovic and Jirka Hlinka from the Institute of Physics (AS CR) are kindly acknowledged.

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Presenter: KULDA, Jiri

Session Classification: Session 6 : Material Science II

Contribution ID: 19

Type: **Oral**

Hydrogen mobility and reactivity in MoS₂ catalyst

Tuesday, 13 September 2022 11:35 (25 minutes)

Catalyst materials are an essential component in hydrogen production and for the operation of fuel cells. Today, however, they are mostly based on platinum, which is expensive and rare. Molybdenum sulfide, MoS₂, which is more abundant and significantly cheaper, has shown interesting catalytic activity and has been a focus point of research in recent years [2]. MoS₂ is a van-der-Waals bonded 2d material that, theoretically, provides a high density of active sites, but little is known about the mobility and the reaction steps of hydrogen and water in MoS₂.

In this presentation we will discuss our recent studies on hydrogen mobility and reactivity in MoS₂ [1]. To shed light on the possible pathways for improving the performance of MoS₂ and other layered catalyst materials, we have studied the diffusion of hydrogen and water by means of neutron scattering and X-ray photoelectron spectroscopy combined with nuclear reaction analysis and molecular dynamics simulations.

We observed a very fast hydrogen diffusion parallel to the basal planes and a very slow diffusion perpendicular to the MoS₂ basal planes. Water, on the other hand, cannot penetrate the perfect crystal, but can intercalate within volume defects, where it can access edge sites of the material. MD simulations were essential for the identification of the contributions of the different hydrogen species (H(+), H₂, H₂O) to the chemistry in MoS₂.

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Presenter: FOUQUET, Peter

Session Classification: Session 2 : Catalysis & Porous materials I

Contribution ID: 20

Type: Oral

Diffusion mechanisms in sodium-ion battery materials using polarized neutrons

Wednesday, 14 September 2022 09:45 (35 minutes)

The demand for energy storage is expected to increase dramatically due to the introduction of electric vehicles and the need for load levelling in the wind, tidal and solar renewables industries. The scarcity of lithium together with issues over supply from remote or politically sensitive areas, has led to concerns over cost. Sodium-ion batteries are a particularly attractive alternative for current lithium-ion battery manufacturers, since they are a drop-in replacement. $\text{Na}_x\text{Fe}_{1/2}\text{Mn}_{1/2}\text{O}_2$ has been identified as a potential cathode material for sodium-ion batteries since it has comparable electrochemical performance to commercially available lithium-ion cathodes and it is composed entirely of abundant elements. We have studied the diffusion mechanisms of $\text{Na}_x\text{Fe}_{1/2}\text{Mn}_{1/2}\text{O}_2$ for $x=1$ and $2/3$ using quasi-elastic neutron scattering (QENS) using the ThALES spectrometer with XYZ polarization analysis. In order to perform quantitative modelling of the QENS data we show that it is necessary to isolate the spin incoherent cross section from the spin-independent nuclear and magnetic cross sections. For $x = 1$ it has the same crystal structure as $\text{O}_3\text{-Li}_x\text{CoO}_2$, whereas for $x = 2/3$ it has the P2- Na_xCoO_2 structure. In both cases the planes of sodium ions are sandwiched between oxygen planes, but the difference in the stacking sequence of hexagonal planes leads to very different diffusion mechanisms. We find that the P2 material is a promising cathode material with high rate capability.

