QENS/WINS2018

Program

Sunday, 15 July 2018,

Registration: 15:00 – 18:00; Senate Room, 19/F, Lau Ming Wai Academic Building

Welcome Reception: 18:00 – 19:00; Senate Room

Monday, 16 July 2018, Senate Room

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
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<tbody>
<tr>
<td>8:20</td>
<td>Opening</td>
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<tr>
<td>8:30</td>
<td>Plenary Chair: Victoria García Sakai</td>
<td>Mark R. Johnson</td>
<td>QENS – Experiment, simulation and application</td>
<td>P_01</td>
</tr>
<tr>
<td>9:10</td>
<td>5 minutes break</td>
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<tr>
<td>9:15</td>
<td>Proteins Chair: Xiangqiang Chu</td>
<td>Tilo Seydel</td>
<td>Dynamics of proteins in aqueous solutions - recent advances using high-resolution spectroscopy</td>
<td>QK_02</td>
</tr>
<tr>
<td>9:45</td>
<td>Liang Hong</td>
<td>Gradual cross-over from sub-diffusion to normal-diffusion: a many-body effect in protein surface water</td>
<td>QI_04</td>
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<tr>
<td>10:05</td>
<td>Coffee</td>
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<tr>
<td>10:20</td>
<td>Biomacromolecules and Membranes</td>
<td>Xiangqiang Chu</td>
<td>Dynamics of Biopolymers under Confinement and Extreme Conditions Studied by QENS</td>
<td>QK_11</td>
</tr>
<tr>
<td>10:50</td>
<td>5 minutes break</td>
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<tr>
<td>10:55</td>
<td>Ralf Biehl</td>
<td>Influence of PEGylation on protein dynamics</td>
<td>QI_15</td>
<td></td>
</tr>
<tr>
<td>11:15</td>
<td>Alexei Sokolov</td>
<td>General Picture of Protein Dynamics: Combining Neutron Scattering with Dielectric and MD-Simulations Studies</td>
<td>QI_10</td>
<td></td>
</tr>
<tr>
<td>11:35</td>
<td>Michihiro Nagao</td>
<td>Towards understanding lipid membrane transport properties using quasi-elastic neutron scattering techniques</td>
<td>QI_17</td>
<td></td>
</tr>
<tr>
<td>11:55</td>
<td>Vereendra Sharma</td>
<td>Dynamical Transitions and Diffusion Mechanism in the Lipid Bilayer</td>
<td>QI_11</td>
<td></td>
</tr>
<tr>
<td>12:15</td>
<td>R. Mukhopadhyay</td>
<td>Dynamical landscape in bio-mimetic membrane systems: Neutron scattering and MD simulation studies</td>
<td>QN_15</td>
<td></td>
</tr>
<tr>
<td>12:30</td>
<td>Lunch</td>
<td></td>
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<tr>
<td>14:00</td>
<td>Biology, Medicine and Water</td>
<td>Eugene Mamontov</td>
<td>QENS studies of living multicellular organisms</td>
<td>QK_01</td>
</tr>
<tr>
<td>14:30</td>
<td>Heloisa Bordallo</td>
<td>Nano-scale mobility of cellular water can discriminate cancer development or recession</td>
<td>QK_04</td>
<td></td>
</tr>
<tr>
<td>15:00</td>
<td>Osamu Yamamuro</td>
<td>Dynamics of Water-in-Salt and Water-in-Bisalt Electrolytes</td>
<td>QI_23</td>
<td></td>
</tr>
<tr>
<td>15:20</td>
<td>Marcella C. Berg</td>
<td>Nanoscale mobility in dental restorative cements</td>
<td>QN_09</td>
<td></td>
</tr>
</tbody>
</table>
### Neutron Facilities in China

**Chair:** Xun-Li Wang  
**Tuesday, 17 July 2018, Room 6207, 6/F, Lau Ming Wai Academic Building**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
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</thead>
<tbody>
<tr>
<td>16:00</td>
<td>Heshen Chen</td>
<td>Status of the China Spallation Neutron Source</td>
<td>WK_10</td>
</tr>
<tr>
<td>16:30</td>
<td>Jian Gong</td>
<td>The Progress of CMRR Neutron Scattering</td>
<td>WI_08</td>
</tr>
<tr>
<td>16:50</td>
<td>Yuntao Liu</td>
<td>Current status of neutron scatterings at CARR</td>
<td>WI_26</td>
</tr>
<tr>
<td>17:10</td>
<td><strong>Posters &amp; Discussions, Drinks</strong></td>
<td></td>
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</tr>
</tbody>
</table>

Note: P_## - Plenary talk (40 minutes); QK_## - QENS Keynote talk (30 minutes); QI_## - QENS Invited talk; (20 minutes); QN_## - QENS normal talk (15 minutes).

Note: WK_## - WINS Keynote talk (30 minutes); WI_## - WINS Invited talk (20 minutes); WN_## - WINS normal talk (15 minutes).

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### Confinement and Ionic Liquids

**Chair:** Jan Peter Embs / Jean-Marc Zanotti  
**Tuesday, 17 July 2018, Room 6207, 6/F, Lau Ming Wai Academic Building**

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<tr>
<th>Time</th>
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</thead>
<tbody>
<tr>
<td>10:55</td>
<td>Jean-Marc Zanotti</td>
<td>Ionic liquids in bulk and under 1D nanometric confinement:</td>
<td>QI_14</td>
</tr>
<tr>
<td>11:15</td>
<td>Jan Peter Embs</td>
<td>Structure, Dynamics and Magnetism in Ionic Liquids</td>
<td>QI_13</td>
</tr>
<tr>
<td>11:35</td>
<td>Osamu Yamamuro</td>
<td>Dynamics of ions in alkylammonium-based ionic liquids with plastic-crystalline phases</td>
<td>QN_05</td>
</tr>
<tr>
<td>11:50</td>
<td>Lucile Mangin-Thro</td>
<td>Separation of coherent and incoherent scattering with polarization analysis on D7 at the Institut Laue-Langevin</td>
<td>QN_06</td>
</tr>
<tr>
<td>12:05</td>
<td>Juan F. Mora Cardozo</td>
<td>H-Bonding influence on the dynamics of imidazolium-based ionic liquids as probed by QENS</td>
<td>QN_11</td>
</tr>
<tr>
<td>12:20</td>
<td><strong>END</strong></td>
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<tr>
<td>12:30</td>
<td><strong>Lunch</strong></td>
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### Industry Materials

**Chair:** Alexander O’Malley / Margarita Russina  
**Tuesday, 17 July 2018, Room 6207, 6/F, Lau Ming Wai Academic Building**

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<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
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</thead>
<tbody>
<tr>
<td>14:00</td>
<td>Margarita Russina</td>
<td>Molecular transport in porous materials and adsorption induced phenomena observed through the lens of neutron spectroscopy</td>
<td>QK_10</td>
</tr>
<tr>
<td>14:30</td>
<td>Alexander O’Malley</td>
<td>Molecular behaviour in established and emerging microporous catalysts</td>
<td>QK_06</td>
</tr>
<tr>
<td>15:00</td>
<td>Sandrine Lyonnard</td>
<td>Water Confined in Fuel Cell Membranes</td>
<td>QI_12</td>
</tr>
<tr>
<td>15:20</td>
<td>Toshiji Kanaya</td>
<td>Dynamics of rubbers reinforced with metallic diacrylate as studied by QENS and μSR</td>
<td>QN_07</td>
</tr>
<tr>
<td>15:35</td>
<td><strong>Coffee</strong></td>
<td></td>
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<tr>
<td>17:10</td>
<td><strong>Posters &amp; Discussions, Drinks</strong></td>
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Note: P_## - Plenary talk (40 minutes); QK_## - QENS Keynote talk (30 minutes); QI_## - QENS Invited talk; (20 minutes); QN_## - QENS normal talk (15 minutes).
**Tuesday, 17 July 2018, Senate Room**

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</thead>
<tbody>
<tr>
<td>8:30</td>
<td>Victoria García Sakai</td>
<td>QENS and Soft Matter – What does the future look like?</td>
<td>P_02</td>
</tr>
<tr>
<td>9:10</td>
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<td><strong>5 minutes break</strong></td>
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</tr>
<tr>
<td>9:15</td>
<td>Arantxa Arbe</td>
<td>Unraveling the properties of systems based on single-chain nano-particles</td>
<td>QK_09</td>
</tr>
<tr>
<td>9:45</td>
<td>Antonio Faraone</td>
<td>QENS insights on the nanoscopic origin of rheological properties in some well-dispersed polymer nanocomposites</td>
<td>QI_21</td>
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<tr>
<td>10:05</td>
<td></td>
<td><strong>Coffee</strong></td>
<td></td>
</tr>
<tr>
<td>10:20</td>
<td>Olaf Holderer</td>
<td>Neutron spin echo spectroscopy as a sensitive tool to study membrane elasticity in microemulsions</td>
<td>QI_02</td>
</tr>
<tr>
<td>10:40</td>
<td>Margarita Krutyeva</td>
<td>Polymer dynamics in nanoconfinement</td>
<td>QI_03</td>
</tr>
<tr>
<td>11:00</td>
<td>Yuuya Nagata</td>
<td>Elucidation of Molecular Dynamics of Poly(quinoxaline-2,3-diyl)₆ Exhibiting Solvent-dependent Helix Inversion Through Quasielastic Neutron Scattering Measurements</td>
<td>QN_10</td>
</tr>
<tr>
<td>11:15</td>
<td>Abhijit Pramanick</td>
<td>Microscopic insights into atomic level dynamics in PVDF-based copolymers and terpolymers using QENS</td>
<td>QN_12</td>
</tr>
<tr>
<td>11:30</td>
<td>Hua Li</td>
<td>The Revised Jump-Diffusion and Rotation-Diffusion Model for QENS Data Analysis</td>
<td>QN_14</td>
</tr>
<tr>
<td>11:45</td>
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<td><strong>END</strong></td>
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<tr>
<td>12:00</td>
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<td><strong>Lunch</strong></td>
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<tr>
<td>13:30</td>
<td>Yang Zhang</td>
<td>How to Walk on Water?– Ioffe-Regel Localization of Acoustic Excitations in Liquids</td>
<td>QK_03</td>
</tr>
<tr>
<td>14:00</td>
<td>Andreas Meyer</td>
<td>On the Relation of Structural Relaxation, Diffusion of Mass, and Viscous Flow in Viscous Metallic Liquids</td>
<td>QI_09</td>
</tr>
<tr>
<td>14:20</td>
<td>Marcus Cicerone</td>
<td>Activated Relaxation and Transport in Liquids well above Tₘ</td>
<td>QI_08</td>
</tr>
<tr>
<td>14:40</td>
<td>Henriette Wase Hansen</td>
<td>Simultaneous dielectric and neutron spectroscopy under high pressure – applied to glass-forming liquids</td>
<td>QN_03</td>
</tr>
<tr>
<td>14:55</td>
<td></td>
<td><strong>Coffee</strong></td>
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<tr>
<td>15:20</td>
<td>Limei Xu</td>
<td>Supercritical phenomenon in liquids</td>
<td>QI_22</td>
</tr>
<tr>
<td>Time</td>
<td>Name</td>
<td>Title</td>
<td>Abstract ID</td>
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<tr>
<td>15:40</td>
<td>Yun Liu</td>
<td>Short-Time Glassy Dynamics in Viscous Protein Solutions with Competing Interactions Studied by Neutron Spin Echo</td>
<td>QI_18</td>
</tr>
<tr>
<td>16:00</td>
<td>Suresh M. Chathoth</td>
<td>Microscopic origin of the logarithmic relaxation process in molecular glass-forming liquids</td>
<td>QN_16</td>
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<tr>
<td>16:15</td>
<td>END</td>
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<tr>
<td>17:30</td>
<td>Posters &amp; Discussions, Drinks</td>
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**Tuesday, 17 July 2018, Room 6207, 6/F, Lau Ming Wai Academic Building**

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<tr>
<th>Time</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>10:20</td>
<td>Catherine Pappas</td>
<td>Magnetic Fluctuations, Precursor Phenomena, and Phase Transition in skyrmion hosting chiral magnets</td>
<td>QI_19</td>
</tr>
<tr>
<td>10:40</td>
<td>Timothy D'Adam</td>
<td>The first user experiment on PELICAN utilising polarisation analysis</td>
<td>QN_01</td>
</tr>
<tr>
<td>10:55</td>
<td>Yinguo Xiao</td>
<td>Spin-wave and electromagnon dispersions in multiferroic MnWO4 as observed by neutron spectroscopy</td>
<td>QN_08</td>
</tr>
<tr>
<td>11:10</td>
<td>Benqiong Liu</td>
<td>Lattice dynamics and coupled quadrupole-phonon excitations in CeAuAl3</td>
<td>QN_04</td>
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<tr>
<td>11:25</td>
<td>END</td>
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<tr>
<td>12:00</td>
<td>Lunch</td>
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**Lattice Dynamics**

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<tr>
<th>Time</th>
<th>Speaker</th>
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</thead>
<tbody>
<tr>
<td>13:30</td>
<td>Kacper Druzbicki</td>
<td>Exploring Local Ordering in Molecular Materials: Vibrational Spectroscopy Perspective</td>
<td>QK_07</td>
</tr>
<tr>
<td>14:00</td>
<td>Jie Ma</td>
<td>Neutron scattering study on the thermoelectric material ZrNiSn1-xSbx with half-heusler alloy</td>
<td>QI_06</td>
</tr>
<tr>
<td>14:20</td>
<td>Yue Chen</td>
<td>Engineering phonon scattering in perovskite MAPbI3 via hydrostatic pressure</td>
<td>QI_16</td>
</tr>
<tr>
<td>14:40</td>
<td>Andreas Schönhals</td>
<td>Vibrational density of states and molecular mobility in a polymer with intrinsic microporosity PIM-1 as revealed by inelastic neutron scattering</td>
<td>QN_02</td>
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<tr>
<td>14:55</td>
<td>Coffee</td>
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**Software Development**

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<th>Abstract ID</th>
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<tbody>
<tr>
<td>15:20</td>
<td>Timmy Ramirez-Cuesta</td>
<td>Neutrons and Numbers: Studying materials and processes with VISION and VirtuES. Modeling INS data with DFT methods</td>
<td>WI_01</td>
</tr>
<tr>
<td>15:40</td>
<td>Yasuhiro Inamura</td>
<td>Current Status for software environment and developments at MLF, J-PARC</td>
<td>WI_10</td>
</tr>
<tr>
<td>16:00</td>
<td>Douglas Abernathy</td>
<td>Applications of MCViNE software at SNS</td>
<td>WN_02</td>
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<tr>
<td>16:15</td>
<td>5 minutes break</td>
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**16:20 – 17:20: Round table discussion on software development for QENS**

Chair Persons: Mark R. Johnson and Victoria García Sakai

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<tr>
<td>17:30</td>
<td>Posters &amp; Discussions, Drinks</td>
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### Wednesday, 18 July 2018, Senate Room

<table>
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<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
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</thead>
<tbody>
<tr>
<td>8:30</td>
<td>Math Karlsson</td>
<td>Ionics and protonics studied with INS and QENS</td>
<td>P_03</td>
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<tr>
<td>9:10</td>
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<td>5 minutes break</td>
<td></td>
</tr>
<tr>
<td>9:15</td>
<td>Maiko Kofu</td>
<td>Dynamics of atomic hydrogen in bulk and nanocrystalline palladium</td>
<td>QK_05</td>
</tr>
<tr>
<td>9:45</td>
<td>Artur Braun</td>
<td>The discovery of the proton polaron</td>
<td>QI_01</td>
</tr>
<tr>
<td>10:05</td>
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<td>Coffee</td>
<td></td>
</tr>
<tr>
<td>10:20</td>
<td>Yukinobu Kawakita</td>
<td>QENS study for functional materials and reduction of time-space correlation function</td>
<td>P_04</td>
</tr>
<tr>
<td>11:00</td>
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<td>5 minutes break</td>
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</tr>
<tr>
<td>11:05</td>
<td>Ivana Evans</td>
<td>Oxide ion conductors for energy applications: Structure and dynamics</td>
<td>QK_08</td>
</tr>
<tr>
<td>11:35</td>
<td>Mattia Gaboardi</td>
<td>Suppression of the long-range order in polycyclic aromatic hydrocarbons</td>
<td>QI_20</td>
</tr>
<tr>
<td>11:55</td>
<td>Tatsiana Burankova</td>
<td>QENS Studies of Reorientational Hydrogen Dynamics in Complex Hydrides</td>
<td>QI_07</td>
</tr>
<tr>
<td>12:15</td>
<td>Gavin J. Irvine</td>
<td>In-situ QENS studies of superionic conductivity in barium hydride</td>
<td>QN_13</td>
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<tr>
<td>12:30</td>
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<td>Conference photo</td>
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<tr>
<td>12:45</td>
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<td>Lunch</td>
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<tr>
<td>13:45 – 17:30</td>
<td></td>
<td>Excursion to Victoria Peak, Leave at 13:45</td>
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Note: P_## - Plenary talk (40 minutes); QK_## - QENS Keynote talk (30 minutes); QI_## - QENS Invited talk; (20 minutes); QN_## - QENS normal talk (15 minutes).
### Facility Overviews I

<table>
<thead>
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<tbody>
<tr>
<td>8:30</td>
<td>Kenneth Herwig</td>
<td>Overview of the Proposed Oak Ridge National Laboratory Spallation Neutron Source Second Target Station Instruments</td>
<td>WK_07</td>
</tr>
<tr>
<td>9:00</td>
<td>Bernhard Frick</td>
<td>The ILL spectroscopy group – overview and future directions</td>
<td>WK_08</td>
</tr>
<tr>
<td>9:30</td>
<td>Jamie Schulz</td>
<td>Status of the Neutron Scattering Capabilities at the OPAL Research Reactor</td>
<td>WK_06</td>
</tr>
</tbody>
</table>

**10:00 Coffee**

### New Instruments

<table>
<thead>
<tr>
<th>Time</th>
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</tr>
</thead>
<tbody>
<tr>
<td>10:20</td>
<td>Félix J Villacorta</td>
<td>Recent progress in MIRACLES, the time-of-flight backscattering spectrometer at the European Spallation Source</td>
<td>WI_05</td>
</tr>
<tr>
<td>10:40</td>
<td>Robert Bewley</td>
<td>The Mushroom, a new type of spectrometer</td>
<td>WI_04</td>
</tr>
<tr>
<td>11:00</td>
<td>Gabriele Sala</td>
<td>CHESS: A look into the next generation of neutrons instruments</td>
<td>WI_20</td>
</tr>
<tr>
<td>11:20</td>
<td>Stéphane Longeville</td>
<td>CSPEC- the cold time of flight spectrometer for the ESS</td>
<td>WI_23</td>
</tr>
<tr>
<td>11:40</td>
<td>Meng Wang</td>
<td>A high energy direct geometry time-of-flight neutron spectrometer at CSNS</td>
<td>WI_15</td>
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**12:00 Lunch**

### New Technologies

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<tbody>
<tr>
<td>13:30</td>
<td>Oliver Kirstein</td>
<td>Neutron scattering instrument systems and technical challenges with ESS being a high-power long pulse neutron source.</td>
<td>WK_02</td>
</tr>
<tr>
<td>14:00</td>
<td>Nikolaos Tsapatsaris</td>
<td>Standardisation rediscovered: Neutron Chopper System Developments at ESS</td>
<td>WI_18</td>
</tr>
<tr>
<td>14:20</td>
<td>Richard Hall Wilton</td>
<td>New developments in detector technology at ESS</td>
<td>WI_16</td>
</tr>
<tr>
<td>14:40</td>
<td>Fankang Li</td>
<td>The status of the ultra-high-resolution neutron spectroscopy at ORNL</td>
<td>WI_14</td>
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<tr>
<td>15:00</td>
<td>Kristijan Kuhlmann</td>
<td>Breakthrough in neutron backscattering spectroscopy: A tenfold enhanced energy resolution using GaAs 200</td>
<td>WN_01</td>
</tr>
</tbody>
</table>

**15:15 Coffee**

### Polarization

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>15:35</td>
<td>Tetsuya Yokoo</td>
<td>Polarized neutron spectrometer POLANO, its construction and commissioning</td>
<td>WI_11</td>
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<tr>
<td>15:55</td>
<td>Gøran Nilsen</td>
<td>Polarization analysis on the LET spectrometer at ISIS</td>
<td>WI_25</td>
</tr>
</tbody>
</table>

**16:15 Posters & Discussions**

**18:00 Conference Dinner**
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Talk length</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:20</td>
<td>Leland Harringer</td>
<td>Survey of Advances in Cold Triple Axis Spectroscopy Design.</td>
<td>WI_03</td>
</tr>
<tr>
<td>10:40</td>
<td>Henrik. M. Rønnow</td>
<td>CAMEA—A novel multiplexing analyzer for neutron spectroscopy</td>
<td>WI_17</td>
</tr>
<tr>
<td>11:00</td>
<td>Matteo Zanetti</td>
<td>Recent developments on TOSCA and VESPA</td>
<td>WI_24</td>
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<tr>
<td>11:20</td>
<td>Kenji Nakajima</td>
<td>Nine years of AMATERAS—a cold-neutron disk-chopper spectrometer</td>
<td>WI_22</td>
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<tr>
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<tr>
<td>12:00</td>
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</tr>
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**Instrument Reports II**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Talk length</th>
</tr>
</thead>
<tbody>
<tr>
<td>13:30</td>
<td>Markus Appel</td>
<td>IN16B at ILL—Workhorse for users and testbed for advanced backscattering</td>
<td>WI_13</td>
</tr>
<tr>
<td>13:50</td>
<td>Nicolas de Souza</td>
<td>EMU spectrometer progress report - towards steady-state operation</td>
<td>WI_07</td>
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<tr>
<td>14:10</td>
<td>Michaela Zamponi</td>
<td>Upgrades at SPHERES</td>
<td>WI_12</td>
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<tr>
<td>14:30</td>
<td>Madhusudan Tyagi</td>
<td>Ongoing upgrades at the high Flux Backscattering spectrometer at the NCNR</td>
<td>WI_19</td>
</tr>
<tr>
<td>14:50</td>
<td>Hitoshi Endo</td>
<td>Current status of neutron resonance spin echo spectrometers</td>
<td>WI_21</td>
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<tr>
<td>15:10</td>
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**Instrument Reports III**

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<tbody>
<tr>
<td>15:35</td>
<td>Xinzhi Liu</td>
<td>Inelastic neutron scattering in very strong magnetic fields on EXED</td>
<td>WN_03</td>
</tr>
<tr>
<td>15:50</td>
<td>Bingfeng Hu</td>
<td>The Construction Progress of CMRR Thermal Triple-Axis Spectrometer DRAGON</td>
<td>WN_04</td>
</tr>
<tr>
<td>16:05</td>
<td></td>
<td>Posters &amp; Discussions</td>
<td></td>
</tr>
<tr>
<td>18:00</td>
<td></td>
<td>Conference dinner</td>
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</tbody>
</table>

Note: WK_## - WINS Keynote talk (30 minutes); WI_## - WINS Invited talk (20 minutes); WN_## - WINS normal talk (15 minutes).
Friday, 20 July 2018, Senate Room

### Facility Overviews II

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>Masatoshi Arai</td>
<td>Overview of the ESS spectrometers - Difference from short pulse instruments</td>
<td>WK_03</td>
</tr>
<tr>
<td>9:00</td>
<td>Russell Ewings</td>
<td>Developments in spectroscopy at the ISIS pulsed neutron and muon source</td>
<td>WK_04</td>
</tr>
<tr>
<td>9:30</td>
<td>Ryoichi Kajimoto</td>
<td>Overview of the neutron spectrometers at J-PARC</td>
<td>WK_05</td>
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<tr>
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<td><strong>Coffee</strong></td>
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### Instrument Reports IV

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>10:20</td>
<td>Douglas Abernathy</td>
<td>Science and performance trends at the ARCS spectrometer of the SNS</td>
<td>WI_02</td>
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<tr>
<td>10:40</td>
<td>Matthew Stone</td>
<td>SEQUOIA, the fine resolution thermal chopper spectrometer at the SNS</td>
<td>WI_06</td>
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<tr>
<td>11:00</td>
<td>Jörg Voigt</td>
<td>T-REX, a bi-spectral chopper spectrometer for the ESS</td>
<td>WI_09</td>
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### Future Trend

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<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
<th>Abstract ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:25</td>
<td>Matthew Stone</td>
<td>The inelastic neutron scattering instrument suite at ORNL and the future direction of its development</td>
<td>WK_01</td>
</tr>
<tr>
<td>11:55</td>
<td>Ferenc Mezei</td>
<td>Opportunities for further advances in time-of-flight spectroscopy</td>
<td>WK_09</td>
</tr>
<tr>
<td>12:25</td>
<td>Ferenc Mezei</td>
<td>Closing Remarks</td>
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<tr>
<td>12:35</td>
<td><strong>Lunch and Good Bye!</strong></td>
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</tbody>
</table>

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<table>
<thead>
<tr>
<th>Presenter</th>
<th>Title</th>
<th>Abstract ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>Olaf HOLDERER</td>
<td>A better view through new glasses: Developments at the Jülich Neutron Spin Echo Spectrometers</td>
<td>QP_01</td>
</tr>
<tr>
<td>V. K. Sharma</td>
<td>Microscopic mobility in alkylamide based deep eutectic solvents</td>
<td>QP_02</td>
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<tr>
<td>S. Mitra</td>
<td>Change in dynamical and phase behaviour of DODAB bilayer with addition of NSAIDs</td>
<td>QP_03</td>
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<tr>
<td>Juan F. MORA CARDOZO</td>
<td>Proton diffusion in the protic ionic liquid 2-Aminoethanaminium Triflate: A computational approach</td>
<td>QP_04</td>
</tr>
<tr>
<td>Takeshi YAMADA</td>
<td>In situ Quasi Elastic Neutron Scattering of Nafion Membrane with Water Vapor Pressure Control System.</td>
<td>QP_05</td>
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<tr>
<td>Kaoru Shibata</td>
<td>QENS study of tetrahedron dynamics in the Zn6Sc 1/1 approximant to the quasicrystal</td>
<td>QP_06</td>
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<tr>
<td>H. SRINIVASAN</td>
<td>Dynamics of acetamide in acetamide+LiNO3 deep eutectic solvents</td>
<td>QP_07</td>
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<tr>
<td>Qianli CHEN</td>
<td>Proton Polaron in Ceramic Metal Oxides</td>
<td>QP_08</td>
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<tr>
<td>Shuhau Yao</td>
<td>Further understanding of better thermoelectric properties of BiCuTeO compared to BiCuSeO</td>
<td>QP_09</td>
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<td>Chenchen YUAN</td>
<td>Slowing down of dynamics with less dense packing in metallic glass-forming liquids modulated by alloying Al element</td>
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<td>Zhendong FU</td>
<td>Magnetic excitations in the ferromagnetic molecular ring (Cr8Y8)</td>
<td>QP_11</td>
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<tr>
<td>Sheng Yun Wu</td>
<td>Role of iron doping in short range antiferromagnetic NiO nanoparticles</td>
<td>QP_12</td>
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<tr>
<td>Alice Klapproth</td>
<td>Inelastic neutron scattering of methane double hydrates</td>
<td>QP_13</td>
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<tr>
<td>Sanghamitra MUKHOPADHYAY</td>
<td>QENS data analysis on Mantid: A modern approach</td>
<td>QP_14</td>
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<tr>
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<td>Nicolò VIOLINI</td>
<td>The design of T-REX, a bi-spectral chopper spectrometer for the ESS</td>
<td>WP_01</td>
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<tr>
<td>Claudia SCATIGNO</td>
<td>Assessing the limits of detection and quantitation on the upgraded TOSCA spectrometer</td>
<td>WP_02</td>
</tr>
<tr>
<td>Masato Matsuura</td>
<td>QENS and INS studies using TOF type Si crystal analyzer backscattering spectrometer DNA <del>from basic sciences to industrial applications</del></td>
<td>WP_03</td>
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<tr>
<td>Russell EWINGS</td>
<td>How we lost most of the flux on MAPS, and how we got it back again</td>
<td>WP_04</td>
</tr>
<tr>
<td>Russell EWINGS</td>
<td>Completion of the MAPS time-of-flight spectrometer upgrade</td>
<td>WP_05</td>
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<tr>
<td>Olaf HOLDERER</td>
<td>The Neutron Spin Echo Spectrometer @ SNS (SNS-NSE)</td>
<td>WP_06</td>
</tr>
<tr>
<td>Shinichio ITOH</td>
<td>Progress in High Resolution Chopper Spectrometer HRC by improving collimator and Fermi chopper</td>
<td>WP_07</td>
</tr>
<tr>
<td>Ryoichi KAJIMOTO</td>
<td>Time-of-flight direct-geometry spectrometer 4SEASONS at J-PARC</td>
<td>WP_08</td>
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<tr>
<td>Tetsuya YOKOO</td>
<td>Suite of the neutron spectrometers in J-PARC</td>
<td>WP_09</td>
</tr>
<tr>
<td>Ian Silverwood</td>
<td>Imaging spectroscopy through parallel beam collimation: A new way to look at scattering</td>
<td>WP_10</td>
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<tr>
<td>Seiko OHIRA-</td>
<td>Sample environment commonly used at the chopper spectrometers in J-PARC MLF</td>
<td>WP_11</td>
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<tr>
<td>KAWAMURA</td>
<td>Update of TOF spectrometer NEAT at Helmholtz Zentrum Berlin</td>
<td>WP_12</td>
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<td>Margarita RUSSINA</td>
<td>A new era for the TOSCA vibrational spectrometer</td>
<td>WP_13</td>
</tr>
<tr>
<td>Alexandre IVANOV</td>
<td>From IN8 to THERMES – development of the thermal three-axis spectrometer at ILL</td>
<td>WP_14</td>
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<tr>
<td>Mitsutaka NAKAMURA</td>
<td>Applicability and limitations of G(r,E) analysis transformed from the inelastic neutron scattering data</td>
<td>WP_15</td>
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<td>Xiaoyan Ma</td>
<td>The effect of putting a neutron velocity selector before the monochromator in the thermal neutron triple-axis spectrometer</td>
<td>WP_16</td>
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<tr>
<td>Lijie HAO</td>
<td>Inelastic neutron spectrometers at China Advanced Research Reactor (CARR)</td>
<td>WP_17</td>
</tr>
<tr>
<td>Dehong Yu</td>
<td>PELICAN – a Time of Flight Cold Neutron Spectrometer - Scientific Outcomes of the First Four Years Operation</td>
<td>WP_18</td>
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<td>Nicolas R. DE</td>
<td>EMU – the high-resolution neutron spectrometer at the</td>
<td>WP_19</td>
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<td>Souza</td>
<td>Australian Centre for Neutron Scattering</td>
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<tr>
<td>Gøran NILSEN</td>
<td>RAMP: a prototype software package for faster neutron instrument simulations</td>
<td>WP_20</td>
</tr>
</tbody>
</table>
Abstract Contents

Plenary Talks

P01  QENS – Experiment, Simulation and Application ............................................. 1
P02  QENS and Soft Matter – What does the future look like? .................................. 2
P03  Ionics and protonics studied with INS and QENS .............................................. 3
P04  QENS study for functional materials and reduction of time-space correlation function. 4

QENS Keynote Talks ........................................................................................................ 5

QK_01  QENS studies of living multicellular organisms .............................................. 5
QK_02  Dynamics of proteins in aqueous solutions – recent advances using high-resolution spectroscopy ........................................................................................................ 7
QK_03  How to Walk on Water? – Ioffe-Regel Localization of Acoustic Excitations in Liquids ... 9
QK_04  Nano-scale mobility of cellular water can discriminate cancer development or recession .......................................................................................................................... 10
QK_05  Dynamics of atomic hydrogen in bulk and nanocrystalline palladium ............. 11
QK_06  Molecular behaviour in established and emerging microporous catalysts ........ 13
QK_07  Exploring Local Ordering in Molecular Materials: Vibrational Spectroscopy Perspective .................................................................................................................... 15
QK_08  Oxide ion conductors for energy applications: Structure and dynamics ........... 17
QK_09  Unraveling the properties of systems based on single-chain nano-particles ....... 18
QK_10  Molecular transport in porous materials and adsorption induced phenomena observed through the lens of neutron spectroscopy ........................................... 19
QK_11  Dynamics of Biopolymers under Confinement and Extreme Conditions Studied by QENS .................................................................................................................... 21

QENS Invited Talks ............................................................................................................ 23

QI_01  The discovery of the proton polaron ................................................................... 23
QI_02  Neutron spin echo spectroscopy as a sensitive tool to study membrane elasticity in microemulsions ........................................................................................................... 25
QI_03  Polymer dynamics in nanoconfinement ............................................................. 26
QI_04  Gradual cross-over from sub-diffusion to normal-diffusion: a many-body effect in protein surface water ........................................................................................................... 27
QI_06  Neutron scattering study on the thermoelectric material ZrNiSn1-xSbX with half-heusler alloy ...................................................................................................................... 28
QI_07  QENS Studies of Reorientational Hydrogen Dynamics in Complex Hydrides ........ 29
QI_08  Activated Relaxation and Transport in Liquids well above $T_m$ ........................................ 31
QI_09  On the Relation of Structural Relaxation, Diffusion of Mass, and Viscous Flow in Visous Metallic Liquids ................................................................. 32
QI_10  General Picture of Protein Dynamics: Combining Neutron Scattering with Dielectric and MD-Simulations Studies ................................................................. 33
QI_11  Dynamical Transitions and Diffusion Mechanism in the Lipid Bilayer ......................... 34
QI_12  Water Confined in Fuel Cell Membranes .................................................................. 36
QI_13  Structure, Dynamics and Magnetism in Ionic Liquids .............................................. 37
QI_14  Ionic liquids in bulk and under 1D nanometric confinement: a multiscale analysis .... 39
QI_15  Influence of PEGylation on protein dynamics ........................................................... 41
QI_16  Engineering phonon scattering in perovskite MAPbI$_3$ via hydrostatic pressure ....... 42
QI_17  Towards understanding lipid membrane transport properties using quasi-elastic neutron scattering techniques ................................................................. 43
QI_18  Short-Time Glassy Dynamics in Viscous Protein Solutions with Competing Interactions Studied by Neutron Spin Echo ......................................................................... 45
QI_19  Magnetic Fluctuations, Precursor Phenomena, and Phase Transition in skyrmion hosting chiral magnets ................................................................. 47
QI_20  Suppression of the long-range order in polycyclic aromatic hydrocarbons .............. 48
QI_21  QENS insights on the nanoscopic origin of rheological properties in some well-dispersed polymer nanocomposites ................................................................. 49
QI_22  Supercritical phenomenon in liquids .......................................................................... 50
QI_23  Dynamics of Water-in-Salt and Water-in-Bisalt Electrolytes ................................... 51

QENS Oral Talks ........................................................................................................... 53
QN_01  The first user experiment on PELICAN utilising polarisation analysis ....................... 53
QN_02  Vibrational density of states and molecular mobility in a polymer with intrinsic microporosity PIM-1 as revealed by inelastic neutron scattering ....................................... 55
QN_03  Simultaneous dielectric and neutron spectroscopy under high pressure – applied to
        glass-forming liquids ................................................................................................. 56
QN_04  Lattice dynamics and coupled quadrupole-phonon excitations in CeAuAl$_3$ ............. 57
QN_05  Dynamics of ions in alkylammonium-based ionic liquids with plastic-crystalline phases ........................................................................................................ 59
QN_06  Separation of coherent and incoherent scattering with polarization analysis on D7 at the Institut Laue-Langevin .................................................................................. 61
QN_07  Dynamics of rubbers reinforced with metallic diacrylate as studied by QENS and $\ce{^{15}N}$SR ........................................................................................................ 62
QN_08  Spin-wave and electromagnon dispersions in multiferroic MnWO4 as observed by neutron spectroscopy .......................................................... 63
QN_09  Nanoscale mobility in dental restorative cements .......................................................... 64
QN_10  Elucidation of Molecular Dynamics of Poly(quinoxaline-2,3-diyl)s Exhibiting Solvent-dependent Helix Inversion Through Quasielastic Neutron Scattering Measurements 66
QN_11  H-Bonding influence on the dynamics of imidazolium-based ionic liquids as probed by QENS ........................................................................... 68
QN_12  Microscopic insights into atomic level dynamics in PVDF-based copolymers and terpolymers using QENS ........................................................................ 70
QN_13  In-situ QENS studies of superionic conductivity in barium hydride ......................... 72
QN_14  The Revised Jump-Diffusion and Rotation-Diffusion Model for QENS Data Analysis .. 73
QN_15  Dynamical landscape in bio-mimetic membrane systems: Neutron scattering and MD simulation studies ................................................................. 75
QN_16  Microscopic origin of the logarithmic relaxation process in molecular glass-forming liquids ............................................................................. 76

**WINS Keynote Talks** ................................................................. 77

WK_01  The inelastic neutron scattering instrument suite at ORNL and the future direction of its development .......................................................... 77
WK_02  Neutron scattering instrument systems and technical challenges with ESS being a high-power long pulse neutron source .................................. 78
WK_03  Overview of the ESS spectrometers - Difference from short pulse instruments - .... 79
WK_04  Developments in spectroscopy at the ISIS pulsed neutron and muon source .......... 80
WK_05  Overview of the neutron spectrometers at J-PARC .................................................. 81
WK_06  Status of the Neutron Scattering Capabilities at the OPAL Research Reactor ........ 82
WK_07  Overview of the Proposed Oak Ridge National Laboratory Spallation Neutron Source Second Target Station Instruments ........................................... 83
WK_08  The ILL spectroscopy group – overview and future directions ................................. 84
WK_09  Opportunities for further advances in time-of-flight spectroscopy ....................... 86
WK_10  Status of the China Spallation Neutron Source ....................................................... 88

**WINS Invited Talks** ................................................................. 89

WI_01  Neutrons and Numbers: Studying materials and processes with VISION and VirtuES. Modeling INS data with DFT methods ......................................... 89
WI_02  Science and performance trends at the ARCS spectrometer of the SNS .................. 91
WI_03  Survey of Advances in Cold Triple Axis Spectroscopy Design ................................. 92
WI_04  The Mushroom, a new type of spectrometer ............................................................... 93
<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>WI_05</td>
<td>Recent progress in MIRACLES, the time-of-flight backscattering spectrometer at the European Spallation Source</td>
</tr>
<tr>
<td>WI_06</td>
<td>SEQUOIA, the fine resolution thermal chopper spectrometer at the SNS</td>
</tr>
<tr>
<td>WI_07</td>
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</tr>
<tr>
<td>WI_10</td>
<td>Current Status for software environment and developments at MLF, J-PARC</td>
</tr>
<tr>
<td>WI_11</td>
<td>Polarized neutron spectrometer POLANO, its construction and commissioning</td>
</tr>
<tr>
<td>WI_12</td>
<td>Upgrades at SPHERES</td>
</tr>
<tr>
<td>WI_13</td>
<td>IN16B at ILL – Workhorse for users and testbed for advanced backscattering</td>
</tr>
<tr>
<td>WI_14</td>
<td>The status of the ultra-high-resolution neutron spectroscopy at ORNL</td>
</tr>
<tr>
<td>WI_15</td>
<td>A high energy direct geometry time-of-flight neutron spectrometer at CSNS</td>
</tr>
<tr>
<td>WI_16</td>
<td>New developments in detector technology at ESS</td>
</tr>
<tr>
<td>WI_17</td>
<td>CAMEA—A novel multiplexing analyzer for neutron spectroscopy</td>
</tr>
<tr>
<td>WI_18</td>
<td>Standardisation rediscovered: Neutron Chopper System Developments at ESS</td>
</tr>
<tr>
<td>WI_19</td>
<td>Ongoing upgrades at the high Flux Backscattering spectrometer at the NCNR</td>
</tr>
<tr>
<td>WI_20</td>
<td>CHESS: A look into the next generation of neutrons instruments</td>
</tr>
<tr>
<td>WI_21</td>
<td>Current status of neutron resonance spin echo spectrometers BL06 “VIN ROSE” at MLF, J-PARC</td>
</tr>
<tr>
<td>WI_22</td>
<td>Nine years of AMATERAS — a cold-neutron disk-chopper spectrometer</td>
</tr>
<tr>
<td>WI_23</td>
<td>CSPEC- the cold time of flight spectrometer for the ESS</td>
</tr>
<tr>
<td>WI_24</td>
<td>Recent developments on TOSCA and VESPA</td>
</tr>
<tr>
<td>WI_25</td>
<td>Polarization analysis on the LET spectrometer at ISIS</td>
</tr>
<tr>
<td>WI_26</td>
<td>Current status of neutron scatterings at CARR</td>
</tr>
<tr>
<td>WN_01</td>
<td>Breakthrough in neutron backscattering spectroscopy: A tenfold enhanced energy resolution using GaAs 200</td>
</tr>
<tr>
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<td>Applications of MCViNE software at SNS</td>
</tr>
<tr>
<td>WN_03</td>
<td>Inelastic neutron scattering in very strong magnetic fields on EXED</td>
</tr>
<tr>
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<td>The Construction Progress of CMRR Thermal Triple-Axis Spectrometer DRAGON</td>
</tr>
</tbody>
</table>

**WINS Oral Talks**

<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>WN_01</td>
<td>A better view through new glasses: Developments at the Jülich Neutron Spin Echo Spectrometers</td>
</tr>
<tr>
<td>QP_02</td>
<td>Microscopic mobility in alkylamide based deep eutectic solvents</td>
</tr>
<tr>
<td>QP_04</td>
<td>Proton diffusion in the protic ionic liquid 2-Aminoethanaminium Triflate: A computational approach</td>
</tr>
<tr>
<td>QP_05</td>
<td>In situ Quasi Elastic Neutron Scattering of Nafion Membrane with Water Vapor Pressure Control System</td>
</tr>
<tr>
<td>QP_06</td>
<td>QENS study of tetrahedron dynamics in the Zn$_6$Sc 1/1 approximant to the quasicrystal</td>
</tr>
<tr>
<td>QP_07</td>
<td>Dynamics of acetamide in acetamide+LiNO$_3$ deep eutectic solvents</td>
</tr>
<tr>
<td>QP_08</td>
<td>Proton Polaron in Ceramic Metal Oxides</td>
</tr>
<tr>
<td>QP_09</td>
<td>Further understanding of better thermoelectric properties of BiCuTeO compared to BiCuSeO</td>
</tr>
<tr>
<td>QP_10</td>
<td>Slowing down of dynamics with less dense packing in metallic glass-forming liquids modulated by alloying Al element</td>
</tr>
<tr>
<td>QP_11</td>
<td>Magnetic excitations in the ferromagnetic molecular ring {Cr$_8$Y$_8$}</td>
</tr>
<tr>
<td>QP_12</td>
<td>Role of iron doping in short range antiferromagnetic NiO nanoparticles</td>
</tr>
<tr>
<td>QP_13</td>
<td>Inelastic neutron scattering of methane double hydrates</td>
</tr>
<tr>
<td>QP_14</td>
<td>QENS data analysis on Mantid: A modern approach</td>
</tr>
<tr>
<td>WP_01</td>
<td>The design of T-REX, a bi-spectral chopper spectrometer for the ESS</td>
</tr>
<tr>
<td>WP_02</td>
<td>Assessing the limits of detection and quantitation on the upgraded TOSCA spectrometer</td>
</tr>
<tr>
<td>WP_03</td>
<td>QENS and INS studies using TOF type Si crystal analyzer backscattering spectrometer DNA <del>from basic sciences to industrial applications</del></td>
</tr>
<tr>
<td>WP_04</td>
<td>How we lost most of the flux on MAPS, and how we got it back again</td>
</tr>
<tr>
<td>WP_05</td>
<td>Completion of the MAPS time-of-flight spectrometer upgrade</td>
</tr>
<tr>
<td>WP_06</td>
<td>The Neutron Spin Echo Spectrometer @ SNS (SNS-NSE)</td>
</tr>
<tr>
<td>WP_07</td>
<td>Progress in High Resolution Chopper Spectrometer HRC by improving collimator and Fermi chopper</td>
</tr>
<tr>
<td>WP_08</td>
<td>Time-of-flight direct-geometry spectrometer 4SEASONS at J-PARC</td>
</tr>
<tr>
<td>WP_09</td>
<td>Suite of the neutron spectrometers in J-PARC</td>
</tr>
<tr>
<td>WP_10</td>
<td>Imaging spectroscopy through parallel beam collimation: A new way to look at scattering</td>
</tr>
<tr>
<td>WP_11</td>
<td>Sample environment commonly used at the chopper spectrometers in J-PARC MLF</td>
</tr>
<tr>
<td>WP_12</td>
<td>Upgrade of TOF spectrometer NEAT at Helmholtz Zentrum Berlin</td>
</tr>
<tr>
<td>WP_13</td>
<td>A new era for the TOSCA vibrational spectrometer</td>
</tr>
</tbody>
</table>
WP_14  From IN8 to THERMES – development of the thermal three-axis spectrometer at ILL ............................................................ 166
WP_15  Applicability and limitations of G(r,E) analysis transformed from the inelastic neutron scattering data .............................................................. 167
WP_16  The effect of putting a neutron velocity selector before the monochromator in the thermal neutron triple-axis spectrometer .................................................. 168
WP_17  Inelastic neutron spectrometers at China Advanced Research Reactor (CARR) .... 169
WP_18  PELICAN – a Time of Flight Cold Neutron Spectrometer - Scientific Outcomes of the First Four Years Operation ................................................................. 170
WP_19  EMU – the high-resolution neutron spectrometer at the Australian Centre for Neutron Scattering ................................................................................. 171
WP_20  RAMP: a prototype software package for faster neutron instrument simulations ... 172
Neutron techniques for QENS cover orders of magnitude in time and length scales - neutrons are therefore perfectly suited to studying a wide range of diffusion processes in hard and soft condensed matter, including biology. Since neutrons are scattered primarily by nuclei, the data can be directly compared with atomistic simulations, in particular those based on empirical force fields, which treat electrons implicitly and cover the widest range in time and length scales. A range of examples will be shown that illustrate how neutrons and atomistic simulations give critical insight into energy and bio-related materials and processes.