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Session Classification: Session 4 : Batteries & ionic conductors

Contribution ID: 21

Type: Oral

Local structure and dynamics of tungsten oxide-based glasses: insights from concurrent neutron diffraction and Compton scattering

Thursday, 15 September 2022 09:45 (25 minutes)

In this work, following our previous work on molybdate glasses, we employ a combination of neutron diffraction and neutron Compton scattering, augmented by ab initio harmonic lattice dynamics and Reverse Monte Carlo modelling to characterise the force-constant disorder in the tungsten oxidebased glasses. Specifically, we discuss the correlations between the average interatomic force constant magnitudes inferred from neutron Compton scattering and the glass formation ability, measured in terms of the value of the glass transition temperature, as well as the average bond-lengths and interatomic distances obtained from diffraction data analysis. Moreover, we provide a comparative analysis of the widths of force-constant distributions of individual atomic species in glasses and their precursor metal oxides based on the distributions of the widths of nuclear momentum distributions. Furthermore, we assess the degree of softening of atom-projected vibrational densities of states induced by the force-constant disorder in the glasses

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Presenter: Dr MATTHEW, Krzystyniak (Rutherford Appleton Laboratory)

Session Classification: Session 6 : Material Science II

Contribution ID: 22

Type: **Poster**

First results from the wide angle spin echo spectrometer WASP

Tuesday, 13 September 2022 18:15 (15 minutes)

The first neutron spin echo (NSE) instrument IN11 was in user operation for 40 years at ILL. The newest spin echo instrument WASP took the relay and just had its first full year of user operation. We will use this occasion to review how the design of the wide angle NSE spectrometers has developed over the years. Apart from WASP, most functioning NSE spectrometers use the basic IN11A design where the precession field is generated by long solenoids along the neutron beam. This construction dramatically limits the angular detector coverage and count rate of the instruments. Last century there have been two attempts to make a wide-angle coverage neutron spin echo instrument: IN11C at ILL was equipped with a flattened solenoid downstream of the sample and was in use until recently. It had a 30 degree-wide angular coverage at the cost of reduced resolution. This instrument was practically trading intensity for resolution. The SPAN instrument [1] at HZB used a pair of coils in the anti-Helmholtz configuration creating an azimuthally symmetric magnetic field, which, in theory, could allow a nearly 360 deg. detector coverage. WASP uses an improved SPAN construction, and it provides a 500 times higher detected intensity than IN11A, while the resolution remains the same.

The long construction has finished in 2018, and the instrument has seen 4 full cycles of user operation. We will present the characteristics of the spectrometer and the first published scientific results on collective dynamics of glass formers [2] and the dynamics of confined ionic liquids [3].

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Session Classification: Poster session

Contribution ID: 23

Type: **not specified**

Probing the binding mechanism of toxic gases in Hofmann-clathrates: a combined neutron scattering and DFT study

Wednesday, 14 September 2022 17:10 (25 minutes)

We report a joint experimental and computational characterization of the adsorption process of toxic gases, such as CO, CO₂ and SO₂ in Hofmann-type clathrates with formula $\{\text{Fe}(\text{pz})[\text{MII}(\text{CN})_4]\}$ (M = metal, pz = pyrazine). These metal-organic frameworks have a 2D layered structure where Fe centers are connected through cyanide ligands to an open-metal site MII, typically Pd, Pt or Ni, offering a binding site with a potentially strong affinity for the gas molecules with potential application for gas capture and sensing.

Neutron characterization techniques combined with density functional theory (DFT) calculations have allowed us to understand the binding mechanism at the open-metal site. The high hydrogen content in these samples makes neutron techniques well suited for this study. The changes in the inelastic neutron scattering (INS) spectra upon gas adsorption, interpreted upon comparison with the normal modes of vibrations from DFT calculations, provide us with a clear signature of the binding mechanism between the MOF and the gas molecules. Our work shows that the adsorption process can be fully characterized by using neutron techniques by combining information of the binding configuration, as characterized by neutron diffraction, and the spectral changes specific of each molecule measured by INS.