E-mail for corresponding author: johnson@ill.eu
Quasi-elastic neutron scattering continues to play an important role in accessing the dynamics in the wide range of systems that fall under the soft matter umbrella [1,2]. Albeit structural characterization being the initial step to understanding soft materials, ultimately many of their macroscopic properties such as viscosity, conductivity or enzymatic activity are related to their molecular motions. Advances in technology and experimental methods, theory and simulation, and the search for new ‘smart’ materials and systems to address social and global challenges, continue to invigorate the research in this field. In most cases neutrons can provide more detailed and/or different information as part of a comprehensive suite of characterization tools. In this talk I will review the field, addressing scientific and neutron user trends. More importantly I would like this talk to open the floor to discussion and debate: what considerations are important for existing and new neutron sources, such that QENS can efficiently and effectively answer key questions in our field.


E-mail for corresponding author: Victoria.garcia-sakai@stfc.ac.uk
Over the past 10-20 years, solid-state ionics, i.e., the study of solid ion conducting materials, or so-called electrolytes, and their usage in various technological applications such as batteries, chemical sensors, and fuel cells has developed into a very important and fast-growing field within materials science. 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 solid-state electrolytes limit their wider use. The development of new, more highly ion conducting systems 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), in combination with computer modeling, continue to play a central role [1]. In this contribution, I will summarize recent progresses in relation to the structural and dynamical study of solid state ionic 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 oxides, because of their large technological promise as electrolytes in next-generation, intermediate-temperature, fuel cells [2].


maths.karlsson@chalmers.se
QENS study for functional materials and reduction of time-space correlation function

Yukinobu KAWAKITA

Japan Atomic Energy Agency, J-PARC Center, Tokai Naka-gun, Ibaraki, Japan

At J-PARC, AMATERAS and DNA are frequently used for QENS measurements. The former is the direct geometry inelastic neutron spectrometer with pulse-shaping and monochromating disk choppers which enable us to access a wide range of incident neutron energy from 1 to 80 meV[1]. The multi Ei method is very useful for catching overall features from slow and large-scale dynamics to fast and atomic-scale dynamics simultaneously[2]. The latter is the near back-scattering inelastic neutron spectrometer with a pulse-shaping chopper and Si111 analyzer mirrors which enable us to access energy transfer range of -500 to 1500 μeV with high resolution of 2.4μeV[3]. The extremely high signal-to-noise ratio extends QENS and INS applications widely. In the first half of my talk, current status of such instruments as well as neutron target will be introduced.

In the second half of my talk, relatively new researches on functional materials using AMATERAS and DNA and approaches to fundamental long-standing problem in liquid physics will be discussed.

The first topic is on a photo-voltaic material, an organic-inorganic hybrid perovskite semiconductor, which has been recently focused as a candidate of next generation PV cells. Methyl-ammonium-lead-iodide involves a methyl-ammonium molecular ion in an inorganic framework. The rotational diffusion of the molecule was studied by QENS measurement by DNA and phonon dynamics over a wide energy range was done by INS measurements by AMATERAS. It was revealed that a four-fold jumping rotation of C-N bond forming electrical dipole prevents optical phonon of inorganic framework to propagate which causes extremely low thermal conduction of this material [4].

The second topic is on complexity in structure of liquid metals. Liquid Bi has complex structure that a characteristic shoulder structure aside of the first peak exists both in structure factor and pair distribution function. Coherent QENS measurements and analysis in real time and real space made clear the origin of this complexity from atomic dynamics. In the reduced van Hove dynamical correlation function, the shoulder structure shows characteristic relaxation interpreted as process loosing double-layered structure based on Peierls distortion in liquid Bi [5]. Analyses on liquid Ga, Sb and Ge are now in progress, which will be touched in the talk.


E-mail for corresponding author: yukinobu.kawakita@j-parc.jp
QENS Keynote Talks

QK_01  QENS studies of living multicellular organisms

Eugene MAMONTOV

Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

The choice of QENS as a suitable probe of microscopic dynamics in a living multicellular organism is far from intuitive. Unlike NMR, which can be sensitive to the atomic positions as manifested through the specific chemical shift, QENS measures hydrogen-dominated scattering signal averaged over the entire sample. This lack of selectivity is balanced in part by the sensitivity of QENS not only to the energy, but also momentum transfer, which advantageously allows analysis of time-spatial characteristics of molecular-level diffusion processes. QENS studies of living cells gradually gain acceptance, but feasibility of QENS for probing entire living multicellular organisms remains to be explored. We present the results of two such studies.

In the first study, we probe microscopic diffusion of water in encysted eggs of brine shrimp (*Artemia*) fully hydrated with (1) water, (2) eutectic mixture of water and dimethyl sulfoxide, and (3) an aqueous solution of lithium chloride. The diffusivity of the hydration water is reasonably well defined, despite the considerable morphological complexity of the hydrated organism. The translational diffusivity of pure water hydrating *Artemia* eggs decreases by at least factor of 4 compared to the bulk value. For water-DMSO and water-LiCl hydration mixtures, the decrease in the translational diffusivity compared to the respective bulk values is smaller, yet the penetration inside the eggs of at least some DMSO and LiCl together with H$_2$O is evident from the elimination of the hydration water freezing. Without DMSO and LiCl additives, the hydration water exhibits multi-step freezing on cooling down, completed at ca. 230 K. Together with the at least four-fold reduction in the translational diffusion coefficient, this suggests a distribution of the effective confinement pore size over the range of 2 to 10 nm. Those pores are also accessible to DMSO and LiCl co-solvents. A remarkable absence of the typical characteristics of the intra-cellular cytoplasmic water, such as freezing near 273 K and the translational diffusion coefficient similar to that in bulk water, may be linked to the unique and well documented resilience of *Artemia* eggs against adverse environmental factors not only in the anhydrous, but also hydrated state.

In the second study, we investigate living planarian flatworms to measure, on the pico-to-nanosecond time scale and nanometer length scale, microscopic diffusion of water and cell constituents in the planarians. Measurable microscopic diffusivities were surprisingly well defined in such a complex...
system as living animals. The overall variation in the microscopic diffusivity of cell constituents was found to be far lower than the variation in the microscopic diffusivity of water in planarians in a temperature range of 284.5 to 304.1 K. It has been known that microscopic dynamics of cell constituents is linked to that of intra-cellular water, but we show that this is not universally true.

Finally, we discuss QENS potential to probe even more complex organisms in the future.


E-mail for corresponding author: mamontove@ornl.gov
Dynamics of proteins in aqueous solutions – recent advances using high-resolution spectroscopy

Tilo SEYDEL1, Marco GRIMALDO1, Christian BECK1,2, Fajun ZHANG2,
Felix ROOSEN-RUNGE3, Frank SCHREIBER2

1Institut Max von Laue - Paul Langevin, Grenoble, France
2Institute for Applied Physics, University of Tübingen, Germany
3Physical Chemistry, University of Lund, Sweden

Novel high resolution neutron spectrometers permit new types of experiments probing several hierarchically superimposed levels of protein dynamics on the molecular length scale. Notably, the high cold neutron flux delivered to the samples opens up the possibility to investigate proteins suspended in aqueous solutions.

In this way, the nanosecond time scale internal motion of proteins and other macromolecules in aqueous solutions at comparatively low concentrations of 50 to 200 mg/ml can be explored [1,2]. These novel types of experiments allow investigating the in-solution internal dynamics of proteins and its difference to the previously studied hydrated macromolecular powder dynamics. Simultaneously, the superimposed global center-of-mass motions can be measured and separated into the rotational and translational diffusion contributions [3]. This center-of-mass diffusion can be interpreted in terms of concepts from colloid physics [4,5]. High-resolution incoherent neutron spectroscopy provides a unique access to the short-time self-diffusion of proteins and other macromolecules in aqueous solutions [4]. On this time scale, hydrodynamic and electrostatic interactions prevail, as opposed to the longer time scales accessible for instance by nuclear magnetic resonance experiments, on which direct interactions (collisions) between the suspended proteins dominate.

The new possibilities permit to address the current topics [1-10], amongst others, of macromolecular crowding [4], of “patchy” colloid physics [5,6], of protein cluster formation [2,5], of protein unfolding [7,8], of the in situ study of dynamic precursor processes to the crystallization of proteins from aqueous solutions, and of intrinsically disordered proteins [9].

The talk will present a selection of recent results highlighting the link between protein biophysics and colloid physics.

E-mail for corresponding author: seydel@ill.eu
Long wavelength longitudinal phonons can propagate in liquids, but whether transverse phonons exist in liquids has been debated since the 1970s. The classic hydrodynamic theory refutes the existence of the latter because the transverse current fluctuation does not directly couple with density fluctuations and the Brillouin zone is not well-defined. However, such arguments fail to describe the non-linear viscoelastic response of liquids. We performed coherent Inelastic Neutron Scattering (INS) measurements of the phonon dispersion relation of metallic liquids and glasses. Two phonon branches, the longitudinal and the transverse, are clearly identified. These experimental observations are also confirmed in both density and current correlation functions obtained from our Molecular Dynamics (MD) simulations. Furthermore, we found that the Ioffe-Regel delocalization point of these phonon modes coincides with the onset of super-Arrhenius transport and dynamic heterogeneity, and the breakdown of Stokes-Einstein relation. Therefore, we interpreted phonon delocalization as the microscopic driving force of the strongly-correlated behavior of liquids. We have also developed a Viscoelastic Hydrodynamic theory by introducing microscopic viscoelasticity and anisotropy, which directly yield a coupling mechanism between the elastic and viscous stress tensors and give rise to the observed one Rayleigh mode and two Brillouin modes. This work is a major step forward in the understanding of the half-a-century old puzzling problem on the nature of the transverse phonons in liquids.
Nano-scale mobility of cellular water can discriminate cancer development or recession

Murillo L. MARTINS¹,² and Heloisa N. BORDALLO¹,³

¹ Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
² Pontifical Catholic University of Goiás, Goiânia, Brazil
³ European Spallation Source ESS ERIC, P.O. Box 176, SE-22100 Lund, Sweden

Nowadays, different approaches are applied for predicting the behavior exhibited by cancer cells in patients before and after starting a specific treatment. Usually, levels of enzymes and cell rigidity are used to distinguish normal and cancerous tissues. More recently, the evaluation of the water apparent diffusion coefficient (ADC) within a tissue, obtained from diffusion weighted magnetic resonance imaging (DW-MRI) analysis or multiparametric magnetic resonance imaging (mpMRI), has become a promising tool in diagnosing clinical conditions. However, while MRI techniques can provide crucial information on the microscopic scale, neutron spectroscopy is the perfect choice to evaluate cellular water dynamics on sub-micrometric and sub-nanosecond scales. In this talk, we discuss on very promising results of this approach by comparing results obtained using quasi-elastic and inelastic neutron scattering combined to thermal analysis on treated and non-treated breast cancer cells. The ensemble of our results allowed correlating changes on the mobility of cellular water to cancer development or recession.

Finally, we show that neutron spectroscopy combined to DFT calculations permits direct comparison of the dynamics of an encapsulated anti-cancer drug to that of the pure form. This approach allows for answering one of the major questions that hinders the development of drug delivery systems: how confinement influences drug dynamics? This information is a key step in understanding and controlling carrier/drug interactions and releasing mechanisms [2].


E-mail for corresponding author: bordallo@nbi.ku.dk
Dynamics of atomic hydrogen in bulk and nanocrystalline palladium

Maiko KOFU$^{1,2}$, Naoki HASHIMOTO$^2$, Hiroshi AKIBA$^2$, Hirokazu KOBAYASHI$^3$, Hiroshi KITAGAWA$^3$, Madhusudan TYAGI$^4$, Antonio FARAONE$^4$, John COLEY$^5$, Wiebke LOHSTROH$^5$, Kazuki IIDA$^6$, Mitsutaka NAKAMURA$^1$, Osamu YAMAMURO$^2$

$^1$Japan Atomic Energy Agency, J-PARC Center, Tokai, Japan
$^2$University of Tokyo, Institute for Solid State Physics, Kashiwa, Japan
$^3$Kyoto University, Graduate School of Science, Kyoto, Japan
$^4$NIST Center for Neutron Research, Gaithersburg, USA
$^5$Technische Universität München, Heinz Maier-Leibnitz Zentrum, Garching, Germany
$^6$Comprehensive Research Organization for Science and Society, Tokai, Japan

The behavior of hydrogen in metals has attracted much attention in fundamental and applied research areas. Palladium hydride (PdH$_x$; $x < 1$) is a typical metal-hydrogen system and has been studied for many decades. Pd has remarkable abilities to absorb plenty of H atoms and the H atoms are highly mobile in the Pd lattice. It is interesting to examine how the properties are changed as the particle size is reduced to a nanometer-scale. We have investigated structure [1], diffusion [2] and vibrational dynamics [3] by means of neutron scattering techniques for both bulk and nanocrystalline PdH$_x$/ PdD$_x$ with a diameter of ca. 8 nm.

Neutron diffraction work on nanocrystalline PdD$_{0.36}$ demonstrated that hydrogen atoms are accommodated both at the octahedral (O) sites (1/2, 1/2, 1/2) and the tetrahedral (T) sites (1/4, 1/4, 1/4). This is in contrast to bulk PdH$_{0.7}$ with the occupation of only octahedral (O) sites. Quasielastic neutron scattering measurements were carried out to probe the diffusion of H atoms. With respect to bulk PdH$_{0.7}$, two relaxation processes were found. For both processes, the variation of the relaxation times with momentum transfer was well reproduced by the jump diffusion (Chudley-Elliott) model involving instantaneous jumps among the O sites. The fast relaxation fraction decreased upon cooling. By comparing the activation energies for the diffusion processes and the energy gap between the ground and excited states, we conclude that the slow relaxation corresponds to jumps between the ground states and the fast one between the first excited states. In nanocrystalline PdH$_{0.5}$, we found a new faster diffusion process with a smaller activation energy in addition to the one observed in the bulk sample. The fast relaxation process was more pronounced at higher temperatures, which is consistent with the temperature dependence of the T-site occupancy. Furthermore, the vibrational spectra of hydrogen in bulk and nanocrystalline Pd were investigated by inelastic neutron scattering.
The spectrum of bulk PdH$_{0.7}$ is roughly described by quantum harmonic oscillators. On the other hand, nanocrystalline PdH$_{0.5}$ exhibits two distinct vibrational excitations; one resembles that observed in bulk PdH$_{0.7}$ and the other is new excitations which appeared at higher energies. Our analysis demonstrated that the new excitations are attributed to the hydrogen vibrations in a highly anharmonic trumpetlike potential. The additional diffusion process and vibrational states are attributed to the H atoms at the T sites in the subsurface region where the potential energy surface is substantially modified by surface strain/distortion effects.


E-mail for corresponding author: maiko.kofu@j-parc.jp
The potential of quasielastic neutron scattering (QENS) to give a unique and detailed insight into the behaviour of active species in both established and emerging microporous catalytic systems is illustrated in 3 case studies, studying methanol-to-gasoline (MTG), ammonia selective catalytic reduction (NH\textsubscript{3}-SCR) catalysis, and the zeotype catalysed Beckmann rearrangement.

We analyse the dynamics of methanol in ZSM-5 catalysts both with and without the hydrocarbon pool, resulting from the MTG reaction taking place at 623K and 673 K, to determine the effects of catalyst use on molecular mobility.[1] Using QENS, we observe that methanol is immobile on the instrumental time scale in the fresh catalyst (ZSM-5-F) and in the sample used to convert methanol for 3 days at 623 K (ZSM-5-623). However, in zeolite ZSM-5-673 (MTG at 673 K for 3 days) we observe isotropic methanol rotation. The observed differences between the zeolites in methanol dynamics are attributed to the development of mesoporosity in ZSM-5-673 due to the high reaction temperature of 673 K, leading to dislodgement of lattice Al as is evident from NMR and porosimetry data.

In collaboration with Johnson Matthey, QENS and MD simulations were combined and applied to the Cu-CHA zeolite catalysed NH\textsubscript{3}-SCR process.[2] The effect of counterion presence on ammonia mobility was studied through comparing the diffusivity in a Cu-CHA sample and a counterion free sample. Our studies of the effect of Cu\textsuperscript{2+} presence in CHA found little impact of the counterion on NH\textsubscript{3} diffusivity, with the NH\textsubscript{3} performing jumps through the 8-rings between cages at the same rate between both samples. The finding was rationalized by MD simulations which observed that coordination shells formed around the Cu\textsuperscript{2+}, shielding other NH\textsubscript{3} molecules which were mobile, allowing the unimpeded intercage jump diffusion. Further studies on the 2-dimensional CHA analogue Levyvine (LEV) using QENS show that while the dynamics on the picoscale are the same with jump between 8-ring cages, mobility on the nanoscale in CHA is higher by a factor of 2 due the increase in 8-ring windows available in the CHA building unit.[3]

In the context of the zeotype catalysed Beckmann rearrangement, we study the mobility of cyclohexanone oxime in a microporous catalyst in comparison with a hierarchical micro/mesoporous analogue. Counterintuitively, we find that the introduction or larger mesopores into the catalyst structure lowers the overall mobility of the oxime due to the presence of a larger immobile fraction. The increase in the immobile fraction is explained by the walls of the mesopore being terminated by strongly adsorbing terminal silanol groups, immobilising the oxime at the low loadings studied.
Many systems of interest to both pharmaceutical and materials science show some extent of disorder, which typically breaks the global positional or orientational molecular arrangement, resulting in occurrence of an amorphous, liquid- or plastic-crystal state. However, the partial disorder may be also manifested at a local scale in the well-defined systems, i.e. the molecular crystals. This might both affect a number of properties of a material, including the stability and dissolution rates of pharmaceutical solids, as well as lead to artefacts in structure elucidation.

Standard X-Ray and neutron diffraction techniques in principle explore the long range, *global ordering* with an infinite time window. On the contrary, techniques like incoherent inelastic neutron scattering (IINS) or time-domain terahertz spectroscopy (THz-TDS) use a dynamic probe at the picosecond timescale. Combining these two perspectives provides a new insight into the structure of materials, facilitated by the rapid progress in the field of computational chemistry.

This talk presents several examples from the field of materials chemistry [1] and pharmaceutical science [2-5] to illustrate how computationally-supported vibrational spectroscopy might be used in refining the crystallographic models. The role of the first-principles computations in understanding of the structural features and dynamic phenomena is assessed along with the limitations and challenges of modern, computational solid-state chemistry.[4,6]

E-mail for corresponding author: kacper.druzbiicki@amu.edu.pl
An in-depth understanding of the structure – property relationships is essential for the successful discovery and preparation of new functional materials capable of overcoming the limitations of the currently used ones. As materials’ complexity increases, characterisation using a range of scattering-based techniques and complementary methods, as well as state-of-the-art data analysis approaches and computational simulations, is essential in providing this insight.

This presentation will give an overview of our recent work on oxide ion conductors: the elucidation of key design principles, defects and mechanisms giving rise to ionic mobility; the development and use of advanced structural data analysis methodologies capable of tackling exceptionally complex crystallographic problems arising from phase transitions; the complementary use of long-range and local structural probes in understanding the structure, properties and disorder. In particular, it will illustrate the insight into the oxide-ion dynamics in solid electrolytes which inelastic and quasielastic neutron scattering, supported by ab-initio calculations can provide.


E-mail for corresponding author: ivana.radosavljevic@durham.ac.uk
Unraveling the properties of systems based on single-chain nano-particles

Arantxa ARBE

Centro de Física de Materiales (CFM) (CSIC-UPV/EHU), San Sebastián, Spain

Single-Chain Nano-Particles (SCNPs) obtained by intra-molecular cross-linking of linear macromolecules (precursors) are emerging soft nano-objects showing unique and remarkable physicochemical and rheological properties as a result of their locally collapsed structure and ultrasmall size. Sensing capabilities, controlled drug delivery and catalytic applications of SCNPs have been demonstrated in dilute conditions. Also, one of the first envisaged applications for SCNPs was to be used as ‘fillers’ in all-polymer nano-composites. The impact of internal cross-linking on the structural and dynamical properties of systems containing these nano-objects is the key question to answer in this context. During the last years we have applied neutron scattering techniques supported by coarse grained molecular dynamics simulations to contribute to this field (see, e. g., [1-7]). Our studies include dilute and crowded solutions of SCNPs, all-polymer nano-composites and melts of SCNPs. Here we show the microscopic insight provided by our investigations on these intriguing systems.


E-mail for corresponding author: a.arbe@ehu.eus
Molecular transport in porous materials and adsorption induced phenomena observed through the lens of neutron spectroscopy

Margarita Russina

Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, Berlin, Germany

The adsorption of liquids and gasses in porous materials is important for many areas of science and applications ranging from energy storage for hydrogen economy to applications in catalysis or to the development of novel drug carriers. In this context, the fundamental understanding of criteria governing the molecular mechanism of adsorption and the process of hydrogen bonds formation is of high importance.

Using neutron scattering and in particular TOF spectrometer NEAT as a powerful magnifying glass we have followed in situ the process of gas adsorption on molecular scale. NEAT has a long history of successful application to the study of nanoscale dynamics over broad time and length scales. Recent upgrade of the instrument resulted in 300 fold higher count rate compared to the predecessor and placed NEAT at the same level as a world leader INS [1]. High count rate and new instrumental capabilities provide optimal experimental conditions for in-situ investigations of the confinement processes in porous systems. Targeted selection of the confining systems and the gradual change in the amount of adsorbed molecules allowed us to tune the degree of guest-host interactions and to follow the molecular behavior systematically.

We observe that even in systems with weak guest-host interactions the molecular mobility depends in a very sensitive way on the structural properties of the host such as pore size and shape [2], [3]. Thus, we have found that the intra-cage diffusive mobility of molecular hydrogen confined into clathrate hydrates can be modified in both directions, i.e. substantially reduced or enhanced compared to those in the bulk material at the same temperatures just by a moderate variation of the pore size by about 20-30%. With an increase of guest-host interactions we see the onset of adsorption induced changes in the structure of porous host and the formation of new structural phases of guest molecules [4], [5]. These molecular scale phenomena ultimately control macroscopic properties such as sorption storage capacity, isotherm behavior etc. Smart tuning of the guest host interactions can serve as one of the strategies for achieving enhanced storage properties or for the utilization of novel phenomena such as negative gas adsorption [4], [6].

E-mail for corresponding author: margarita.russina@helmholtz-berlin.de
Biopolymers such as proteins undergo sophisticated changes in space and time, in order to keep the cells functioning. These motions are believed to ultimately govern the biological function and activities of the biopolymer. Quasi-elastic neutron scattering (QENS) provide exceptional tools for studying the dynamics of protein and other biopolymers in the time range of 10ps to 1ns at the molecular level. Here we provide several examples of using QENS technique to study the dynamic behavior of biopolymers under different environments.

The first example is to study the effects of pressure on the conformational flexibility and relaxation dynamics of a hyperthermophilic protein, IPPase, that is found in the deep-sea [1]. Our results indicate that under a pressure of 100 MPa, close to that of the native environment deep under the sea, IPPase displays much faster relaxation dynamics than a mesophilic model protein, hen egg white lysozyme (HEWL) at all measured temperatures, opposite to what we observed previously under ambient pressure [2]. These contradictory observations imply that high pressure affects the dynamical properties of proteins by distorting their energy landscapes. Accordingly, we derived a general schematic denaturation phase diagram that can be used as a general picture to understand the effects of pressure on protein dynamics and activities.