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Session Classification: Session 5 : Catalysis & Porous materials II

Contribution ID: 24

Type: **Poster**

Ion dynamics in soft electrolytes for fuel cells and batteries

Tuesday, 13 September 2022 17:30 (15 minutes)

Energy conversion and storage devices as fuel cells or lithium-ion batteries contain an electrolyte to transport ions from the negative to the positive electrode. This electrolyte can be a salt-containing liquid as in state-of-the-art Li-ion batteries, a polymer as in proton exchange membrane fuel cells and solid-state batteries, or inorganic conductors as oxides or glass ceramics. In all cases, understanding the relation between elementary diffusion mechanisms, as well as their dependence on solvent content, molecular architecture, structure, temperature, materials fabrication process and integration into real systems, is key and requires characterization of the ion dynamics at multiple scales. Typically, the performance of an electrolyte is determined in terms of macroscopic ion conductivity, but microscopic-scale information is needed to establish the driving forces and limiting factors, in view of optimizing materials design. In this talk we will show examples of multi-resolution QENS studies performed on different types of soft electrolytes (ionomers, membranes, ionic liquids) to identify the nature of motions as well as their characteristics (relaxation times, diffusion coefficients, jump distances, activation energies). We will also highlight the need for complementary tools e.g. NMR and molecular dynamics simulation to provide a mechanistic understanding of the interplay between ion conduction and the matrix / polymer / solvent motions, and provide the full multi-scale picture of ion dynamics in complex soft ionic systems.

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Session Classification: Poster session

Contribution ID: 25

Type: **Oral**

Nanoconfining H₂ - manipulation of the phase diagram and consequences of reduced freedom

Wednesday, 14 September 2022 15:35 (35 minutes)

Condensed phases of molecular hydrogen (H₂) are highly desired for clean energy applications ranging from hydrogen storage to nuclear fusion and superconductive energy storage. However, in bulk hydrogen, such dense phases typically only form at exceedingly low temperatures or extremely high (typically hundreds of GPa) pressures, reducing accessibility of application.

Formation of solid-like H₂ at atmospheric pressure at temperatures above the critical point has been indicated in when H₂ is confined in nanoscale pores of carbon nanomaterials indicating an alternative route to access condensed phases at more accessible pressures and temperatures.^{1–3} To understand the potential of nanoconfinement for manipulation of the hydrogen phase diagram, we explore which H₂ solids form and why when confined inside carbonaceous nanoscale pores, and investigating pore size and geometry effects.

Using a powerful combination of variable temperature and variable pressure inelastic neutron scattering and neutron diffraction we study the rotational dynamics, distribution and arrangement and structure of nanoconfined H₂.^{4,5}

Our results lead us to a general strategy for further manipulation of the H₂ phase diagram via nanoconfinement effects, and for tuning of anisotropic potential through control of confining material composition and pore size.

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Session Classification: Session 5 : Catalysis & Porous materials II

Contribution ID: 26

Type: **Oral**

Thermal conductivity and lattice dynamics in structurally complex materials

Thursday, 15 September 2022 09:00 (45 minutes)

The lattice thermal conductivity of many different materials is displaying a ‘glass like behavior’ [1], with a relatively small value of the lattice thermal conductivity at ambient temperature and an almost independent temperature dependence in the range 20 to 300 K. This is the case for disordered crystals [1], for clathrates [2], but also for aperiodic crystals [3] such as the icosahedral quasicrystal $i\text{-AlPdMn}$ [4], and the Rb_2ZnCl_4 phase that displays an incommensurately modulated phase between 190 and 300 K [5]. The detailed understanding of this behavior and the relationship between the phonon spectrum/phonon lifetime and the thermal conductivity is still a matter of debate.

In this presentation I will review some recent results and show how atomic scale simulations of phonon dispersion and phonon lifetime can reproduce the observed experimental data. The structural complexity might be characterized by two main parameters: the long-range order and number of atoms in the unit cell (up to infinity for aperiodic crystals) [6] and the disorder and short range order. The influence of these two parameters will be discussed [7].

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Session Classification: Session 6 : Material Science II

Contribution ID: 27

Type: **Oral**

Solid state NMR spectroscopy: a tool for the investigation of zeolites as catalysts and adsorbents

Wednesday, 14 September 2022 15:00 (35 minutes)

Solid state nuclear magnetic resonance spectroscopy (ss-NMR) is a very powerful technique for the investigation of all kind of solid materials, including pharmaceuticals, soils, organics, polymers, cements, ceramics or batteries among others. NMR spectroscopy provides evidence at an atomic level on the local environment of the nuclei difficult to obtain by other techniques.

Ss-NMR has been largely used in the investigation of zeolites, which are crystalline microporous silicate or aluminosilicate-based materials with a three-dimensional structure with channels and cavities of molecular dimensions. The unique properties of zeolites are responsible of their application as catalysts in petrochemical and chemical industry and as adsorbents in separation processes. Relevant information on zeolites and their applications that can be obtained by ss NMR will be illustrated here with three case studies:

1.- Structural characterization of RTH type zeolite provides very valuable information for the elucidation of the 3D structure. Zeolites are synthesized using organic molecules as structure directing agents (OSDA) and very often in fluoride medium. The information obtained by combining ^{19}F , ^{13}C and ^{29}Si NMR spectroscopy is essential to determine the structure and the distribution of the atoms in the solid. Moreover, application of 2D ^1H NMR pulse sequences will be used to determine the number of silanol groups involved in structural defects.

2.- The investigation on the mechanism of the Beckmann rearrangement reaction of oximes into amides on zeolite catalysts. The use of ^{15}N -ss NMR in combination with DFT calculation allowed to establish that the reaction intermediates formed is different on zeolites containing Brønsted acid sites or silanol defect groups.

3.- Pulse field gradient (PFG) NMR spectroscopy is used to obtain information on the diffusion of small hydrocarbon molecules within the zeolites pores as this process plays a key role on their applications in gas separation and catalysis. This technique has been allowed to stablish that the diffusion of alkene (ethene, propene) molecules within the pores of the microporous silico-aluminophosphate SAPO-34 is promoted by the presence of Brønsted acid sites, while these sites have no influence on the transport of alkanes.

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Session Classification: Session 5 : Catalysis & Poursous materials II

Contribution ID: 28

Type: **Oral**

Dynamics in functional oxide ion conductors studied with INS and QENS

Wednesday, 14 September 2022 11:15 (45 minutes)

Over the past two decades, the study of solid oxide electrolytes and their usage in various technological applications, such as batteries, chemical sensors, and fuel cells has developed into an extremely important field within materials science research. This development is driven by the need for cleaner and more sustainable sources of energy, which is one of the grand challenges in the 21st century. However, a too low ionic conductivity, and/or a too low chemical stability under operating conditions, of present-day oxide electrolytes often limit their wider use. The development of new, more highly ion conducting oxides is hence critical to future breakthroughs. This requires an increased understanding of the underlying mechanisms of ionic conduction, and in this regard inelastic and quasielastic neutron scattering (INS and QENS, respectively) play an important role. In this contribution, I will summarize recent progresses in relation to the structural and dynamical study of solid oxide ion conductors, using INS and QENS, as well as to discuss challenges and opportunities within this field of research. A special focus will be given on proton conducting perovskite type oxides, because of their high promise for application in technological devices, as well as the emerging class of solid oxide electrolytes based on oxide-hydrides.

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Presenter: KARLSSON, Maths (Chalmers University of Technology)

Session Classification: Session 4 : Batteries & ionic conductors

Contribution ID: 29

Type: **not specified**

Cation Dynamics as a Probe of Local Structure in 3D Hybrid Perovskites: Insights from High-resolution Inelastic Neutron Scattering

Thursday, 15 September 2022 10:45 (25 minutes)

Organometal Halide Perovskites (OHPs) have emerged as a prospective class of materials holding great promises for efficient conversion of solar energy. While understanding their atomic structure and dynamics is critical to rationalize their exceptional photovoltaic performance and improve their environmental and operational stability, this task remains a formidable challenge for both crystallography and spectroscopy.[1-5] In this contribution, we present a novel, complementary strategy developed to explore the local structure around the organic cations, owing to the superb sensitivity of Inelastic Neutron Scattering (INS) to hydrogen motions.[6,7] We also provide an overview of the application of the developed methodology combining broadband high-resolution INS experiments (TOSCA, ISIS; LAGRANGE, ILL) with state-of-the-art ab initio modelling beyond the harmonic picture (AIMD), to interrogate local structure in the archetypal iodoplumbate-OHP, MAPI, across its pressure-temperature phase diagram and under chemical pressure induced by cation engineering.