The second example is to obtain fundamental understanding of the impact of hydrophilic nanodiamond (ND) surface on biomolecules at the molecular level. In this work, the tRNA dynamics on ND surfaces are investigated by QENS and all atom molecular dynamics simulations [3]. Both QENS experiments and MD simulations show faster dynamics of tRNA on ND surface compared to that of the dry tRNA on ND surfaces and freestanding RNA molecules. The strong, attractive interactions between ND, tRNA, and water give rise to unlike dynamical behavior and structural changes of tRNA in front of ND compared to without ND. Our new findings may provide new design principles for safer, improved drug delivery platforms.

We also used QENS to study the microscopic dynamics of the dark-state rhodopsin versus the ligand-free opsin, to answer how the dynamics of rhodopsin change during photoactivation [4]. These observations and further investigation using QENS can reveal important macromolecular dynamic behaviors that cannot be otherwise measured by other techniques.

E-mail for corresponding author: xqchu@gscaep.ac.cn
QENS Invited Talks

QI_01  The discovery of the proton polaron

Artur BRAUN, Qianli CHEN

1Empa. Swiss Federal Laboratories for Materials Science and Technology High Performance Ceramics, Dübendorf, Switzerland

2University of Michigan – Shanghai Jiao Tong University Joint Institute, Shanghai, China

In electrochemical energy storage and conversion, electrodes and electrolytes are the key components of batteries, fuel cells and capacitors. Electrons and ions are the relevant electric charge carriers. The key player in technology for the hydrogen economy is the proton - an elusive charge carrier which cannot be so easily detected [1]. Ceramic proton conductors can be used as electrolyte membranes in solid state devices. Smart defect engineering makes that oxygen vacancies can be filled with oxygen ions from ambient vapor water molecules. The protons from the water molecule form intermediate OH bonds with proximate oxygen ions. Upon thermal activation, the OH bonds melt and the proton becomes liberated as positive charge carrier. The transport properties of the yttrium doped barium cerate and barium zirconate electrolytes were investigated by thermodynamic parameterization of their structure with temperature 273 K - 773 K and pressure 0 - 6 GPa. The proton conductivity activation energy decreases linear with increasing lattice spacing, suggesting that epitaxial strained films should be promising future electrolyte membranes. The Raman modes increase with increasing pressure and get a slightly higher "pitch" upon protonation. The OH bond breaking occurs at a characteristic temperature range which is accompanied by the onset of a lateral proton diffusivity which accounts for the macroscopic conductivity as measured with electroanalytical methods. At the microscopic scale, ambient pressure XPS and quasi elastic neutron scattering which were carried out operando parallel on the same samples with impedance spectroscopy, confirm that it is exactly this proton phonon coupling which switches the proton conductivity on. The quantitative analysis of the proton jumping frequencies showed that the Ce-O stretching mode is the effective propeller for the proton at work. Moreover, the temperature dependence of the proton jump frequency follows exactly the mathematical model for a Holstein polaron, rendering the proton conductivity process in ceramic proton conductors a genuine proton polaron [2].


E-mail for corresponding author: Artur.Braun@alumni.ethz.ch
Neutron spin echo spectroscopy as a sensitive tool to study membrane elasticity in microemulsions

Olaf HOLDERER¹

¹Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

The high energy resolution of Neutron Spin Echo (NSE) Spectroscopy is perfectly suited for studying thermally driven membrane fluctuations in soft matter systems. Measuring membrane fluctuations allows determining the membrane bare bending rigidity of a membrane patch and is complementary to phase diagram measurements and SANS [1]. Adding co-surfactants such as diblock copolymers or homopolymers to the microemulsion modifies the bending rigidity and has been followed with NSE. A recent topic in microemulsion membrane dynamics was the influence of a rigid interface to the surfactant membrane. Microscopic flat interfaces provided by clay particles [3] as well as macroscopic interfaces were investigated [4]. The latter has been studied in grazing incidence geometry, a new development in NSE Spectroscopy where in analogy to GISANS only the part of the sample at a solid/liquid interface is illuminated with an evanescent neutron wave. Despite the low intensity, a carefully designed low background sample cell together with new neutron optical components such as neutron resonator structures [5] allowed to gather interface specific information and to observe modifications of the undulation dispersion relations in soft membranes such as microemulsions [4] and also phospholipid membranes [6].


E-mail for corresponding author: o.holderer@fz-juelich.de
In functional polymeric nanomaterials the confinement by a solid surface can have crucial effects on the structural and dynamical properties of the polymer. Both in nanocomposites - nanosized particles homogenously dispersed in a polymeric matrix (nanocomposites) - as well as in polymer chains that are confined in porous media, e.g. in long cylindrical nanopores, the number of possible conformations of a polymer chain can be reduced due to the presence of a large amount of solid surface. Effects on the dynamics are particular important for those macromolecules, which are close to the surface [1].

Investigations with neutron spin-echo (NSE) [2, 3] have evidenced that the attractive polymer-surface interaction can have a two-fold effect: The adsorption of polymer to the pore surface favors the formation of a surface layer that slows down the dynamics [2] - as compared to the that of pure polymer; the anchoring of the polymer segments on the surface creates an interphase between the polymer in close vicinity to the solid surface and the pure polymer [3]. It was also observed that under strong confinement conditions [4] the entanglement network becomes diluted.

In absence of specific adsorption of the polymer segment on the Alumina surface, i.e. at locally repulsive polymer-surface interaction, no effect of the confining walls on the local segment relaxation is observed [5]. On the larger scale both the Rouse relaxation rate and the entanglement distance do not differ between bulk and confined polymer melts within experimental accuracy. The neutron scattering experiments clearly show that for a confinement size equaling the polymer end-to-end distance, the entanglement network is not affected, a result that is not so clear from simulations.


E-mail: m.kruteva@fz-juelich.de
Gradual cross-over from sub-diffusion to normal-diffusion: a many-body effect in protein surface water

Pan Tan, Yihao Liang, Xiangjun Xing and Liang Hong

School of Physics and Astronomy & Institute of Natural Sciences, Shanghai Jiao Tong University, Shanghai, China 200240.

Dynamics of hydration water is essential for the functionality of enclosed protein molecules. Diffusing water not only transports enzymatically essential ingredients, e.g., ions, substrates and protons, into the catalytic sites of proteins, but also renders internal flexibility necessary for the functioning of biomacromolecule. It has been demonstrated that water molecules exhibit sub-diffusion on protein surfaces; yet the microscopic mechanism remains vague. Here, we combine neutron scattering experiments with molecular dynamics simulations and analytic modelling to study dynamics of hydration water in perdeuterated protein powders. We find that water molecules jump randomly between trapping sites on protein surfaces. The trapping times of these sites follow a broad, power-law distribution, which results in sub-diffusion. Moreover, the sub-diffusive exponent gradually increases with observation time towards normal diffusion due to a many-body volume-exclusion effect.

Email for corresponding author: hongl3liang@sjtu.edu.cn
QI_06 Neutron scattering study on the thermoelectric material ZrNiSn1-xSbx with half-heusler alloy

Qingyong Ren1, Chenguang Fu2, Yingtu Liu2, Jiong Yang3, Tiejun Zhu2, Jie Ma1

1School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China
2Department of Materials Science and Engineering, Zhejiang University, Hangzhou, Zhejiang 310027, China
3Materials Genome Institute, Shanghai University, Shanghai, 200444, China

Due to the narrow band gap and sharp slope of the density of states near the Fermi level [1, 2], Half-Heusler (HH) alloy was recognized as a potential high temperature thermoelectric (TE) material, which could directly convert the waste heat into usable electricity and solve the energy crisis. After it was first reported on 1999, the TE performance had been significantly optimized and a maximum zT~1 had been obtained. However, most efforts had been devoted to tune the carrier concentration and reduce the lattice thermal conductivity by doping [3, 4], which only qualitatively analyzed the mechanism. And it was hard to find the original driving force of low zT and designed an advanced TE material due to the limited information. We synthesized a series of ZrNiSn1-xSbx (x=0, 0.04, 0.08 and 0.12) compound, and applied neutron scattering technique to study both the static and dynamic spectra. We found that the anti-site disorder was not important in the system, while extra Ni-vacancy and a specific double-domain effect were obtained. Moreover, the composition- and temperature-dependence of the phonon density-of-states were analyzed by the density functional theory.


E-mail for corresponding author:jma3@sjtu.edu.cn
QI_07  QENS Studies of Reorientational Hydrogen Dynamics in Complex Hydrides

Tatsiana BURANKOVA1, Elsa ROEDERN2, Léjo DUCHÊNE2,4, Aristea E. MANIADAKI3, Zbiegniew ŁODZIANA3, Hans HAGEMANN4, Arndt REMHOF2, Jan EMBS1

1Paul Scherrer Institute, Villigen PSI, Switzerland
2Empa, Dübendorf, Switzerland
3Polish Academy of Sciences, Kraków, Poland
4Université de Genève, Geneva, Switzerland

All-solid-state batteries employing solid-state electrolytes (SSE) promise higher energy densities through the use of high voltage cathodes and metallic anodes and improved operational safety compared to batteries based on liquid organic electrolytes [1]. Moving beyond lithium electrochemistry also offers more sustainable and cost-effective solutions. Development of practical SSEs with high conductivity is, however, a major challenge, which requires a synergistic experimental and computational approach.

QENS has proved to be an informative method for describing reorientational dynamics in a recently emerged SSE class of borohydrides and polyborates, contributing to the increased understanding of fundamental mechanisms underlying superionic conductivity in these materials. A profound characterization of complex systems can, nevertheless, be achieved only with the input from complementary methods. Thus, in this work we demonstrate detailed dynamical portraits of novel SSEs for Li [2,3], Mg [4] and Na [5] batteries obtained by means of the QENS analysis supported by DFT simulations, IR, Raman and NMR spectroscopy. Using deuterium labeling we disentangle contributions of different components of the studied electrolyte systems and build comprehensive models of molecular motions (Figure 1, 2).

Figure 1. Scheme of BH$_4^-$ motions in mixed lithium amide-borohydrides [2]

Figure 2. Scheme of BH$_4^-$ and ligand motions in solid-state Mg electrolyte.

E-mail for corresponding author: tatsiana.burankova@psi.ch, jan.embs@psi.ch
Activated Relaxation and Transport in Liquids well above $T_m$

Marcus CICERONE

National Institute of Standards and Technology, Materials Measurement Lab, Gaithersburg, MD, USA

Microscopic molecular theories of supercooled liquids and glasses often posit the presence of long-lived structures in these systems. Such structures are required to produce observed phenomenology such as spatially heterogeneous dynamics. We find evidence for such structures not only in supercooled liquids, but in simple liquids far above the melting temperature. We present neutron scattering [1, 2], simulation [3], and ultrafast optical experiments showing that these structures and associated dynamic heterogeneities arise at much higher temperature than is typically expected. We also show that they play a very important role in overall transport and relaxation, even in the liquid state.


E-mail for corresponding author: cicerone@nist.gov
On the Relation of Structural Relaxation, Diffusion of Mass, and Viscous Flow in Viscous Metallic Liquids

Andreas Meyer

Institute of Materials Physics in Space, German Aerospace Center (DLR), Cologne, Germany

Electrostatic- and electromagnetic levitation of metallic droplets allows to access investigation of chemical reactive metallic liquids and a deep undercooling below their melting point. In combination with quasielastic neutron scattering container-less positioning enables measurements of dynamical properties in a large range of momentum and energy transfer with an exceptional signal-to-noise ratio.

Here results from QENS measurements on various viscous metallic liquids on the time-of-flight spectrometer ToFToF of the Forschungsneutronenquelle Heinz Maier-Leibnitz in Garching, Germany, are presented. Incoherent scattering at small $Q$ values gives access to self-diffusion coefficients – coherent scattering around $Q$ values of the structure factor maximum to structural relaxation times. The data set is complemented with measurements of density and of viscosity via the oscillating drop method on the levitated samples.

The results are discussed in context of the Stokes-Einstein relation, liquid state theory in the hydrodynamic regime and the Maxwell equation.

E-mail for corresponding author: andreas.meyer@dlr.de
We present an overview of protein dynamics based mostly on results of neutron scattering that cover very broad frequency (time) range by combining time-of-flight, backscattering and spin echo data. To broaden the frequency range even more, the neutron scattering data are complimented by dielectric relaxation spectroscopy data. To unravel microscopic details of the protein dynamics we also involve results of molecular dynamics simulations. We identify several major classes of protein motions on the time scale from faster than picoseconds to several microseconds [1-4], and discuss the coupling of these processes to dynamics of hydration water [2,4-6]. Our analysis suggests that the microsecond backbone relaxation process might be the main structural relaxation of proteins, and it defines their glass transition temperature [1,4], while faster processes present kind of localized secondary relaxations [1-5]. Based on the overview, we formulate a general picture of protein dynamics and discuss the challenges in the field of dynamics of biological molecules.


E-mail for corresponding author: sokolov@utk.edu
Cell membrane is a complex heterogeneous mixture of lipids, proteins and carbohydrates. Dynamics of cell membrane is a prime determinant in a number of physiological processes such as cell signaling, permeability, etc. The basic matrix of the cell membrane is a lipid bilayer, which exhibits the rich phase behavior. We have studied detailed dynamical landscapes and phase behavior of lipid bilayer using incoherent elastic and quasielastic neutron scattering [1-5]. Our studies showed presence of four distinct motions: (i) lateral motion of the lipid within the leaflet (ii) localized internal motion of the lipid (iii) bending and (iv) thickness fluctuation of the membrane [1-5]. We have also studied interactions of different membrane active peptides [6-8], drugs [5], antioxidants [9], cholesterol [8] with phospholipid membranes. Various interesting results including a new action mechanism of antimicrobial peptides, mitigation of the destabilizing effect of antimicrobial peptide due to presence of cholesterol, etc. are found and will be discussed in this talk. To understand tunable antimicrobial activity of ionic liquids (ILs), we have recently investigated effects of ILs on the microscopic dynamics and phase behaviour of the phospholipid membrane [10-11]. It is found that interaction of ILs with phospholipid membrane is primarily responsible for their antimicrobial activity and can be tuned by varying the alkyl chain length of the IL.


E-mail for corresponding author: sharmavk@barc.gov.in ; vksphy@gmail.com
In this talk, we will discuss the role and state of water in hydrogen fuel cells, with particular focus on the dynamical behavior of water (and protons) confined within nanostructured proton-conducting polymer electrolyte membranes (PEMs). The PEM is the key component of low temperature fuel cells, which are one of the most promising technologies for powering small portable devices and automobiles. It acts as a separator between the electrodes, electronic insulator and proton conductor. A microscopic understanding of the relation between the chemical structure of the polymer membrane, its morphology, and the proton transfer is essential to improve fuel cell performances. Benchmark materials are PerfluoroSulfonic Acids (PFSA), composed of a hydrophobic PTFE matrix bearing side-chains terminated by hydrophilic SO$_3^-$ groups. In the presence of water, interconnected nanoscale ionic domains are formed upon swelling. The efficiency of proton conduction is directly impacted by the total amount of water and the microscopic properties of the adsorbed molecules. Herein, we will review our recent efforts to probe the water and proton multi-scale dynamics by combining multi-resolution Quasi Elastic Neutron Scattering (QENS) [1-4], PFG-NMR and Molecular Dynamics simulations [5,6]. We demonstrate that the mobility of species is controlled by the balance between short range interactions and connectivity. Confinement at the nano-scale and direct interaction with the interfaces are shown to produce anomalous sub-diffusion within the ionic nanochannels [7]. In conclusion, we elucidate the true nature of water confined in soft ionic nanostructures and provide a general understanding of the complex multi-scale structure-function interplay in advanced materials for use as electrolytes in energy devices.


E-mail for corresponding author: sandrine.lyonnard@cea.fr
Ionic liquids (ILs), having a melting temperature typically below 400K, are a fascinating class of materials showing a huge diversity of interactions (Coulomb, van der Waals, hydrogen bonds, ...) and dynamical processes (long-range diffusion, localized processes like methyl-group rotations, charge transport via proton-hopping, ...) depending on the composition, i.e. the kind and nature (protic vs. aprotic) of ions the liquid is made of. Due to properties like negligible vapor pressure, good electrochemical and thermal stability, and tunable structures, ILs are now extensively used in many relevant applications (biomass processing, pharma-ceutical, biotechnological and electrochemical applications, ...). Even though a huge number of applications involving ILs has been established, many fundamental questions related to the underlying microscopic mechanisms are still unanswered. In our research we focus on basic dynamical processes and the question how these processes are influenced by the structure and composition of ILs. This is especially important with respect to the question how charge transport happens in ILs that are regarded as potential electrolytes in energy applications.

In my talk I will give a review of our research on different IL systems ranging from pyridinium- and imidazolium based ILs to those ionic liquids, which show interesting magnetic features [1-8]. In our investigations we use typical neutron scattering techniques (QENS on tof- and backscattering instruments, diffraction, polarized neutrons) in combination with simulation approaches (classical and ab-initio MD, DFT), complementary characterization methods (DSC, NMR, magnetic measurements) and advanced chemical synthesis methods (methylation, selective deuteration) in order to accomplish a comprehensive understanding of microscopic structures and processes occurring in ILs.


E-mail for corresponding author: jan.embs@psi.ch
We illustrate the potentialities of Quasi-Elastic Neutron Scattering (QENS) in the study of Ionic Liquids (ILs). ILs are pure solutions of charged organic molecules with no solvent. These molecular electrolytes show a property original for a pure liquid: they self-organize in nanometric fluctuating aggregates \[1\]. When probed at the macroscopic scale, ILs behave as highly dissociated (i.e. strong) electrolytes \[2\] while, at the molecular scale, they show clear characteristics of weak ionic solutions \[3\]. In this talk, we report a multi-scale analysis (time-of-flight and spin-echo neutron scattering, PFG-NMR and Dynamic Light Scattering based nano-rheology) that sheds new light on these apparently at odd behaviors \[4,5\].

Due to their remarkable chemical and electrochemical stability, ILs have been identified as prime candidates electrolytes for the development of new safe and sustainable energy storage systems. We show \[6\] a noticeable enhancement (by a factor 3) of the transport properties of a neat IL under CNT (Carbon NanoTube) confinement in a 1D situation. Such CNT membranes are a possible route to boost the transport properties and hence the specific power of lithium batteries \[7\]. We then address the conductivity of electrolytes directly relevant to the field of electrochemical storage systems: ILs charged with lithium salts. We show that these electrolytes confined in 1D CNT membranes show a drastic and unprecedented increase in ionic conductivity. Compared to the bulk analogues, we indeed report conductivity gains by a factor up to 50 upon macroscopic 1D CNT confinement.

Such a disruptive concept of a 1D CNT based separator laying at the cross-road of basic science and applied research is probably of interest for future technological outcomes.


Corresponding Author: jmzanotti@cea.fr
Influence of PEGylation on protein dynamics

Ralf Biehl¹, Karol Ciepluch¹, Karol Ciepluch¹,⁴, Aurel Radulescu², Ingo Hoffmann³, Andreas Raba¹, Jürgen Allgaier¹, Dieter Richter¹

1 Jülich Centre for Neutron Science & Institute of Complex Systems(JCNS-1&ICS-1), Forschungszentrum Jülich, Germany
2 Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich, Germany
3 Institute Laue-Langevin (ILL), 71 rue des Martyrs, 38042 Grenoble, Cedex 9, France
4 Department of Biochemistry and Genetics, Jan Kochanowski University, Kielce, Poland

Protein-polymer conjugation is a widely used technique to develop protein therapeutics with improved pharmacokinetic properties as prolonged half-life, higher stability, water solubility, lower immunogenicity and antigenicity. Combining biochemical methods, small angle scattering (SAXS/SANS) and neutron spinecho spectroscopy here we examine the impact of PEGylation (i.e., the covalent conjugation with polyethylenglycol or PEG) on interaction between protein-polymer conjugates and on structure and internal domain dynamics between them.

We use Phosphoglycerate Kinase (PGK) to elucidate the reason for reduced activity that is connected to PEGylation. PGK is a protein with a hinge motion between the two main domains that is directly related to function.

The interaction between different conjugates shows a double Yukawa characteristic due to the different interaction ranges of protein surface charge and polymer coil attached to the surface.

The overall configuration of PGK is not changed in comparison to the native structure. NSE explores the internal domain dynamics between the main PGK domains. We find that these dynamics is mainly unchanged but we find a second component of translational diffusion in a harmonic potential between polymer coil and protein. This interaction is discussed in terms of the Ornstein-Uhlenbeck process.

E-mail for corresponding author: Ra.biehl@fz-juelich.de
Perovskite MAPbI$_3$ exhibits outstanding optoelectronic properties, but its thermal instability still hinders its practical applications. Previous studies showed that the thermal properties are closely related to the combined characteristics of the inorganic framework lattice vibrations and the organic cations jumping rotational modes, but the detailed microscopic mechanisms are yet to be fully understood. In this presentation, the pressure effects on phonon scattering in MAPbI$_3$ are discussed based on the results obtained from molecular dynamics simulations and inelastic neutron scattering measurements. Using the mode decomposition technique, we have obtained the phonon lifetimes, including those of the optical modes which have very large linewidths. Most interestingly, we find that the phonon scattering in the tetragonal phase is very sensitive to compression. A small hydrostatic pressure of several kbar can lead to significant changes of phonon lifetimes due to the four-fold rotation of the MA$^+$ cations around the C-N axis. Our results provide a better understanding of the lattice dynamics of MAPbI$_3$ and important insight into the pressure phonon relationship. The large pressure response of phonon scattering is expected to pave the way for further thermal engineering of MAPbI$_3$ and related perovskites.
Lipid molecules are the basic building block of biological membranes. These membranes are dynamic in nature across a wide range of length and time scales. Among these diverse dynamics, quasi-elastic neutron scattering (QENS) techniques cover dynamics ranging from molecular movements of lipids, water molecules, and/or additives [1] to collective motions of two or more lipid molecules. Recently some of us showed that neutron spin echo spectroscopy (NSE) can be used to measure lipid membrane viscosity, $\eta_m$, by measuring the collective thermal thickness fluctuations. [2] The membrane viscosity is one of two key parameters that characterize the membrane transport properties, such as diffusion of molecules in the membranes to accommodate biological functions. As is widely known, the other key parameter is the molecular diffusion constant, $D$, in the membrane which is also accessible by QENS. [3] While there are various ways to measure $D$ in membranes, such as fluorescence microscopy, nuclear magnetic resonance, as well as QENS, very few techniques can be used to measure $\eta_m$ directly. As NSE can access $\eta_m$ through the thermal fluctuations of membranes, a combination of these QENS techniques offers an opportunity to directly compare $D$ and $\eta_m$ experimentally.

Here we prepared large unilamellar vesicles with the radius $R$ of about 50 nm in water, and the same concentration samples were used to measure a backscattering spectrum using DNA in J-PARC [4] and compared the result with the one measured by NSE. The temperature dependence of $D$ and $\eta_m$ both showed Arrhenius type behavior, and the estimated activation energies were similar to each other. A direct comparison between these parameters confirmed the two-dimensional diffusion model of a cylindrical inclusion in a membrane by Saffman and Delbrück. [5] As biological membranes contain various types of molecules including proteins, the present methodology with proper deuteration schemes may start providing a deeper understanding of membrane transport properties in such complex environments.