1 Ferreira *et al.*, Commun. Phys., 2020, 3:48

[2] Druzicki *et al.*, Polymers, 2021, 13(9), 1440

[3] Breternitz *et al.*, Angew. Chem. Int. Ed., 2020, 59, 424

[4] Wiedemann *et al.*, J. Phys. Chem. Lett. 2021, 12, 2358

[5] Kubicki *et al.*, Nat. Rev. Chem., 2021, 5, 624

[6] Druzicki *et al.*, J. Phys. Chem. Lett., 2016, 7, 4701

[7] Druzicki *et al.*, J. Phys. Chem. Lett., 2021, 12, 3503

Primary author: Dr DRUZBICKI, Kacper (Materials Physics Center, CSIC-UPV/EHU)

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Session Classification: Session 6 : Material Science II

Contribution ID: 30

Type: **Oral**

Ion dynamics in solid electrolytes for batteries

Wednesday, 14 September 2022 09:00 (45 minutes)

Fast ion-conductors, especially those conductive for lithium and sodium cations, have been the subject of intense (re)investigation lately in the context of electrochemical applications, most notably as solid electrolytes in all-solid-state-batteries. In that context, ions need to travel macroscopically (i.e. in the μm -mm scale) between electrodes to charge and discharge the cell. As such, the main functional property of interest in solid electrolyte materials is macroscopic ionic diffusivity/conductivity, but application to next-generation batteries also imposes a host of other requirements, namely, processability, (electro)chemical- and mechanical stability during operation etc.

In this talk, recent advancements in the fundamental understanding of ion-conduction in solid electrolytes will be elaborated, using topical example materials such as the thiophosphates Na_3PS_4 and Li_3PS_4 . The use of multiple complementary spectroscopic probes (neutron-, NMR-, Raman-, impedance- spectroscopies) along with atomistic simulation techniques (molecular dynamics, nudged elastic band) is paramount to obtaining a complete multiscale picture of solid-state ionics, and thus allow for further advancements.

Key outstanding questions will be posed for discussion such as a) the role of harmonic vs. unharmonic dynamics in predicting, understanding and tuning ionic conductivity in solids and b) the interplay between host anion (lattice) dynamics and mobile cation mobility/diffusivity.

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Presenter: FAMPRIKIS, Theodosios

Session Classification: Session 4 : Batteries & ionic conductors

Contribution ID: 31

Type: **Poster**

Proton Dynamics in Potassium Dihydrogen Phosphate (KDP) at Pressures up to 2.5 GPa by Inelastic Neutron Scattering

Tuesday, 13 September 2022 18:30 (15 minutes)

In the crystal structure of KDP (KH_2PO_4) the phosphate tetrahedra are linked together by a net of O-H-O hydrogen bonds. At ambient pressure and temperature protons are disordered in a two-minimum potential along the bonds. At a temperature of 123 K a ferroelectric phase transition takes place related to the locking of protons in one of these two energy minima. We used inelastic neutron scattering to follow pressure and temperature variation of bond-stretching and bond-bending vibrations of hydrogen. A compact high-pressure cell of a generic “piston-cylinder” type has been designed in order to make use of a special scattering geometry of the neutron spectrometer IN1-Lagrange at ILL with large solid angle open for scattered neutrons. The most informative energy range for hydrogen bond vibrations stays above the vibration range of the cell materials what makes the consequences of trade-off on sample volume and attainable pressure experimentally less penalising. The proton vibration spectra in KDP up to quasi-hydrostatic pressures of 25 kbar and temperatures around the phase transition have been recorded and analysed in the model of double-well interatomic potential with varied oxygen-hydrogen distance.