E-mail for corresponding author: mnagao@indiana.edu
At low salt conditions, it is common for the protein-protein interaction to have both a short-range attraction (SA) and a long-range repulsion (LR). These kinds of competing potential features result in the rich phase behavior of protein solutions which is important for protein formulations in the pharmaceutical industry.[1] Depending on the potential parameters, it has been recently proposed that protein solutions can have different liquid states, such as dispersed fluid state, clustered fluid state, random percolated state, and cluster percolated state.[2] Using purified lysozyme proteins, we have investigated concentrated protein solutions at a very wide range of concentrations and temperatures. We observed the localized glassy like behavior at the short time scale for highly concentrated solutions at low temperatures using a neutron spin echo while the same samples remain Newtonian fluid for the investigated range of the shear rates determined by a microcapillary viscometer.[3] The inter-protein structure investigated by small angle neutron scattering revealed that this interesting behavior is introduced by the formation of intermediate range order (IRO) due to the competition of the SA and LR interaction. The IRO causes the localized heterogeneous density distribution only at the intermediate range length scale, i.e., frustrated or localized phase transition. And the same samples have uniform density distribution at larger length scales. This is intrinsically different from commonly studied colloidal gel systems where the heterogeneous density distribution tends to extend to the whole system. Our results demonstrated the importance of the structure at the IRO length scale to understand the properties of protein solutions.

E-mail for corresponding author: yunliu@nist.gov
Magnetic Fluctuations, Precursor Phenomena, and Phase Transition in skyrmion hosting chiral magnets

Catherine PAPPAS¹, Lars J. BANNENBERG¹, Eddy LELIEVRE-BERNA², Fenjiao QIAN¹, Robert M. DALGLIESH³, Peter FALUS²

¹Delft University of Technology, Mekelweg 15, 2629 JB Delft, Netherlands
²Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France
³STFC, ISIS, Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom

The phase diagram of skyrmion hosting chiral helimagnets like MnSi, Mn₃₋ₓFeₓSi or Fe₁₋ₓCoₓSi follows the same generic scheme composed of helical spiral, conical spiral and skyrmion crystal phases. At zero magnetic field and for weak disorder the transition to the helimagnetic state is of first order. Above Tc in a region dominated by precursor phenomena, neutron scattering shows the buildup of strong chiral fluctuating correlations over the surface of a sphere with radius 2\pi/\ell where \ell is the pitch of the helix. We present a comprehensive inelastic neutron scattering study of the precursor phenomena using high resolution Neutron Spin echo spectroscopy also under magnetic fields [1,2]. The magnetic field does not alter the sharp first order transition although it has a strong influence on the spatial distribution of the fluctuating correlations. The results are discussed in the context of literature, the debate on the existence of a tricritical point and the relevance of a scenario proposed by Brazovskii [3,4] for liquid crystals to describe the first order nature of the transition in chiral magnets.


E-mail for corresponding author: c.pappas@tudelft.nl
Suppression of the long-range order in polycyclic aromatic hydrocarbons

Mattia GABOARDI,1 Ian SILVERWOOD,1 Jay SIEGEL,2 and Felix FERNANDEZ-ALONSO,1,3

1ISIS Facility, Rutherford Appleton Laboratory (Harwell Campus, Chilton, Didcot, OX110QX, UK)
2School of Pharmaceutical Science and Technology (Tianjin University, Nankai District, Tianjin, P.R. China)
3Department of Physics and Astronomy (University College London, Gower Street, London, WC1E6BT, UK)

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds entirely made of aromatic carbon and hydrogen that can range from the simplest case of anthracene toward the limit of graphene (when all the edges are saturated by hydrogens). Such molecules are abundant in the Universe and thought to be the starting material for the earliest forms of life. Intercalated with alkali metals, they can lead to new materials of interest for energy storage applications, such as organic superconductivity,1 hydrogen storage,2 and batteries.3

A curious case is given by the bowl-shaped Corannulene (C20H10), that resemble a 1/3 fragment of fullerene and crystallizes in a monoclinic (P21/n) lattice. Although crystalline and thermodynamic parameters of C20H10 are known since decades, an elusive transition has been revealed only recently and might shed more light on the intermolecular order of such interesting compounds.

Figure 1 C20H10 molecule and QENS profile across the pre-melting transition.


E-mail for corresponding author: mattia.gaboardi@stfc.ac.uk
QI_21  QENS insights on the nanoscopic origin of rheological properties in some well-dispersed polymer nanocomposites

Erkan SENSES¹, Antonio FARAONE²

¹Koç University, Department of Chemical and Biological Engineering, Istanbul, Turkey
²National Institute of Standards and Technology, NIST Center for Neutron Research, Gaithersburg, U.S.A.

Polymer nanocomposites (PNCs) with attractive polymer–nanoparticle (NP) interactions, are often reported to disperse individually, enabling the investigation of interfacial effects on the rheological properties without contribution from particle percolation. By taking advantage of selective isotope labeling of the chains, neutron scattering techniques uniquely allow the possibility of investigating the structural and dynamical properties of the polymers in the matrix. In particular, high-resolution QuasiElastic Neutron Scattering (QENS) techniques, such as backscattering and Neutron Spin Echo, allow directly observing the chain motions at the nanoscale by simultaneously accessing a broad range of time-scale (from sub-nanoseconds to hundred nanoseconds), and length-scales (from monomer size to entanglement mesh sizes); specifically important for polymers are the localized fast dynamics on sub-monomer level, the segmental dynamics at the monomer level and the entangled/collective dynamics at larger scales.

Here, I will present results on the nanoscale dynamics of polymer chains in hard [1] and soft (all-polymers) [2] composites with dynamically asymmetric interphases. The effect of the presence of the NPS on the polymer matrix Rouse dynamics and entanglements explains how both a reinforcing and an unusual softening can be induced in the same material. Similarly, the viscosity reduction often observed in composites with NPs of sizes comparable to that of the polymer coils in the matrix, can be explained by chain disentanglement. [3]


E-mail for corresponding author: afaraone@nist.gov
For a group of substances with different chemistry but sharing similar anomalous properties (e.g., density anomaly, diffusivity anomaly), the existence of a liquid-liquid critical point as well as liquid-liquid phase transition is assumed to be the key. However, the experimental confirmation remains challenging since the hypothesized critical point and phase transition are located in the phase region below the homogeneous crystallization line which is difficult for experiments to detect directly. In this talk, I will discuss our recent studies on the liquid-liquid phase transitions from supercritical region using supercritical phenomenon. Our results show that the structure change reflected in the potential energy surface is directly connected to the change in dynamic properties, which is important for the investigation of glass transition at low temperature and thus can also be employed to investigate the liquid-liquid transition occurring in supercritical phase region.

E-mail for corresponding author: limei.xu@pku.edu.cn
A “water in-salt” (WIS) electrolyte, 21m LiTFSI in water, has been used as a parent hydrate salt to dissolve another lithium salt containing an anion of similar fluorinated structure, LiOTf. The mixed salt system, abbreviated “water-in-bisalt” (WIBS), consisting of 21m LiTFSI and 7m LiOTf, provides an aqueous electrolyte with 28m Li⁺, or cation/water ratio of approximately 1:2, for lithium-ion batteries [1]. Compared with the parent WIS system, a more compact and protective solid electrolyte interphase is formed at higher efficiency in this highly ionic aqueous media, allowing a 2.5 V aqueous Li-ion full cell based on the electrochemical couple of LiMn₂O₄ and TiO₂ that delivers the highest voltage and energy density amongst all aqueous battery systems to date. We have measured the dynamics of the WIS electrolyte at two concentrations, 13.9m and 21m and the WIBS electrolyte at (21+7) m at the DNA facility at J-PARC. QENS data were obtained with both H₂O and D₂O solution to get information about both solute and solute dynamics. We complement the QENS measurements with molecular dynamics (MD) simulations using a many-body polarizable force field. Since even the H₂O solutions had appreciable coherent contributions, both coherent and incoherent intermediate scattering functions were extracted from the MD simulations and the appropriate combinations compared with the QENS results.

E-mail for corresponding author: dlongprice@gmail.com
The polarised neutron option for PELICAN [1] has recently been commissioned. This major advance in instrumentation allows the full power of a cold-neutron time-of-flight spectrometer to be realised with a polarised neutron beam. Thus high resolution neutron spectra can be obtained whereby the coherent nuclear, incoherent and magnetic scattering cross sections can be completely separated. As such one should be able to separate magnetic only signals from hydrogenous samples – it is also possible to systematically isolate the vibrational signals (both coherent and incoherent) from the data. Such an experimental configuration is perfect for studying vibronic coupling in molecular magnetism.

We have recently measured the excitations from the fully hydrogenous wheel compound Cr₇Co, [[Me₂NH₂]₂[Cr₇CoF₆(O₂CCMe₃)]₂]. The 1.5 K spectra from Cr₇Co obtained using PELICAN showed a potential magnetic excitation at 1.8 meV. The signal was assigned as magnetic based on its Q and temperature dependence, however overlap of the Hydrogen contribution made analysis difficult. Polarised neutron scattering allows us to completely separate the magnetic effect – which can then be analysed in the conventional manner without need for deuteration. The work presented herein details the first such XYZ polarisation analysis user experiment carried out on PELICAN including a discussion of the instrumentation, experimental setup and the subsequent data analysis employed. It is hoped that the techniques utilised here can be used to analyse hydrogenous molecular magnets whose structure may not lend itself to deuteration. Such improved experimental techniques have the potential to increase the operating performance of future SMM’s as highlighted.
in [2].


E-mail for corresponding author: timd@ansto.gov.au
Polymers with intrinsic microporosity are promising candidates for the active separation layer in gas separation membranes. Here, by means of inelastic neutron scattering, the vibrational density of states (VDOS) and the molecular mobility were investigated for PIM-1, the prototypical polymer with intrinsic microporosity. The results are compared to data measured for a more conventional high-performance polyimide used in gas separation membranes (Matrimid).

The measured data show the characteristic low frequency excess contribution to the VDOS above the Debye sound wave level, generally known as the Boson peak in glass-forming materials. In comparison to the Boson peak of Matrimid, that of PIM-1 is shifted to lower frequencies. This shift is discussed considering the microporous, sponge-like structure of PIM-1 as providing a higher compressibility at the molecular scale than for conventional polymers [1].

Elastic fixed window scans were measured on a neutron backscattering spectrometer to have an overview about the molecular dynamics at a time scale of ca. 1 ns. The temperature dependence of the estimated mean squared displacement shows a step-like increase in the temperature range from 100 K to 250 K indicating the onset of some molecular mobility. The nature of this motional process was analyzed in detail by quasielastic neutron scattering where the data are discussed with regard to both the q- and the temperature dependence.


E-mail for corresponding author: andreas.schoenhals@bam.de
Simultaneous dielectric and neutron spectroscopy under high pressure – applied to glass-forming liquids

Henriette Wase Hansen¹, Alejandro Sanz¹, Karolina ADRIANOWICZ², Bernhard FRICK³, Kristine NISS³

¹Roskilde University, Department of Science, Roskilde, Denmark
²University of Silesia, Institute of Physics, Katowice, Poland
³Institut Laue-Langevin, Grenoble, France

By combining dielectric spectroscopy (DS) and neutron scattering (NS) in our newly developed high-pressure DS-NS cell [1], we show that both the fast and slow dynamics in a glass-forming liquid along isochrones, i.e. constant relaxation time $\tau_\alpha(T,P)$, is invariant, as predicted by isomorph theory using DS and QENS from IN16B and IN5 at Institut Laue-Langevin [2].

The main dynamical feature in glass-forming liquids is the $\alpha$-relaxation. There is no common understanding yet of what governs the timescale and the spectral shape of the relaxation. It has several times been suggested that there is a close connection between fast and slow dynamics, even though they can differ in timescales by more than ten orders of magnitude.

A recent theoretical development in the physics of liquids, the isomorph theory, rationalises this [3]. The fundamental prediction of isomorph theory is the existence of isomorphs, i.e. curves in the phase diagram along which all dynamical phenomena and structure are invariant.

The dynamics in real glass-forming systems is rich and includes a large range of dynamical processes taking place on different timescales. Experimentally, possible isomorphs can be identified by the isochrones; if they are isomorphs, all dynamic processes are expected to be invariant on all timescales.

We investigate the dynamics on pico- and nanosecond timescale with backscattering and time-of-flight combined with dielectric spectroscopy. We show the difference in behaviour between two simple van der Waals liquids and a complex hydrogen bonding liquid in agreement with predictions from isomorph theory along the glass transition isochrone, i.e. $\tau_\alpha$ =100 s [2], and along isochrones found from IN16B, i.e. $\tau_\alpha$ ~ nanoseconds [4].


E-mail for corresponding author: hansenhw@ill.fr
Lattice dynamics and coupled quadrupole-phonon excitations in CeAuAl$_3$

Benqiong LIU$^{1,2}$, Petr ČERMÁK$^{2,3}$, Christian FRANZ$^4$, Christian PFLEIDERER$^4$, Astrid SCHNEIDEWIND$^2$

$^1$Key Laboratory of Neutron Physics, Institute of Nuclear Physics and Chemistry, CAEP, Mianyang 621900, PR China

$^2$Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstrasse 1, 85748 Garching, Germany

$^3$Department of Condensed Matter Physics, Charles University in Prague, Prague, Czechia

$^4$Physik Department E21, Technische Universität München, 85748 Garching, Germany

Cerium intermetallic compounds of CeTX$_3$ type (T=transition metal d element and X=Si, Ge or Al) have attracted considerable attention, due to the discovery of many interesting physical phenomena such as magnetic properties, heavy-fermion behavior and unconventional superconductivity. In most of these systems, the crystal electronic field (CEF) excitations and phonons can be studied independently since they are considered to decouple with each other. However, strong magneto-elastic (MEL) coupling could result in the formation of a bound state of CEF and phonons that shows up in the magnetic cross section as described by a vibronic model for cubic CeAl$_2$ [1, 2] or recently for tetragonal CeCuAl$_3$ [3].

In order to study if such interesting feature exists or not in CeAuAl$_3$ system, neutron scattering experiments have been performed on a single crystal sample in the paramagnetic phase. Except for the transition from the ground state to the first excited doublet, an additional weak magnetic excitation at $E=7.9$ meV has been observed. In order to explain this result, the bound state model for a cubic system [1] is generalized to tetragonal point-group symmetry. Magnetic inelastic neutron scattering spectrum can be calculated by the magnetic dipole transition matrix elements, determined by the eigenstates of the total Hamiltonian including the MEL coupling term [4]. We will present python software package CrysFiPy [5] allowing to fit both single crystal and powder averaged experimental data considering MEL coupling.

In addition, “mixed-mode” excitations (anticrossing of phonons and CEF) have been observed for the first time. By considering the one-ion MEL interaction [6, 7], which corresponds to the direct coupling between the shear deformations of the lattice and the 4f shell, an analytical expression for the mixed-mode excitations has been obtained using group theory. The calculated spectrum agrees well with experimental data. In this work, the second order MEL interaction as well as the linear rotational interaction is neglected [8].

E-mail for corresponding author: b.liu@fz-juelich.de
One of the characteristic and interesting features of ionic liquids (ILs) is nanometer-sized structure (nanostructure). For example, imidazolium-based ILs (ImILs) have nanostructures consisting of the polar-domains with imidazolium rings and anions and the non-polar domains with alkylchains of the cations. We have revealed that the nanostructure is essentially the same as that of a liquid-crystalline (LC) phase [1-3,5] and investigated the dynamics of ImILs by means of quasielastic neutron scattering (QENS) [1,2,4,5]. Recently, Yamada et al. found that some of alkylammonium-based salts, which are another popular ILs, have plastic-crystalline (PC) phases that are the counterparts to the LC phase; the LC phase has an orientationally-ordered positionally-disordered structure, while the PC phase an orientationally-disordered positionally-ordered one.

We have measured the DSC, neutron diffraction and QENS data of methyltriethylisopropyl-ammonium bis(trifluoromethylsulfonylimide (abbreviated as N\textsubscript{1223}Tf\textsubscript{2}N) and the methyl-
ethylpropylisopropylammonium salt ($N_{1233}^1\text{Tf}_2\text{N}$) in a temperature range between 4 and 400 K. They have crystalline (C), liquid (L) and two PC phases; one may be a normal isotropic PC phase and the other an anisotropic PC phase where the cations undergo uniaxial rotations. The QENS data were collected in a time range between 0.1 ps and 10 ns by means of HFBS and DCS spectrometers in NIST.

Figure 1 shows the Arrhenius plot of $N_{1233}^1\text{Tf}_2\text{N}$; a similar result was obtained for $N_{1223}^1\text{Tf}_2\text{N}$. There are basically 5 relaxations in a wide time range of 4 orders of magnitude. By analyzing the $Q$-dependence of the relaxation times and elastic incoherent structure factors (EISF), we have succeeded to specify the relaxation modes as given in the figure. The comparison between the dynamics of ImILs and ammonium-based ILs will be shown in the meeting.


E-mail for corresponding author: yamamuro@issp.u-tokyo.ac.jp
Neutron scattering is a powerful method to determine position and motion of hydrogen in condensed matter samples, however the scattering suffers from the enormous incoherent contribution from the hydrogen. This contribution can easily dominate the signal and mask important information given by the coherent scattering. Neutron polarization analysis can be used to account for the incoherent contribution.

The D7 spectrometer at the Institut Laue-Langevin [1] is a neutron scattering instrument with permanent polarization analysis, capable of determining the incoherent contribution and thus to separate this contribution from the coherent scattering. The instrument works well in both diffraction and spectroscopic modes. In diffraction mode, the instrument can measure momentum transfers up to 4 Å\(^{-1}\). Spectroscopy is possible using a Fermi chopper to determine the neutron time-of-flight, giving an energy resolution of \(0.1 \leq \Delta E \leq 0.5\) meV depending on the incident wavelength [2].

We will present a description of the methods and limitations of using polarized neutrons for coherent/incoherent separation. We will also present the capabilities of D7, along with a selection of recent examples for diffraction from liquids, powders and single crystals, and for quasielastic spectroscopy. Finally, we will present a brief description of a proposed upgrade to the instrument that would boost flux by more than an order of magnitude and also improve the resolution.


E-mail for corresponding author: mangin-throl@ill.fr
Dynamics of rubbers reinforced with metallic diacrylate as studied by QENS and SR

Ryo MASHITA¹, Rintaro Inoue², Toshiji KANAYA³, Hiroyuki KISHIMOTO¹

¹SUMITOMO Rubber Industries, LTD., Kobe, Japan
²Research Reactor Institute, Kyoto University, Osaka, Japan
³J-PARC, Material and Life Science Division, KEK, Ibaraki, Japan

We have studied structure and dynamics of rubber polymers reinforced with metallic diacrylate. Rubber polymers are utilized in various industrial products such as tires for automobile, airplane and base-isolating devices and are indispensable in industry and our daily life. In such industrial uses, rubber materials are usually reinforced with an addition of filler materials such as carbon black, silica and clay. Among them, rubber crosslinked with zinc diacrylate (ZDA) exhibits strong reinforcement properties without an addition of fillers. Hence the structure of such rubber has been extensively studied. Dynamics studies are very few although they are very important to understand the properties. In the study, we have therefore studied the structure and dynamics of rubbers crosslinked by ZDA [1-4]. It is found that the bound rubber layer is located on the aggregated of ZDA, and as for the dynamics the so-called β-process which dominates the glass transition directly is very much affected by ZDA but the so-called picosecond fast process is not. The results will be discussed from molecular viewpoint in the meeting.

References

E-mail for corresponding author: tkanaya@post.kek.jp
Spin-wave and electromagnon dispersions in multiferroic MnWO₄ as observed by neutron spectroscopy

Yinguo XIAO¹,², C. M. N. KUMAR³, Shibabrata NANDI⁴, Yixi SU⁴, Wentao JIN⁴, Zhendong FU⁴, Enrico Faulhaber⁵, Astrid SCHNEIDEWIND⁴, Thomas BRÜCKEL²,⁴

¹ Peking University Shenzhen Graduate School, Shenzhen, China
² Jülich Centre for Neutron Science, Forschungszentrum Jülich, Jülich, Germany
³ Jülich Centre for Neutron Science, Outstation at SNS, Oak Ridge, USA
⁴ Jülich Centre for Neutron Science, Outstation at MLZ, Garching, Germany
⁵ Heinz Maier-Leibnitz Zentrum, Technische Universität München, Garching, Germany

Multiferroics with strong coupling between ferroelectric and ferromagnetic degrees of freedom have attracted intense research effort due to their application potential in tunable multifunctional devices [1-2]. As a prototypical multiferroic material with spiral magnetic order, MnWO₄ has been widely studied concerning its magnetic and ferroelectric properties [3-4]. High-resolution inelastic neutron scattering reveals that the elementary magnetic excitations in multiferroic MnWO₄ consist of low-energy dispersive electromagnons in addition to the well-known spin-wave excitations [5]. The latter can well be modeled by a Heisenberg Hamiltonian with magnetic exchange coupling extending to the 12th nearest neighbor. They exhibit a spin-wave gap of 0.61(1) meV. Two electromagnon branches appear at lower energies of 0.07(1) and 0.45(1) meV at the zone center. They reflect the dynamic magnetoelectric coupling and persist in both the collinear magnetic and paraelectric AF1 phase and the spin spiral ferroelectric AF2 phase. These excitations are associated with the Dzyaloshinskii-Moriya exchange interaction, which is significant due to the rather large spin-orbit coupling.


E-mail for corresponding author: xiaoyg@pkusz.edu.cn
Despite great progress in oral health related issues, dental caries is still a major problem that affects both children and adults. Especially dental restorative work is very costly in industrialized countries and therefore developing and improving restorative materials can beneficially impact the public health system. Among dental restorative materials glass ionomer cements (GICs) are of great interest, since they have the ability to bond to the tooth structure without the need for preconditioning the surface with an acid or unnecessary removal of tooth substance. Furthermore, fluoride is slowly released during setting adding to the anticariogenic benefits of the material. GIC’s poor mechanical strength is however a disadvantage, and improved knowledge on this subject can bring potential development. One possibility is to advance our understanding of the dynamics of the aqueous solution used to prepare the GIC. In this study, we applied quasi-elastic scattering (QENS) in a time range from picoseconds (ps) to nanoseconds (ns), to understand how the nanoscale mobility of the aqueous solution of polyacrylic acid (PAA) used in conventional GICs changes under confinement. By exploding that the system is dynamically heterogeneous and thereby that different types of hydrogen motions can be superimposed independently we were able to separate distinct motions within the liquid and in the GIC’s. The QENS analysis revealed that the self-diffusion translational motion identified in the liquid is also visible in the GIC. However, as a result of the formation of the cement matrix and its setting, both translational diffusion and residence time differed from the PAA solution. When comparing the local diffusion obtained for the selected GIC, the only noticeable difference was observed for the slow dynamics associated to the polymer chain originating from PAA solution. Additionally, over short-term ageing, progressive water binding to the polymer chain occurred in one of the investigated GIC. Finally, further analysis showed a considerable change in the density of the
GIC without progressive water binding indicates an increased polymer crosslinking. A deep understanding of polymer-water binding, polymer crosslinking as well as material density changes occurring during the maturation process of GIC are necessary for development of advanced dental restorative materials.

E-mail for corresponding author: marcellac.berg@gmail.com
Elucidation of Molecular Dynamics of Poly(quinoxaline-2,3-diyl)s Exhibiting Solvent-dependent Helix Inversion Through Quasielastic Neutron Scattering Measurements

Yuuya Nagata,¹ Michinori Suginome,¹ Taiki Tominaga,² Rintaro Inoue,³ Sugiyama Masaaki³

¹ Graduate School of Engineering, Kyoto University, Kyoto, Japan
² Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society (CROSS), Ibaraki, Japan
³ Institute for Integrated Radiation and Nuclear Science, Kyoto University, Osaka, Japan

Increasing attention has been paid to the structural control of artificial helical polymers because of their scientific and industrial applications for asymmetric catalysts, chiral stationary phase, and chiroptical materials. So far, we found that single-handed helical poly(quinoxaline-2,3-diyl)s (PQXs) bearing chiral side chains exhibit a solvent-dependent helix inversion,¹ which can serve as effective scaffold for chirality-switchable materials.

Recently, in order to elucidate the mechanism of the solvent-dependent helix inversion of PQXs, we have revealed detailed structures of 2oct with right- or left-handed structures in THF-d₈ or a mixed solvent of 1,1,2-TCE-d₃ and THF-d₈ (8/2, v/v) by using small-angle neutron scattering (SANS) experiments, in conjunction with theoretical calculations.² The obtained structures of 2oct suggested that the right-handed 2oct in THF-d₈ is well solvated, while the left-handed 2oct in 1,1,2-TCE-d₃/THF-d₈ (8/2, v/v) is less solvated, i.e., the accumulation of small energy differences in the solvation of the chiral side chains alters the conformation of the two chiral side chains per repeating unit, resulting in absolute control over the macromolecular helical chirality. In this study, we carried out quasielastic neutron scattering measurements to elucidate the impact of the molecular dynamics on the solvent-dependent helix inversion of the PQX at BL-02 DNA in J-PARC (Figure 2). We also discuss molecular dynamics (MD) simulations for detailed analyses of QENS measurements.

E-mail for corresponding author: nagata@sbchem.kyoto-u.ac.jp, suginome@sbchem.kyoto-u.ac.jp, and sugiyama@rri.kyoto-u.ac.jp
Room temperature ionic liquids (RTILs) typically have melting temperatures below 100 °C and are entirely composed of ions. Task-specific synthesis of RTILs opens a huge variety of applications for these compounds. Currently, ILs are intensively used in advanced chemical processes, in nanotechnology and furthermore in applications such as catalysis, biomedicine, electrochemistry etc. In our work, we will present results from QENS experiments performed on a series of RTILs based on the imidazolium cation (see figure below). The aim was to investigate the effect of switching off one of the hydrogen-donor sites in the cation [1]; chemically this can be achieved by a methylation of the acidic proton located between the two nitrogen atoms in the imidazolium ring. We combined the imidazolium-based cations with a series of H-free anions (thiocyanate [CNS], dicyanamide [C₂N₃]⁻ and tricyanomethanide [C₄N₃]⁻), variable both in size and in the number of hydrogen-donor sites.

Chemical structure of the a) [C₂mim]⁺ and b) the [C₂C₁mim]⁺ (methylated) cations.

Suppression of hydrogen-bond sites through cation methylation has also been investigated by infrared spectroscopy; the thus obtained data help to explain changes in physical-chemical properties of the system, such as the decrease/increase of the melting point and differences in the viscosity [1]. The aim of our investigations was to decipher the dynamical processes underlying the observed changes induced by the methylation of the acidic proton. The temperature range covered during the QENS experiments performed on FOCUS at SINQ (40K to 410K) explored several thermal phases of the ILs, such as crystallization, glass-transition, cold crystallization, and melting (investigated via DSC investigations). A detailed analysis of the spectra revealed two well-separated dynamical processes:
the slower one describes long-range diffusion, while the faster one can be attributed to confined dynamical processes [2]. Differences in the spectral linwidths of [C2mim]+ and [C2C1mim]+ clearly manifest the impact of H-bonding sites on the dynamics of the investigated liquids.


E-mail for corresponding author: juan.mora@psi.ch
PVDF-based ferroelectric polymers have emerged as a unique class of materials, distinct from their ceramic counterparts, with attractive electrical, thermal and electromechanical properties. As electroactive materials, they provide advantages of high breakdown strength, low dielectric loss, relatively fast charge/discharge rates and greater flexibility. Microscopic understanding of functional behavior in polymeric ferroelectrics has presented new challenges since unlike traditional ceramic ferroelectrics, electric-field-induced response in polymers is a consequence of short-range molecular dynamics that are difficult to measure directly. In recent studies, using careful analysis of Quasi-elastic Neutron Scattering (QENS) patterns, we have been able to provide new insights into the atomic-level H-atom dynamics of PVDF-based co-polymers and terpolymers. In one set of studies, we showed the presence of two energetically distinct types of molecular motions in the copolymer PVDF-TrFE, viz. localized rotational motion of methylene groups and a jump diffusion process, and their respective variations across ferroelectric-to-paraelectric phase transition. In another set of studies on PVDF-based terpolymers, we showed that the relaxor behavior in these materials cannot be ascribed alone to short range molecular dynamics within crystalline domains. Instead, from multiscale quantitative microstructural characterization, a clear correlation between the amount of crystalline-amorphous interfaces and dielectric relaxation is observed, which indicates that such interfaces play a central role. These results provide critical insights into the role of atomic and microscopic structures towards relaxor behavior in ferroelectric polymers, which will be important for their future design.

E-mail for corresponding author: apramani@cityu.edu.hk
In-situ QENS studies of superionic conductivity in barium hydride

Gavin J. Irvine*, Prof John TS Irvine, Prof Martin Owen Jones

1University of St Andrews, School of Chemistry, St Andrews, Fife.
2ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, UK.

Hydride materials have potential applications in hydrogen storage, and ammonia synthesis [1,2]. Barium hydride in particular has been shown to be a superionic conductor at intermediate temperatures (~500 °C) after undergoing an identical phase change (P n m a to P 63/m m c) observed for other superionic conductors[3,4]. In our present research we use quasi-elastic neutron scattering (QENS) to elucidate the diffusion pathway. The QENS data was fit via the Chudley-Elliot model (CE) and showed a jump pathway of around 3.4 Å. From CE we can extract a diffusion coefficient which we can relate to the ion conductivity via the Nernst-Einstein equation. The QENS data was collected with in-situ electrochemical impedance spectroscopy (EIS), which directly measures the ion conductivity. Thus, by comparing the results of the two techniques we are able to quantify the charge carrier density and relate that to specific crystallographic sites (via neutron powder diffraction data: NPD). Finally, we also utilize total scattering data to compare and contrast the local and global order of the material.

Barium hydride can serve as a model material on which future superionic materials can be developed and thus push forward the ambitious goal of an all solid state battery and/or fuel cell. The system represents one of only a few superionic conducting solids that have been investigated thoroughly. This study is particularly reliant on neutron scattering due to the presence of hydrogen which is difficult to study using other solid state material analysis techniques.


*Corresponding author: gjj4@st-andrews.ac.uk
Quasi-elastic neutron scattering (QENS) has many applications directly related to the development of high-performance functional materials and biological macromolecules, especially those containing some water. QENS results can provide information about both the long-time diffusive motions (on the time scale of 1ns) and short-time rotational motions of water molecules contained in samples. The analysis method of QENS spectral data is important to obtain parameters explaining the dynamics of water. Although there are three kinds of model used to fit QENS data [1], which are the empirical diffusion model (EDM), the relaxing cage model (RCM), and the jump-diffusion and rotation-diffusion model (JRM), none can give very good fitted QENS spectra both for $Q \leq 1 \text{Å}^{-1}$ and $Q > 1 \text{Å}^{-1}$ at the neutron energy transfer larger than 50 μeV.

The JRM combines both the translational and rotational motion of water, so it can give more comprehensive and related parameters describing the water contained in samples. The JRM has already been used for fitting of the QENS spectra by Bordallo et al. [2] in 2006 and by us [3] in 2015, but there exists some approximations about the contribution to QENS spectra by the translational and rotational motion of water.

Here we deduced a revised JRM for fitting QENS spectra, by adding the contribution to elastic part from the translational motion and taking into account the contribution of the scattering lengths in sears expansion to deal with the rotational motion. The new revised JRM can give a very good fit of QENS spectra from magnesium–silicate–hydrate (MSH) based samples. Figure 1 and 2 shows an example of QENS spectra fitted by using the JRM and the revised JRM for a pure MSH sample, respectively.
Figure 1 MSH QENS data fitted by JRM.

Figure 2 MSH QENS data fitted by revised JRM.


*E-mail: tlihua@jnu.edu.cn
Amphiphilic molecules such as surfactants and lipids undergo self-association under specific conditions to form aggregates such as micelles, vesicles, membrane etc. The phase behaviour and dynamical features in the different phases of various biomembrane mimetic lipids/membrane systems are of immense interest. It is known that basic nature of the dynamical processes in these model membrane systems is very similar to that in the actual cell membrane. Cell membrane is a complex heterogeneous mixture of lipids, proteins and carbohydrates. Dynamics of membrane is a prime determinant in a number of physiological processes such as cell signaling, permeability, cell fusion, etc. However, the complex composition of cell membrane does not allow understanding of the detailed role of each membrane component (e.g. individual lipid species) in the physiological processes. Information towards these aspects can be obtained by looking into simplified model systems. Direct comparison of the MD simulation helps to interpret the experimental results data. Combining neutron scattering and MD simulation techniques, we have successfully described the dynamical behaviour in various self-assembled molecular systems [1-7]. We will discuss results from some of our studies on micelles, vesicles, lipid bilayer, membrane etc as obtained by combination of neutron scattering and MD simulation [3,5,7]. We will also discuss our recent study of interaction of ionic liquids ILs, potential candidates for new antimicrobials, with phospholipid membranes [6].


*E-mail for corresponding Author: mukhop@barc.gov.in
Microscopic origin of the logarithmic relaxation process in molecular glass-forming liquids

Changjiu Chen¹, Rithin P. Krishnan¹, Kaikin Wong¹, Dehong Yu², Fanni Juranyi³, and Suresh M. Chathoth¹⁴

¹ Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, P. R. China.
² Australian Nuclear Science and Technology Organization, Lucas Heights, NSW 2234, Australia.
³ Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland.
⁴ City University of Hong Kong Shenzhen Research Institute, Shenzhen, 518057, P. R. China.

Logarithmic relaxation is a unique relaxation process exhibited by a few molecular liquids and biomolecules. However, the microscopic origin of logarithmic relaxation is still unclear. To understand the origin of this process, we studied two liquids that exhibit logarithmic relaxation in confinement state using quasi-elastic neutron scattering (QENS) and depolarized dynamic light scattering (DDLS). Although the intermolecular potential of the liquids is drastically different in the soft-confined state from the bulk liquids, we observed that the logarithmic relaxation still persists. Our results indicate that the intermolecular potential does not play a role in determining the logarithmic relaxation process. The coupling of rotational and translational relaxation processes could be the origin of the logarithmic relaxation process exhibited by the molecular liquids [1].

Email: smavilac@cityu.edu.hk
The Oak Ridge National Laboratory (ORNL) operates two powerful neutron sources, the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS). The international user community has access to a total of 30 instruments that are taking part of the user program, and 10 of these are dedicated to inelastic or quasielastic scattering. I will give an overview of the presently operating instrument suite in the first part of the presentation.

Both facilities are looking ahead to major changes within the next 5-10 years. At HFIR the beryllium reflector will be replaced in 2023-24, which presents an opportunity to install major upgrades to the instruments and neutron guide systems. One of the cold guide end stations will host a new multi-analyzer cold triple axis instrument (MANTA) which is currently being designed. An IN15-style neutron spin echo instrument is also being considered for another guide end station. A future second target station at the Spallation Neutron Source would make room for an additional approximately 20 instruments optimized to make best use of cold neutron peak brightness.

E-mail for corresponding author: ehlersg@ornl.gov
The European Spallation Source (ESS) is a European Research Infrastructure Consortium (ERIC), a multi-disciplinary research facility based on the world’s most powerful neutron source, and one of the largest science and technology infrastructure projects being built today [1].

The need for a high-power neutron spallation source in Europe was discussed for the first time around 20 years ago, and construction began in summer 2014. The ESS Construction project is a pan-European effort with 15 European nations as members and Sweden and Denmark as host nations. The project is strongly dependent on in-kind contributions from partner laboratories, universities and research institutes, which amount to up to 40 percent of the overall construction budget of 1.843BEuro.

Since the ESS is a green-field site project, there is no host laboratory that can provide technical support. Consequently, the infrastructure required to operate the facility needs to be established in parallel to designing the main systems such as the Accelerator, the Target or the neutron scattering instruments. Also, ESS is being designed and built as an integrated facility, which will minimize the long-term operation cost but requires significant effort when it comes to e.g. integrating complex instrument systems into a site-wide control or timing system [2]. Similarly, the expected unprecedented flux ESS will provide to the neutron instruments requires in many cases new systems such as detectors in combination with low backgrounds, which, for example, do not saturate at high-countrates [3,4,5]. Of course, such systems need to be integrated into a computational framework to allow the end user performing experiments to fully utilise the neutron scattering instruments, which are currently being designed and build by in-kind partners throughout Europe.

The presentation will discuss how technical challenges were – and still are being - addressed, or why it is necessary to start related and complementary development activities early to not only provide the best possible systems to the instruments but maximise the long term return on investment.

ESS is the first long pulsed spallation source. The proton power will be 5 MW with the repetition rate at 14 Hz and the pulse duration of 3 ms. The brightness from a thin moderator benefited from the unique neutronic character of para-Hydrogen would be one order of magnitude higher than existing other spallation sources. Because of these source characters, instruments are essentially long and focusing on use of cold to thermal neutrons. Pulse shaping chopper will be the key technology to adjust time resolution with much flexible manner with long pulse duration on taking the multiplicity technique[2]. By taking a cutting edge design of optics, useful neutrons would be delivered under less dissipation condition, and furthermore the curved long guide system would extremely diminish high energy contamination for instrument to almost realize a background free environment. On the contrarily ability on epithermal experiments would be abandoned and left to other facilities. This demarcation might make clearly a role of facilities in the world in the future. In the talk, I will show the present situation of the instrument development including a characteristic feature of target-moderator system. Especially comparison between the ESS instruments and ones in short spallation facilities will be highlighted [3].

Developments in spectroscopy at the ISIS pulsed neutron and muon source

Russell EWINGS1, Rob BEWLEY1, Duc LE1, Tatiana GUIDI1, Ross STEWART1, Toby PERRING1, Stewart PARKER1, Franz DEMMEL1

1ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, United Kingdom

In this talk I will give an overview of developments on the spectrometers at ISIS over the last couple of years, as well as giving a few recent examples of scientific highlights that some of the new instrumentation has enabled. Since the last WINS conference, supermirror guides, as well as some other upgrades, have been installed on TOSCA, MAPS and MARI, with the former two instruments now fully operational and back in the user program. I will show some results that illustrate the gains in performance of all of these instruments, as well as commenting on some of the lessons learned from the process of going from design to implementation. I will also present a few results from the new polarized neutron option that is being commissioned on LET.

Looking to the future I will discuss some of the spectroscopy instrument development projects that are underway at ISIS. These include a new Si analyzer for OSIRIS and a major software project (PACE – Proper Analysis of Coherent Excitations) for improving the ease, quality and rapidity of data analysis from time-of-flight spectrometers.

Finally I shall also give an update on some of the new instrumentation that is being designed – MUSHROOM (Multi-Use Spectrometer for High Rate Observations of Ordered Materials) and OSIRIS++.

E-mail for corresponding author: russell.ewings@stfc.ac.uk
Overview of the neutron spectrometers at J-PARC

Ryoichi KAJIMOTO¹,², Tetsuya YOKOO¹,³, Mitsutaka NAKAMURA¹,², Yukinobu Kawakita¹,², Masato MATSUURA⁴, Hitoshi ENDO¹,³, Hideki SETO¹,³, Shinichi ITOH¹,³, Kenji NAKAJIMA¹,², and Seiko OHIRA-KAWAMURA¹,²

¹J-PARC Center, Tokai, Ibaraki, Japan
²Japan Atomic Energy Agency, Tokai, Ibaraki, Japan
³High Energy Accelerator Research Organization, Tsukuba, Ibaraki, Japan
⁴Comprehensive Research Organization for Science and Society, Tokai, Ibaraki, Japan

The MLF Spectroscopy Group consists of six time-of-flight instruments for inelastic and quasi-elastic neutron scattering in the Materials and Life Science Experimental Facility (MLF) at J-PARC [1]. 4SEASONS, HRC, AMATERAS, and POLANO are direct geometry spectrometers; 4SEASONS is a thermal neutron chopper spectrometer covering the range of 10⁰-10² meV. HRC can access higher energies, while AMATERAS is optimized for lower energies. POLANO is characterized by the capability of using polarized neutrons. DNA is a near-back scattering spectrometer with a pulse-shaping chopper. Measurements with micro-eV resolution can be performed on this instrument. Neutron spin echo spectrometer VIN ROSE can access even slower dynamics. 4SEASONS, HRC, AMATERAS have been open for users earlier than the other instruments, and now continuously produce significant scientific outcomes. DNA, which is a little younger, is catching up to the former three instruments recently. VIN ROSE has just started the user program with a part of its instrument suite, while POLANO has started the on-beam commissioning. By a combination of these instruments, MLF gives opportunities to study dynamics in widely spread fields including solid state physics, amorphous materials and liquids, soft and biological matters, as well as industrial applications such as tire rubbers and battery materials. In this presentation, we review the characteristic features, scientific outcomes, and continued progresses in the instrumentation of these 6 instruments.


E-mail for corresponding author: ryoichi.kajimoto@j-parc.jp
The Australian Centre for Neutron Scattering (ACNS) utilises neutrons from Australia’s multi-purpose research reactor, OPAL, to solve complex research and industrial problems for Australian and international users via merit-based access and user-pays programs.

An overview of the ACNS neutron scattering capabilities at the OPAL reactor will be given including an update on the status of OPAL, its neutron beam facilities, cold neutron source and our future plans.

E-mail for corresponding author: jamie.schulz@ansto.gov.au
The Oak Ridge National Laboratory (ORNL) Spallation Neutron Source was constructed to enable a significant increase in proton beam power and the addition of a Second Target Station (STS). The Proton Power Upgrade (PPU) will double the proton power capability of the SNS accelerator from 1.4 to 2.8 MW. PPU will deliver 2 MW to the current SNS target station and will provide the proton power required by STS. The PPU project has received Critical Decision-1 from the U.S. Department of Energy Office of Science. STS is proposed to operate at a frequency of 15 Hz with 0.7 MW of proton beam power delivered to a rotating tungsten target. The strength of the STS will be the production of high peak brightness beams of cold neutrons, complementing the strengths of the current ORNL neutron sources. This talk will discuss the current status of PPU and describe instrument concepts which have been developed for STS, emphasizing the complementarity of the ORNL neutron sources.

E-mail for corresponding author: herwigkw@ornl.gov
We give an overview over the instruments in the Spectroscopy Group at the Institut Laue-Langevin [1] and its ongoing or upcoming instrument projects. The ILL Spectroscopy Group operates four different classes of instruments that measure the atomic, molecular and crystal motions of samples in hard and soft matter:

1) Direct Time-of-flight spectrometers, which analyse the change of the initially monochromatic neutron velocity after the sample scattering by measuring their time of arrival. We present the cold neutron multi-chopper TOF spectrometer IN5 and its upgrade program, the cold neutron time-focussing TOF spectrometer IN6 which upgrades to SHARP (CRG), the thermal neutron TOF spectrometer IN4 with its upgrade to PANTHER and the Brillouin spectrometer BRISP (CRG). Finally a TOF ‘Rapid Measurement Special Environment Spectrometer’ RAMSES will be introduced with the modernisation programme ENDURANCE2.

2) Backscattering spectrometers, which are hybrids between three-axis and inverted TOF spectrometers and which achieve highest energy resolution by using neutron optics with perfect crystals but maintaining normal incidence at monochromator and analyser: we discuss the thermal backscattering spectrometer IN13 with its upgrade to IN13+ and the versatile cold neutron backscattering spectrometer IN16B on which for the first time an inverted time-of-flight backscattering spectrometer option was commissioned on reactors [2].

3) Spin-echo spectrometers (NSE) which measure very precisely small changes in neutron velocities by analysing how their spins precess before and after interaction with the sample. All NSE are located on cold n-guides: the ‘classical’ IN11 including IN11C, the world highest resolution NSE IN15 which just underwent an upgrade and the new wide angle NSE WASP [3] which is under commissioning.

4) Three-axis spectrometers, in which the monochromator, sample and analyser can each be aligned independently on their axis: We present the cold triple axis spectrometer ThALES with its multiplex array upgrade project MARMOT and IN12 (CRG), the thermal triple axis IN8, IN20 with upgrade and IN22 (CRG) as well as the hot triple axis spectrometer IN1 and the vibrational spectrometer LAGRANGE.

[1] https://www.ill.eu/users/scientific-groups/spectroscopy/
[3] P. Falus, presentation at this conference

E-mail for corresponding author: frick@ill.eu
WK_09  Opportunities for further advances in time-of-flight spectroscopy

Ferenc MEZEI$^{1,2}$

$^1$European Spallation Source ESS ERIC, Lund, Sweden

$^2$Hungarian Academy of Sciences, Wigner Research Center for Physics, Budapest, Hungary

Time-of-flight (TOF) spectroscopy looks back to more than half a century of successful use in neutron scattering research. Nevertheless, new opportunities in beam delivery (advanced supermirror based neutron optical design, improved chopper system layout and detector system) allow us today to substantially enhance instrument performance. The rebuilt NEAT spectrometer at Helmholtz Zentrum Berlin (HZB) offers a good illustration. Amongst others by its about 5 times more efficient beam delivery to the sample than that of world leader IN5 at ILL in terms of neutron flux on the sample at a given resolution related to the brightness of the cold neutron source used. Important ingredients of high efficiency in beam delivery are the capability of adjusting the energy resolution to the needs of the experiment or the beam profile at the sample to the sample size.

Most recent achievements in enhancing moderator efficiency are by now untapped for high performance TOF spectroscopy: namely bi-spectral cold and thermal neutron simultaneous beam extraction into the same neutron beam guide and the use of advanced low dimensional moderator design for 2–3 times higher source brightness. Both methods have been extensively worked out at ESS by simulations. Conclusive evidence was experimentally obtained on bi-spectral beam extraction at the high magnetic field beam-line EXED at HZB.

Another not yet implemented opportunity of particular relevance for quasi-elastic scattering is the adjustment / optimization of the chopper modulation pattern not only to the energy resolution needs of the experiment but also to the type of spectral features to be studied. Here the application of correlation spectroscopy with quasi-random modulation of the incoming neutron beam (instead of the conventional repetition a single pulse) opens up the way to a new domain of sensitivity. With statistical choppers the resolution can be changed without changing the chopper speed or slit width by adjusting the beam width at the chopper and in the data reduction process after the experiment. Thus the same quasi-random statistical chopper disc can cover a large range of experimental resolution needs [1]. The data collection rate compared to conventional single pulse beam chopping was found to be about an order of magnitude higher for relatively large intensity spectral features in a TOF spectrum (such as a quasi-elastic line) and by up to 2 orders of magnitude for the whole spectrum if the sample independent back-ground count rate is dominant, as in the case of very small samples [2].

Thus, in the end, a TOF spectrometer with the basic NEAT design facing an ESS style advanced bi-spectral low dimensional moderator on an ILL class neutron source – such as the upcoming PIK reactor
at NRC KI PNPI in Gatchina, Russia – and including a statistical chopper as an optional alternative to a
conventional chopper (straightforward to realize by placing the two choppers close to each other and
stopping one of them fully open), can provide for the various features of the TOF spectra intensity
gains over best existing at ILL by a factor between about 20 to 2000.