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Presenter: Dr IVANOV, Alexandre (Institut Laue-Langevin)

Session Classification: Poster session

Contribution ID: 32

Type: **Oral**

Photon-in/photon-out spectroscopy in materials science

Tuesday, 13 September 2022 09:45 (35 minutes)

Instruments for photon-in/photon-out spectroscopy have become available on many X-ray absorption spectroscopy beamlines at synchrotron radiation sources. This makes the technique visible and accessible to many researchers in the materials science community. In particular, in situ and operando studies in catalysis and research related to energy storage greatly benefit from the larger information content when X-ray emission spectroscopy (XES) is added to X-ray absorption spectroscopy. Beamline ID26 at the ESRF features XES instruments for the hard and tender X-ray range. Their design maximizes detection efficiency for low analyte concentrations and time-resolved studies. In situ cells for tender X-rays must be inserted into the vacuum of the spectrometer chamber and windows have to be adapted to the short penetration depth of the tender X-rays. I will present the tender X-ray spectrometer and some examples for the application of photon-in/photon-out spectroscopy in materials science. I will furthermore discuss a new protocol for time-resolved and imaging studies using X-ray emission spectroscopy.

1 J. Synchrotron Rad. (2021) 28 362 - 371

[2] J. Synchrotron Rad. (2020) 27 813 - 826

[3] Inorg. Chem. (2022) 61 869 -881

[4] Nanoscale, 2020 12 16270 - 16284

[5] Inorg. Chem. (2020) 59 12518 - 12535

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Presenter: GLATZEL, Pieter (ESRF)

Session Classification: Session 2 : Catalysis & Porous materials I

Contribution ID: 33

Type: **Oral**

Ionic Liquids: bulk vs 1D CNT confinement. Towards better batteries?

Wednesday, 14 September 2022 12:00 (35 minutes)

composite polymer membranes made out of vertically aligned carbon nanotube (CNT) forests. As this system shows no tortuosity and no friction at the electrolyte / CNT interface, the transport properties within the pore system (the interior of the CNTs) are expected to be tremendously enhanced. We actually have recently shown¹ that, compared to the bulk situation, such 1D CNT nanometric confinement induces a conductivity gain of the electrolyte as high as 50. We interpret this result as a possible revelation of a superlubricity phenomenon under confinement². Such 1D CNT membrane making possible an ultra-fast travel of the ions in between the electrodes of a battery separator is an appealing route to boost the power density of batteries (Fig. 1). A patent has been filed³.

In this framework, a thorough multiscale characterization of the confined electrolyte is essential. The competition between electrostatic and van der Waals interactions leads to a property original for pure ILs: they self-organize in fluctuating nanometric aggregates. So far, this transient structuration has escaped direct clear-cut experimental assessment. In bulk, we have taken advantage of the alliance of QENS (Tof and NSE), PFG-NMR and particle-probe rheology to i) catch this phenomenon and ii) highlight an unexpected consequence: a one order of magnitude difference of the transport quantities, depending whether they are inferred at the molecular or at the micrometric scale⁴. Along with electrochemical impedance spectroscopy data, we will also show Tof and PFG-NMR measurements of the same IL confined in the CNT membranes.

1. Berrod, Q. et al. Ionic liquids confined in 1D CNT membranes: gigantic ionic conductivity. ArXiv171006020 Cond-Mat (2017).
2. Heiranian, M. & Aluru, N. R. Nanofluidic Transport Theory with Enhancement Factors Approaching One. *Acs Nano* 14, 272–281 (2020).
3. Berrod, Q., Ferdeghini, F., Judeinstein, P. & Zanotti, J.-M. Nanocomposite membranes for electrochemical devices. Patent WO 2016151142 A1. (2016).
4. Berrod, Q. et al. Ionic Liquids: evidence of the viscosity scale-dependence. *Sci. Rep.* 7, (2017).

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Session Classification: Session 4 : Batteries & ionic conductors