E-mail for corresponding author: ferenc.mezei@esss.se
The China Spallation Neutron Source (CSNS) is a multidiscipline research platform with neutron scattering. The site of CSNS is Dongguan, Guangdong Province. The facility comprises an 80-MeV Linac, a 1.6 GeV proton rapid cycling synchrotron, a tungsten target station, and the experimental hall for 20 neutron spectrometers. The RCS provides a beam power of 100 kW on the target in the phase I. There are three initial spectrometers in the experimental hall: general purpose powder diffractometer, small angle neutron scattering meter and magnetic reflectometer. The construction of CSNS was finished last August on schedule. The first neutron beam obtained August 28, 2017. CSNS through the acceptance review organized by Chinese Academy of Sciences March 25, 2018. CSNS runs smoothly with the proton beam power on the target more 20kW. It is opened to users. The first papers of the user experiments were published. The design and construction of several user spectrometers are started. CSNS provides scientists of a unique opportunity for the neutron scattering research and applications. The talk will report the design, construction, commissioning and applications of CSNS.
Molecular spectroscopy is a very powerful tool to study the dynamical properties of solid, liquid and gases. With the development of neutron spallation sources, and the use of epithermal neutrons, inelastic neutron scattering can measure the vibrational spectra of materials on the whole range of vibrational motions (0-4400 cm⁻¹) and effectively opening up the field of neutron spectroscopy [1]. INS is a technique that was mostly used to study hydrogen-containing materials due to the high cross section of hydrogen [2].

The VISION spectrometer at the SNS in Oak Ridge Tennessee has an increased overall flux at low energy transfers up to 4000 times over its predecessors and it has unprecedented sensitivity. I will show the limits of what is now possible in INS thanks to VISION. From the determination of INS spectra of publishable quality in minutes (for samples in the gram quantity range) [3], measuring the signal of samples in the milligram range to the direct determination of the signal of 2 mmol of CO₂ adsorbed on catalysts [4].

Finally, the major challenges that we are facing will be discussed, in particular methods to automate data analysis and interpretation through computer modelling. We have computer cluster: VirtuES (VIRTUal Experiments in Spectroscopy) dedicated to analyse VISION data. We are also developing ICEMAN (Integrated Computer Environment; Modeling and Analysis for Neutron data) a new software to simplify the link between computer modelling and neutron scattering data and maximise the
benefits of the VirtuES cluster. As part of ICEMAN we have the O’Climax software that allows the calculation of INS spectra from powder and crystals samples, including coherent effects if required for any type INS instrument (example in figure).

The wide angular-range chopper spectrometer ARCS at the Spallation Neutron Source (SNS) is optimized to provide a high neutron flux at the sample position with a large solid angle of detector coverage. The instrument incorporates modern neutron instrumentation, such as an elliptically focused neutron guide, high speed magnetic bearing choppers, and a massive array of $^3$He linear position sensitive detectors. ARCS began user operations in 2008 and has enjoyed a successful ramp up of publications with a significant proportion in high-impact journals. This has been enabled by continual improvements in the instrument capabilities. An oscillating radial collimator was added to improve the background performance from complex sample environment equipment. Examples include high temperature furnaces, a large volume dilution refrigerator and an electrostatic sample levitation device. The capabilities of ARCS enable a wide variety of science, such as the exploration of the momentum distribution in Bose-Einstein condensates, and characterizations of the effects of anharmonic interactions on phonons in thermoelectrics and novel lattice dynamics in single crystals. Ongoing efforts for instrument improvement include continued advances for data acquisition and analysis software to maximize the scientific output. Future developments such as a new chopper to enable a higher resolution mode are currently being explored.
The development of high m ballistic guides, focusing geometries and multiplexed analyzer backends has produced a host of new spectroscopy designs. Many new instruments can boast one to two orders of magnitude increase in collection over traditional triple axis spectroscopy. The NCNR is currently undertaking the design of a new instrument. Monte-Carlo results for the primary spectrometer will be presented detailing the tailoring of neutron transport through a ballistic guide to match the neutron volume acceptance of a double focusing monochromator. Several different backend designs are currently under consideration. Resolution selection, versatility, survey and parametric study capabilities vary significantly between designs. An examination of several secondary spectrometers will be provided detailing the tradeoff between these capabilities.
Not long ago measuring 3D systems on a direct geometry time of flight spectrometers was a difficult and inefficient task and not often done as it was far better to go to a triple axis machine. However, these days instruments like LET(ISIS) and IN5(ILL) with a large coverage of position sensitive detectors and new software [1] routinely map out the whole of S(Q,w) space in single crystals. These measurements are very time consuming though, typically taking a day or two per scan. This can make measurements on small/weakly scattering crystals or parametric studies either impossible or impractical.

In this presentation I will present a concept for a new type of time of flight indirect geometry spectrometer which is also capable of mapping out the whole of S(Q,w) space, but in time scales at least an order of magnitude faster than the direct geometry machines. It also has the advantage of being much cheaper and having a small footprint.


E-mail for corresponding author: robert.bewley@stfc.ac.uk
MIRACLES is the high-resolution time-of-flight backscattering spectrometer at the European Spallation Source. Conceptually, [1] the instrument is optimized for quasielastic neutron scattering (QENS) experiments around the Si(111) backscattering reflection covering an energy transfer range of $\Delta E \approx \pm 500 \, \mu eV$. The expected highest resolution of $\delta(\hbar \omega) \approx 2.5 \, \mu eV$ can be easily tuned to match the observation time (and consequently flux) of the system under study. MIRACLES' users will also be able to carry out inelastic neutron scattering (INS) experiments scanning an energy range of $\sim 20$ meV with constant inelastic resolution.

Currently, the project continues its pathway towards detailed design and construction. In the last few months, significant modifications with respect to the conceptual design have been achieved, oriented mainly to the optimization of the primary spectrometer. [2] The guide has been adapted to the instrumental hall layout and several improvements, concentrated mainly on the neutron beam extraction, curved guide and focusing nose, have been implemented. In the latter case, two different focusing options are proposed, allowing for studying smaller samples, thus facilitating studies limited by the amount of available material such as biological systems. Moreover, the updated chopper cascade will provide an even more versatile performance with very flexible selection of configuration modes, taking advantage of the long ESS pulse and tailoring the instrument resolution ad hoc, from high-resolution to high-flux. The newer detailed design of the secondary spectrometer pays special attention to improve the analyzer-detector configuration, and minimizing the sample-detector distance, allowing simultaneously a minimization of the energy resolution contribution from the secondary spectrometer and making room for a cryomagnet that will be easily adapted, expanding
MIRACLES science case. These points, as well as future design efforts will be oriented to provide MIRACLES with an outstanding performance that will unfold new opportunities in neutron spectroscopy.


E-mail for corresponding author: fjimenez@essbilbao.org
SEQUOIA is a fine resolution thermal direct geometry chopper spectrometer located at the Spallation Neutron Source at Oak Ridge National Laboratory. The instrument has been operating since 2010. This presentation will review the current capabilities of the instrument along with some of the scientific highlights from its tenure. There are upgrade projects which are being developed for the SEQUOIA instrument to improve its reliability and expand its scientific mission. These include a revision of the vacuum system, the addition of detectors at small scattering angles, the possibility of a co-mounted third Fermi chopper, and the installation of a post sample radial collimator. These upgrades will also be discussed.

E-mail for corresponding author: stonemb@ornl.gov
EMU, the high-resolution neutron spectrometer installed at the OPAL reactor, ANSTO [1] delivers 1.2 μeV FWHM energy transfer resolution for an accessible ± 31 μeV energy transfer range. The spectral resolution is achieved by neutron backscattering from Si (111) on the primary and second flight paths, which also determines the accessible 0.35 to 1.95 Å⁻¹ momentum transfer range.

Two years of user operation document strong demand for QENS characterization of microscopic diffusion processes in energy materials such as solid-state electrolytes, and increasingly in bio-related soft materials [2,3]. Over the same time frame the spectrometer has serviced a ~ 2:1 Australian/Overseas distribution of scientific user groups, while most experiments were carried out with standard cryo-furnaces (2 to 800 K temperature range). Spectrometer beam-time access is merit-based, thus welcoming experiments beyond the first two-year ‘sample’, and including experiments that may require other ancillary equipment such as (existing) controlled-gas delivery, pressure, applied fields, etc.

Representative examples of the spectrometer capabilities will be given, thus with an emphasis on QENS line shape and mean-square displacements analyses.

Scientific support emphasis is presently on enabling initial data analysis of the collected data, and on the instrumental side reaching the design 0.1 Å⁻¹ minimum momentum transfer range and growing signal-to-noise ratio beyond its current ~ 1000:1 value.


E-mail for corresponding author: nds@ansto.gov.au
The China Mianyang Research Reactor (CMRR) with the power of 20 MW is located in Mianyang city, Sichuan Province. The measured thermal and cold fluxes for neutron scattering experiments are $2.4 \times 10^{14}$ n/cm$^2$·s and $10^9$ n/cm$^2$·s, respectively. CMRR has two neutron halls, a thermal neutron hall and a cold one. The reactor has opened to users officially since 2012. It ran 120 days in 2016 and more than 150 days in 2017. Now CMRR is included in the website: Neutronsources.org.

Eight neutron scattering instruments have been installed, which began commissioning in the middle of 2014. Four thermal neutron instruments were installed in the reactor hall, including the High Resolution Neutron Diffractometer (HRND), Residual Stress Neutron Diffractometer (RSND), Thermal Neutron Radiography Station (TNR) and High Pressure Neutron Diffractometer (HPDC). Four cold neutron instruments were installed in the guide hall, including the Small-Angle Neutron Spectrometer (SANS), Time-of-flight and Polarized Neutron Reflectometer (TPNR), Cold-neutron Triple-Axis Spectrometer (CTAS) and Cold Neutron Radiography Station (CNR). The texture measurement was realized on the RSND by utilizing the Kappa goniometer. The HPDC was upgraded with new 6.7 m focusing neutron guide before monochromator. The flux was raised about one order of magnitude and reached to $3 \times 10^6$ n · cm$^2$ · s$^{-1}$. At present high pressure loading in HPDC can realize a maximum pressure of 15 GPa. Now the upgrade plan in HRND, the high resolution and high intensity modes, is launched and will be finished in the future few years. SANS has been equipped with a new neutron velocity selector and the collimation system was optimized. The cold neutron flux at the sample position reaches $2 \times 10^7$ n·cm$^2$·s$^{-1}$ at present. The characteristics of the TPNR are the time-of-flight and polarization modes. Relative resolution of momentum transfer is $\Delta q/q = (0.5\sim5)\%$ for $q = (0.05\sim3.0)$ nm$^{-1}$. CTAS has an energy resolution $\Delta E/E \leq 2\%$ and energy transformation range 0~10 meV.

In situ neutron diffraction measurements on zircaloy-4 alloy have been performed and RSND plays more important role in the engine material field. Several measurement results performed on the HPDC, such as magnetic and hydrogen materials research progress, have been published in the SCI journals. The research results of soft matter using SANS have been published on Macromolecules and Advanced Materials. The magnetic film study by TPNR has been published on Scientific Reports and Physical Review Applied. Some new experiment results and analysis will also be presented on the conference.
Recently, the second phase for neutron scattering instruments development has been launched. Three new instruments will be built within next 3-5 years, which includes a Polarized Thermal Neutron Triple-Axis Spectrometer (TTAS), an Ultra Small-Angle Neutron Spectrometer (USANS), and a Neutron Standard-Test Beam Line (NSTB). More sample environment systems will be equipped for the present spectrometers, such as high/low temperature, high pressure, superconducting magnetic field and chemical loading (hydrogen/deuterium gas environment).

E-mail for corresponding author: gongjian@caep.cn
T-REX is a bispectral direct-geometry chopper spectrometer under construction at the European Spallation Source (ESS). Currently the project is in the engineering design phase. We report on technical solutions for various instrument components.

The instrument will provide neutrons in the energy range $2 \text{ meV} < E_i < 160 \text{ meV}$ and therefore will allow detailed exploration of reciprocal space to study excitations in condensed matter with an emphasis on collective dynamics of the nuclear and spin structure.

The chopper layout [1] is designed for polychromatic experiments using multiple incident neutron energy in Repetition Rate Multiplication. Moreover, the chopper configuration can be tuned to high energy resolution, i.e. achieving $20 \mu\text{eV}$ elastic energy resolution at $2 \text{ meV}$ incident energy for the investigation of relaxations and diffusive processes, or to a relaxed resolution providing a flux gain up to a factor of 5. By limiting the beam collimation, the $Q$ resolution can be tailored to the experimental needs, as investigated in the study of the instrumental resolution function [2].

Many of the scientific questions to be addressed by the spectrometer will be tackled by means of neutron Polarization Analysis (PA) to probe not only the energy of spin excitations but also the eigenstates or to distinguish the spin-incoherent from the coherent scattering.

The incoming neutron beam is polarized by Spin Optical exchange pumping in the thermal spectral range [3] and supermirror devices for cold neutrons. XYZ neutron spin analysis in a wide angular range is realized using the magic PASTIS setup [4]. Here we base on our experience developing large high quality $^3\text{He}$ spin filter cells [5]. These components enable a long decay time of the polarization of the gas, which is crucial for long lasting inelastic scattering experiments.

In collaboration with the ESS detector group we are designing the PSD detectors based on the $^{10}\text{B}$ multigrid technology [6] to cover the large area (20 m$^2$ in the full scope) with minimal gaps and a high detection efficiency for neutrons of energy up to 200 meV.

E-mail for corresponding author: j.voigt@fz-juelich.de
The software is playing a large role in both the performance of experiments and the data treatment. The software utilized in most of instruments at the Materials and Life Science Experimental Facility (MLF) in J-PARC are based on several software frameworks. One is IROHA2 developed for the control and management of the hardware devices installed in the instrument, including the data acquisition system DAQ middleware [1] which realizes an event recording method. To control and manage the whole instrument more easily and efficiently, IROHA2 have a web interface to access all functions to achieve a platform-independent user interface. The other is the software series of data analysis and visualization. We've developed a framework software Manyo Library [2] for the development of data treatments software to unify the data container and to share the developed codes among instruments in MLF, for example unit-conversion function and data correction to obtain scientific results. Utsusemi [3] is one of the software suite developed with Manyo Library, which enables MLF users to convert event-recording data to histogram data to apply various corrections and visualization. The Utsusemi software has been already introduced into many instruments. These software developments are now ongoing to improve user experiences.

One topic of our recent successful developments is about the “quasi-real-time” data reduction and visualization method, named a live data reduction. From the beginning of MLF running, users have strongly required to see the current data during the measurement to decide next experimental conditions and schedules. To realize “real-time” data treatment we considered that the message queue technology of an asynchronous communications protocol should be utilized for our data acquisition system and data reduction software. In these years, we decided to adopt a Publisher-Subscriber model using this technology and developed new modules working in our DAQ middleware, which send event-recorded data to a message queue server as a data publisher. In addition, we have successfully demonstrated the live data reduction using Utsusemi or the other codes developed to be applied to obtain data from the server as a subscriber at several instruments in MLF.

In this presentation, we will introduce the structure of software utilized in MLF and recent topics in our developments.

E-mail for corresponding author: yasuhiro.inamura@j-parc.jp
Polarized neutron spectrometer POLANO, its construction and commissioning

Tetsuya YOKOO\textsuperscript{1,2}, Yoichi IKEDA\textsuperscript{3}, Shinichi ITOH\textsuperscript{1,2}, Masaki FUJITA\textsuperscript{3}
Manabu OHKAWARA\textsuperscript{3}, Naokatsu KANEKO\textsuperscript{1,2}, Takashi INO\textsuperscript{1,2}, Seiji SUGAI\textsuperscript{1,2}

\textsuperscript{1}High Energy Accelerator Research Organization (KEK), Institute of Materials Structure Science, Tsukuba, Japan
\textsuperscript{2}J-PARC Center, Materials and Life Science Experimental Facility, Tokai, Japan
\textsuperscript{3}Tohoku University, Institute for Materials Research, Sendai, Japan

POLANO is the chopper type spectrometer with a polarization analysis capability now under commissioning in the Materials and Life Science Experimental Facility (MLF), J-PARC. After spending several years for designing, manufacturing and construction of the spectrometer, finally commenced the beam commissioning of the POLANO with unpolarized condition \cite{1,2}. For instrumentation, pumping tests of the functional large vacuum chamber, adjust of detectors (PDSs), rotational and phasing test of choppers, operating communication tests, device control computing tests, and others were proceeded before opening shutter to ensure the neutron beam commissioning. With using neutron beam, its intensity, divergence, tof profiles and direct imaging were measured. Since POLANO is targeting high-energy polarization experiment, all those components are designed as optimizing for 100 meV neutron. In particular, 4Qc converging super mirror guide tube can effectively transport such a relatively high energy neutrons to the sample position \cite{3}. Also, we are making our efforts to eliminate unintended contamination (backgrounds). Direct beam catcher made of B$_4$C are placed just in front of detectors, which can prevent cross talks between detectors. We also install massive stainless steal collimator to adjust the cross section of incoming beam and to reduce unnecessary beam.

As mentioned above, POLANO principal concept is to achieve higher-energy polarization analysis of inelastic scattering beyond a reactor-based neutron source. We target the energy range over $\Delta E=40$ meV with using SEOP for a polarizer and bender supermirror as an analyzer (phase I). We are now working on developing \textit{in situ} SEOP system, achieve 70\textperthousand\textperthousand of $^3$He spin polarization \cite{4}. Also, magnetic devices and system are under development \cite{5}. In the next summer both SEOP system and magnetic systems will be installed in the beam line, and will start polarization beam commissioning. In the second phase, we focus on higher energy experiments ($0$ meV $< \Delta E < 100$ meV) with a wide solid angle SEOP/MEOP analyzer. In order to achieve a high flux polarized neutron experiment, we plan to adopt cross correlation method. R&D of the correlation chopper is now under way.

E-mail for corresponding author: tetsuya.yokoo@kek.jp
The SPectrometer for High Energy RESolution (SPHERES) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. It provides high energy resolution with a good signal-to-noise ratio [1]. Different components of the instrument have been upgraded to further improve the instrument performance.

Some recent years ago the PST chopper has been renewed. The new more compact one-wing chopper can be operated with the desired frequency with a crystal speed of 225m/s close to the optimum velocity for the phase space transformation. Together with the exchange of the chopper also the graphite deflector crystals on its circumference were replaced with ones of a higher reflectivity and mosaicity. Thanks to the increased velocity and the better deflector crystals, the intensity in most detectors had been doubled.

Just recently the focusing neutron guide has been replaced with an elliptic guide. It had been optimized based on simulations, which also considered the new PST chopper. With the new elliptic guide another intensity gain at the sample position of about 30% was obtained. Together with the exchange of the focusing guide also a new background chopper has been installed about 2m upstream of the PST chopper to further reduce background. This will then also allow for a high signal-to-noise setup by eliminating every second pulse, albeit at the cost of intensity.


E-mail for corresponding author: m.zamponi@fz-juelich.de
We report on the current progress of the IN16B backscattering spectrometer at the Institut Laue-Langevin in Grenoble, France [1]. It served the user community with about 400 beam days for experiments since late 2013, while exciting new options and experimental opportunities have been developed in parallel. Altogether, the instrument today is of extreme flexibility and the applications are manifold.

In its classical configuration with Si 111 Doppler monochromator and analyser, spectroscopy with sub-\(\mu\)eV resolution within a \(\pm 31\ \mu\)eV energy transfer window can be performed for momentum transfers up to 1.8 \(\text{Å}^{-1}\). Larger momentum transfers up to 3.7 \(\text{Å}^{-1}\) are available by using Si 311 crystals (2 \(\mu\)eV resolution with a \(\pm 59\ \mu\)eV transfer window). The possibility to perform elastic and inelastic fixed window scans are valued by our users, as they help to easily observe temperature or pressure dependent changes of the sample dynamics [2]. After a short presentation on IN16B we focus on a novel mode of operation with substantially increased signal-to-noise ratio reaching values above \(10^4\) in typical experiments [3], and the inverted time-of-flight option BATS that was commissioned in early 2018.

The principle of BATS was described first by van Eijck et al. [4] and is a major extension of the spectrometer, realised in collaboration with FAU Erlangen-Nürnberg and funded by the German Ministry of Education and Research (BMBF). A high speed pulse chopper system with two counter-rotating disc pairs of 750 mm diameter turning at up to 19000 rpm was installed 34 m upstream of the sample position. BATS opens the available energy transfer window beyond the limits of the conventional Doppler configuration and is the first implementation of such an instrument option on a reactor-based instrument. It provides high flexibility by using a complex slit pattern on the chopper discs which enable the use of 7 different slit widths. With Si 111 analysers, the energy resolution can be selected between 1.4 and 9.8 \(\mu\)eV in an energy transfer window with a width of 340 \(\mu\)eV that can be offset into the inelastic region. High repetition rate modes with a pulse frequency of 237 Hz are available for increasing intensity at the cost of reducing the available energy transfer window. Moreover,
BATS is compatible with the use of Si 311 analysers (to be commissioned).

To achieve the necessary, short pulse lengths for BATS, the slit width on the discs needed to be reduced below the width of the existing guide. We present the concept of a future adaptive focusing and defocusing guide system with variable width that matches the flexibility of the chopper system, where its mechanical feasibility has recently been demonstrated.

Another important development, the GaAs option for highly improved energy resolution, is reported by K. Kuhlmann in a separate contribution.


E-mail for corresponding author: appel@ill.eu
WI_14 The status of the ultra-high-resolution neutron spectroscopy at ORNL

Fankang Li¹, Jaime A. FERNANDEZ-BACA¹, Lowell CROW¹, Steven R. PARNELL³, Masaaki MATSUDA¹ and Roger PYNN¹,²

¹ 1 Bethel Valley Road, Oak Ridge, TN, USA, 37831 (Oak Ridge National Laboratory, Oak Ridge, TN, USA).
² 2401 N Milo B Sampson Ln, Bloomington, IN, USA, 47408 (Indiana University, Bloomington, IN, USA)
³ Mekelweg 15, 2629 JB Delft, Netherlands (Delft University of Technology, Delft, The Netherlands)

To measure the crystal lattice distortion or the lifetime of weak interactions among quasiparticles, such as phonons, electrons and magons, with high resolution, the key is to break the inverse relationship between the resolution and useable flux. By using the Larmor precession of the neutron spin inside a given magnetic field, its momentum or energy change during the interactions with sample can be measured with ultra-high resolution. Therefore, this unique property of neutron provides us with another approach to overcome some of the limitations of conventional neutron scattering instruments. Also, it can make the best use of all the available neutrons by allowing the use of large divergent beams. The progress on upgrading the HB-1 polarized triple axis spectrometer at the High Flux Isotope Reactor of ORNL with superconducting magnetic Wollaston prisms will be presented. For neutron diffraction, the achievable resolution of the absolute peak splitting and relative lattice distortion ($\Delta d/d$) can be $2\times10^{-4}$ and $1\times10^{-6}$ relatively [1-2]. While for inelastic scattering, for example phonon linewidth and phonon energy shift measurements, the resolution can be <10µeV [3].


E-mail for corresponding author: fankangli@hotmail.com

Back to the program
A high energy direct geometry time-of-flight neutron spectrometer at CSNS

Meng Wang¹, Taisen Zuo², Fangwei Wang³, Daoxin Yao¹, Yue Zheng¹, Dehong Yu⁴

¹School of Physics, Sun Yat-sen University, Guangzhou, China
²China Spallation Neutron Source, Institute of High Energy Physics Chinese Academy of Sciences, Dongguan, China
³Institute of Physics Chinese Academy of Sciences, Beijing, China
⁴Australian Center for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia

The China spallation neutron source (CSNS) locating at Dongguan in Guangdong province is the first spallation neutron source in China [1]. It was designed with a 100 kW power with the possibility to be upgraded to 500 kW. As a collaborative project between Sun Yat-sen University and CSNS, we are planning to build the first high energy direct geometry time-of-flight neutron spectrometer (Sun-light) at CSNS.

Sun-light spectrometer will be sitting on a neutron guide pointing at a decoupled water moderator. An elliptical supermirror neutron guide is proposed to maximize flux at the sample position. A set of choppers including T0, Disk and Fermi choppers, will be employed to eliminate fast neutron background, remove overlapping frames and optimize energy resolutions suitable for different scientific needs. The desired incident energies (Ei) are from 20 to 1000 meV with an energy resolution of 3-10% of Ei. A multi-Ei mode will be employed below Ei=300 meV. He-3 position sensitive detectors, covering an angular range from -30 to 60 degrees, are temporally proposed to be used. The distance between the sample position and the detectors is 2.5 m. With these preliminary specifications, Sun-light will be able to cover momentum transfer up to 12 Å⁻¹ with 300 meV incident energy. The spectrometer is designed to study material dynamics for a wide range of functional materials in many fields such as physics, material and chemical sciences.


E-mail for corresponding author: wangmeng5@mail.sysu.edu.cn
The European Spallation Source (ESS), a next generation neutron spallation source, is presently under construction in Lund, Sweden. The first 15 instruments have been selected from conceptual proposals submitted by groups from around Europe. These instruments present numerous challenges for detector technology in the post Helium-3 crisis era, which is the default choice for neutron detectors for instruments built until today and due to the extreme instantaneous rates expected across the ESS instrument suite. Additionally a new generation of source requires a new generation of detector technologies to fully exploit the opportunities that this source provides.

During 2016, all the instruments have had the initial scope of the instrument determined within the construction phase of ESS. The current baseline detector requirements are presented. A strategy outline as to how these requirements are being tackled by is shown, as well as ongoing developments [1].

In particular for ESS, over half of the detectors will be based upon thin film converters of $^{10}$Boron Carbide [2,3,4]. The highlights of the developments so far over the past 6 years are shown [5,6,7,8]. In particular, examples of how these have been tested to determine that scientific requirements are met are shown, based upon demonstrating key aspects of scientific performance. Additionally for the first time, simulation of detailed detector and instrumental performance has been used to refine and determine the detector design [9,10]. The state of the art of these simulation techniques is shown as well as future prospects.


E-mail for corresponding author: richard.hall-wilton@esss.se
CAMEA—A novel multiplexing analyzer for neutron spectroscopy

Felix Groitl1,2, Dieter Graf,3 Jonas Okkels Birk,2 Márton Markó,2,4 Marek Bartkowiak,3 Uwe Filges,3 Christof Niedermayer,2 Christian Rüegg,2,5 and Henrik M. Rønnow1,6

1École Polytechnique Fédérale de Lausanne, Laboratory for Quantum Magnetism, 1015 Lausanne, Switzerland
2Paul Scherrer Institute, Laboratory for Neutron Scattering and Imaging, 5232 Villigen, Switzerland
3Paul Scherrer Institute, Laboratory for Scientific Developments and Novel Materials, 5232 Villigen, Switzerland
4Wigner Research Centre for Physics, Neutron Spectroscopy Department, 1525 Budapest, Hungary
5Department of Quantum Matter Physics, University of Geneva, 1211 Geneva, Switzerland
6University of Copenhagen, Niels Bohr Institute, 2100 Copenhagen, Denmark

The analyzer detector system continuous angle multiple energy analysis will be installed on the cold-neutron triple-axis spectrometer RITA-2 at SINQ, PSI. CAMEA is optimized for efficiency in the horizontal scattering plane enabling rapid and detailed mapping of excitations. As a novelty the design employs a series of several sequential upward scattering analyzer arcs. Each arc is set to a different, fixed, final energy and scatters neutrons towards position sensitive detectors. Thus, neutrons with different final energies are recorded simultaneously over a large angular range. In a single data-acquisition many entire constant-energy lines in the horizontal scattering plane are recorded for a quasi-continuous angular coverage of about 60 degrees. With a large combined coverage in energy and momentum, this will result in a very efficient spectrometer, which will be particularly suited for parametric studies under extreme conditions with restrictive sample environments (high field magnets or pressure cells) and for small samples of novel materials. In this talk I will outline the concept, specifications and current status of the instrument currently under construction.


E-mail for corresponding author: henrik.ronnow@epfl.ch
The European Spallation Source (ESS) is a European Research Infrastructure Consortium (ERIC), a multi-disciplinary research facility based on the world’s most powerful neutron source with a vision to enable scientific breakthroughs in research related to materials, energy, health and the environment, and address some of the most important societal challenges of our time [1]. The ESS is realizable only by harnessing the European wide neutron instrumentation, accelerator, target and moderator expertise in the form of the “in kind” model. The initial suite of neutron instruments will consist of 15 instruments delivered by European partners, with further integration of instruments following to complete the projected suite of 22 instruments.

Neutron chopper systems are expected to be present on nearly all of the instruments foreseen for ESS, totaling more than 150 unique systems, once the facility reaches maturity in a wide spanning geographical layout of over 200 m². The pulse structuring and wavelength band selection functions of neutron chopper systems are central to the operation of instruments at all facilities and at the ESS and will be critical to unlocking the full potential of the center’s unique long pulse source. High performance, high reliability and radiation-hard choppers systems are required in order to tailor the long pulse, meet our challenging scheduled beam availability requirements of 95% and withstand the harsh radiation environment, making the ESS neutron chopper systems unique.

In order to meet these challenges and with the help of our European partners the ESS Neutron Chopper Group is leading critical technology development in a horizontal cross section of the ESS neutron instrument chopper needs. The latest developments in Chopper Control Systems, Chopper Mechanical integration, Remote handling of active components, High speed choppers, Prompt pulse suppression (T0), critical chopper materials irradiation tests and finally the latest in vivo vertical integration test of a complete ESS chopper system using the ESS architecture will be presented. The resulting developments are already being integrated in current instrument detailed designs.

This work is the culmination of European neutron chopper expertise and is of utmost importance in the production of high performance, maintainable chopper systems that ensure the highest instrument availability achievable and in turn to fulfill the immediate and long term scientific objectives of the ESS facility.

E-mail for corresponding author: nikolaostaptsaris@esss.se
The high flux backscattering spectrometer (HFBS) installed at the NIST Center for Neutron Research is an inverted geometry spectrometer capable of resolving motions on the time scale of a few nano seconds. As a high-resolution spectrometer, flux at the sample position is always a critical issue. To increase the flux at the sample position, HFBS employed a phase space transformation chopper which increases flux by a factor of 4.2. To increase the flux further, we recently upgraded our focusing guide that enhances flux by a factor of 1.9. The new focusing guide is made of 8 smaller sections of 50 cm each; each section is coated with a material that corresponds to a unique ‘m’ value. This guide also features a distinct taper design. This novel design enhances flux at the guide exit as more neutrons now can be reflected efficiently by the coated material. I will also discuss design of new background suppression chopper that we are working on to bring down the overall background.

E-mail for corresponding author: madhusudan.tyagi@nist.gov
CHESS: A look into the next generation of neutrons instruments

G. Sala¹, G. Ehlers², V. B. Graves² K.W. Herwing², J.Y.Y. Lin³

¹Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
²Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA
³Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

CHESS is the new proposed direct geometry inelastic spectrometer dedicated to the analysis of small samples with modest energy resolution (2.5-5% of E_i). This relatively short instrument will take full advantage of both the increased peak brilliance of the SNS Second Target Station (STS) coupled moderators, and of the recent advances in instrument design and technology, to achieve unprecedented performance for inelastic scattering in the cold energy range [1]. The simulations predict that it will exceed that of CNCS by at least a factor of 200. Two sections of ballistic octagonal guides will transport the beam to the sample position at 29.6 m from the moderator. A new concept for double disk choppers will select the wavelengths and deal with frame overlap. CHESS will take full advantage of Repetition-Rate Multiplication (RRM) to analyze samples at multiple incident energies, maximizing the efficiency of the measurement. Finally, the detector tank will house a large array of curved 8-pack detector ³He tubes giving a total solid angle coverage of 6.0 sr, and it will incorporate Helmholtz coils for polarization analysis.

Detailed Monte Carlo (MC) simulations of a real experiment on K₂V₂O₈ have been performed to optimize the instrument using McStas and MCViNE; these results were verified by running similar calculations on CNCS.


E-mail for corresponding author: salag@ornl.gov
Neutron spin echo spectroscopy (NSE) uniquely enables us to explore the dynamics of various materials spatiotemporally. NSE has already achieved the highest energy resolution with neutrons as a probe [1], that is, the maximum Fourier-time has reached a submicrosecond.

Kyoto University and KEK have been installing two types of neutron spin echo (NSE) spectrometers with neutron resonance spin flippers (RSFs) into BL06 at Materials and Life Science Experimental Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC). The beam line consists of a neutron resonance spin echo (NRSE) instrument and a modulated intensity by zero effort (MIEZE) instrument. NSE with RSFs is a rather new approach [2]. Furthermore, the combination of NSE and a pulsed neutron source makes it possible to scan a wide spatiotemporal space very efficiently. The beam line has been named “VIN ROSE” (Village of Neutron ResOnance Spin Echo spectrometers), which will spawn a new field of spectroscopic methods [3].

We have started the commissioning with the MIEZE spectrometers and verified the characterizations between time-of-flight neutron spectroscopy and MIEZE, TOF-MIEZE, quantitatively [4]. Recently, 400kHz-MIEZE signal was successfully generated. At the NRSE spectrometer, the two-dimensional ellipsoidal neutron-focusing supermirrors are now under development in close collaboration with the RIKEN center for advanced photonics. The ellipsoidal supermirrors are essential for NRSE with high-energy resolution, which is installed before and after the sample position symmetrically to correct the path difference. The optical design is 1250mm semi-major axis and 65.4mm semi-minor axis with 900mm length. Such a large ellipsoidal supermirror was unrealistic due to the difficulties in both the supermirror deposition and the substrate fabrication. Our strategy to develop such large ellipsoidal supermirrors is to assemble the segments deposited by the supermirror. We have established the necessary elemental technique [5], and achieved the reasonable characteristics evaluated by neutron reflectivity measurements. The spin echo signals at the NRSE spectrometer with the ellipsoidal supermirrors (3Qc) have been successfully archived most recently. The detailed status of BL06 “VIN ROSE” will be given at the presentation.


E-mail for corresponding author: hitendo@post.j-parc.jp
Nine years of AMATERAS — a cold-neutron disk-chopper spectrometer

Kenji Nakajima¹, Seiko Ohira-Kawamura¹, Maiko Kofu³, Tatsuya Kikuchi¹,², Yasuhiro Inamura¹

¹Materials and Life Science Division, J-PARC Center, Tokai, Ibaraki, Japan
²Research & Development HQ., Sumitomo Rubber Industries, Ltd., Kobe, Hyogo, Japan

AMATERAS (Figure 1) is a cold-neutron disk-chopper spectrometer installed at BL14 port of the Materials & Life Science Experimental Facility (MLF) at J-PARC [1]. AMATERAS is one of the first generation disk-chopper spectrometers with pulse-shaping operation as with CNCS at SNS and LET at ISIS, and it is designed to carry out inelastic and quasielastic neutron scattering experiments in the range from cold to sub-thermal neutron energy with high intensity and fine and flexible energy resolution.

AMATERAS started its operation and user program from December 2009. Up to now, experiments of more than 140 proposals have been carried out, which resulted in more than 50 papers, 11 theses and 7 press releases. Along with performing a user program, we are continually maintaining and improving the performance of the spectrometer. During the operation, we had have number of technical problems, which we have overcome or are trying to do so.

In this presentation, based on our experience of 9 years of operation of the spectrometer, we will show the current status, issues and future plans of AMATERAS.


E-mail for corresponding author: kenji.nakajima@j-parc.jp
The European Spallation Source (ESS), expected to be the world’s most powerful neutron source, will begin operations in 2022. Among the endorsed instruments foreseen for day one instrumentation at ESS, is the cold time-of-flight spectrometer CSPEC. CSPEC is a joint proposal from the Technische Universität München, Germany, and the Laboratoire Léon Brillouin, Saclay, France. The high performance cold time-of-flight-spectrometer will serve multiple disciplines to address scientific questions from hard and soft matter research, life sciences, geosciences and magnetism. In particular CSPEC will be optimized to address time dependent phenomena under realistic conditions. While current day spectroscopic experiments mainly probe the static state of a sample, neutron spectroscopy experiments that probe the time dependent behaviour, e.g. of electrolytes in an electric field, or laser excited light harvesting proteins, are still in an exploration stage, mainly due to the lack of flux at the instruments available today. CSPEC will benefit from the high brilliance of the ESS spallation in addition to the cumulative flux provided by repetition rate multiplication (RRM) that results in large flux gains making it possible to probe time-dependent phenomena with millisecond to second time resolution.

The unique pulse structure of the ESS with its long pulse duration (2.86 ms) and a repetition rate of 14 Hz requires new concepts for the instrumentation to make optimum use of the available source time frame. With an instrument length of ~160 m, moderator to sample, a wavelength range of $\Delta \lambda \leq 1.8$ Å can be probed within each ESS time period via RRM. The energy resolution can be tuned in the range of $\Delta E/E = 6 - 1\%$, and CSPEC will utilize cold neutrons in the range from $\lambda = 2 - 20$ Å with the focus on the cold part of the spectrum. The guide is optimised to enhance signal to noise and will be able to focus on samples ranging from several mm$^2$ to several cm$^2$ in area. The large detector area, with a radius of 3.5 m, -30° – 140° and 3.5 m in height, will incorporate a sample chamber with cryogenic vacuum to limit the background through sample environment scattering. In addition the sample chamber will, via the use of a gate valve, enable experiments under real and transient conditions. CSPEC is in the preliminary engineering phase and we will present the current design layout and the expected performance.

E-mail for corresponding author: slongeville@cea.fr
Inelastic neutron scattering as a vibrational spectroscopy technique [3] is widely used across chemistry, materials science, biology, and beyond. This presentation focuses on recent developments on two of these spectrometers, namely, TOSCA (ISIS, UK) [4] and VESPA (ESS, Sweden) [5], both joint ventures between CNR (ITA) and ISIS (UK). These two broadband high-resolution chemical spectrometers exploit the time-of-flight technique at a pulsed spallation source in so-called indirect geometry, whereby final-energy selection is attained with crystal analyzers after scattering by the sample. To optimize instrument design, extensive neutron-transport simulations and baseline studies of neutronic response have become a must, along with extensive benchmarking against much-needed experimental data. This combined approach was not the norm in the past (i.e., TFXA or the earlier TOSCA), but has now become an essential ingredient in recent and forthcoming instrument upgrades on TOSCA, or in the design of VESPA.

In the above context, this contribution provides an update of ongoing efforts on TOSCA to quantify its neutronic response before and after a recent and major upgrade of the primary spectrometer [6-8], as well as ongoing feasibility studies aiming at a subsequent upgrade of its secondary spectrometer [9]. This work represents the first opportunity to benchmark a broadband, high-resolution chemical spectrometer in terms of measured vs. simulated response. In the case of VESPA, the current design of both its primary and secondary spectrometers has already capitalized from these joint efforts, including a detailed analysis of expected performance supported by both simulations and analytical models.

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[1] Url: www.isis.stfc.ac.uk/Pages/Tosca.aspx

E-mail for corresponding author: matteo.zanetti@cnr.amministrazione.it
Combining neutron time-of-flight spectroscopy with longitudinal polarization analysis promises the possibility of separating cross-section components over vast regions in \((Q,\Delta E)\) space. This is particularly useful in systems where the scattering component of interest is dominated by other components e.g. proton diffusion in lightly doped ionic conductors or longitudinal spin excitations in quantum magnets. While polarized time-of-flight spectroscopy is conceptually very attractive, it has proven difficult to realize due to the joint requirement of broad-band and wide-angle analysis; indeed, after decades of effort, only a few spectrometers support it world-wide. In this talk, I will describe our recent progress [1,2] towards installing uniaxial longitudinal polarization analysis on the LET time-of-flight spectrometer at the ISIS facility. The polarized beam is generated by a supermirror "V"-cavity polarizer, immediately followed by a Mezei-type precession coil flipper. Analysis of the scattered beam is achieved using a wide-angle \(^4\)He spin filter, providing access to the full \(\pi\) st. covered by the detector array. While polarization analysis on LET most obviously caters to studies of magnetic materials, the possibility of probing quasi-elastic processes (like proton diffusion) with high resolution and isotopic sensitivity represents an interesting future prospect.


E-mail for corresponding author: goran.nilsen@stfc.ac.uk
China Advanced Research Reactor (CARR) was built in China Institute of Atomic Energy (CIAE) locating in Southwest of Beijing. It was a 60 MW tank-in-pool inverse neutron trap type research reactor equipped with a liquid D₂ cold neutron source. The reactor has 9 horizontal beam tubes and 25 vertical channels, the maximum thermal neutron flux is about $8 \times 10^{14}$ n/(cm$^2$·s). On May 13th 2010 the reactor went critical, and reached full power for 72 hours on March 13th 2012. At the end of 2017 CARR project was passed through the official evaluation organized by the government successfully, and the application of operating license is under review. As a multipurpose research reactor, its main applications include neutron scattering, neutron activation analysis, isotope production, silicon doping, fuel element test, fundamental nuclear physics and so on.

Till now nine instruments are constructed through the internal and international cooperation, which are High Resolution Powder Diffractometer, High Intensity Powder Diffractometer, Residual Stress Diffractometer, Texture Diffractometer, Four Circle Diffractometer, Reflectometer, Small Angle Neutron Scattering and two Thermal Triple Axis Spectrometers. Some experiments were carried out to prove the quality of instruments, the results are quite comparable with those obtained from the similar instruments in the world. In June 2017 the cold source was ready.

Furthermore, another 7 instruments were approved and are under construction now, which are Thermal Neutron Imaging, Cold Neutron Imaging, Cold Triple Axis Spectrometer, Multi Axis Crystal Spectrometer, Engineering Neutron Diffractometer, Prompt Gamma Thermal and Cold neutron Activation Analysis Instruments. They are expected to be ready at the end of 2019.


E-mail for corresponding author: ytlhu@ciae.ac.cn
WINS Oral Talks

WN_01  Breakthrough in neutron backscattering spectroscopy: A tenfold enhanced energy resolution using GaAs 200

Kristijan KUHLMANN¹², Markus APPEL¹², Bernhard FRICK², Andreas MAGERL¹

¹ Friedrich-Alexander University Erlangen-Nürnberg, Biophysics group, Erlangen, Germany
² Institut Laue-Langevin, Grenoble, France

A demonstrator neutron backscattering spectrometer using the GaAs 200 Bragg reflection has been developed to bring about a significant increase in energy resolution. The gain in resolution is offered by the narrow intrinsic line width of GaAs 200, an order of magnitude smaller than the line width of the currently used Si 111. Test measurements on the backscattering spectrometer IN16B at the ILL have yielded an unprecedented energy resolution of δE = (76.5 ± 3.3) neV FWHM, a factor of 10 smaller than the current standard of 750 neV FWHM as well as a factor of 4 smaller than the highest currently available resolution in neutron backscattering of 300 neV FWHM. These measurements have provided proof of concept for the construction of a full-scale user instrument.

E-mail for corresponding author: kristijan.kuhlmann@fau.de
MCViNE (Monte-Carlo Virtual Neutron Experiment) is an open-source Monte Carlo (MC) neutron ray-tracing software developed using C++ and Python. Its object-oriented design allows for flexible, hierarchical representations of sophisticated instrument components such as detector systems, and samples with shapes and scattering kernels of various sorts. This flexible design enables many applications of MCViNE simulations at the Spallation Neutron Source (SNS), Oak Ridge National Lab. MCViNE simulations of powder and single crystal samples measured at Direct-geometry TOF spectrometers have shown excellent agreement with experimental datasets, including signals from vibrational and magnetic origins. The predictive power of MCViNE makes it suitable in helping design new instruments. Therefore, MCViNE was used to simulate the CHESS instrument, a new DGS instrument planned for the Second Target Station (STS) at SNS that takes full advantage of high-brightness of STS moderators and is especially suitable for small samples. The simulations allow the designers to optimize the design for the guide and the detector system, and to make reasonable comparisons to the CNCS instrument at SNS. MCViNE simulations were also performed for MENUS, a transformational high flux versatile multi-scale materials engineering beamline at STS to compare its performance to that of VULCAN at SNS. MCViNE simulations were also used to study the effects of instrument resolution on the measured data. Detailed simulations of powder 4He data measured at ARCS and single crystal spinwave data for V2O3 measured at SEQUOIA were used to examine and confirm the material and resolution models. In addition, MCViNE simulations of resolution functions for ARCS powder experiments were carried out to aid in "super-resolution" reconstruction of phonon Density of States.

E-mail for corresponding author: linjiao@ornl.gov
The Extreme Environment Diffractometer at Helmholtz Zentrum Berlin is a time-of-flight (TOF) instrument dedicated to studies of novel spin phenomena in strong (up to 26 T) static magnetic fields and low temperatures\cite{1}. Originally it was designed as an elastic instrument – TOF diffractometer. Later, to maximize the scientific scope it was extended to have a small angle scattering capabilities. Recently an upgrade to achieve a direct geometry inelastic scattering functionality has been implemented successfully. Compromising between the multiple limitations from the permanently installed High Field Magnet\cite{2} and the existing instrument configuration, a variety of instrument parameters were optimized to maximize flux on the sample for given resolution\cite{3}.

In this contribution I will report on the recent progress in installation of the inelastic option on EXED, its commissioning, as well as user experiments. Selected experimental results will be presented to illustrate the capability and performance of the instrument. The successful implementation of inelastic option on Extreme Environment Diffractometer marks a new level for the inelastic neutron scattering in extreme conditions and opens new fields for research in high magnetic fields.

Reference


*E-mail for corresponding author: prokhnenko@helmholtz-berlin.de
DRAGON is a thermal triple-axis spectrometer (TTAS) under construction at China Mianyang Research Reactor (CMRR), which is designed to measure lattice and magnetic excitations in materials. The construction of DRAGON was launched in May 2017 and will be finished in April 2021. The TTAS DRAGON is estimated to be in commission and in full service in 2022. DRAGON is highly configurable and versatile, which has four main characteristics. 1) The neutron velocity selector is employed instead of pyrolytic graphite (PG) to filter high-order neutrons so the incident neutron energy could be selected consecutively. 2) Two double-focusing monochromators are employed: highly oriented pyrolytic graphite HOPG (002) and copper Cu (220). 3) Single 3He tube detector mode is used. 4) The sample environments including high magnetic field (8T), static high pressure (2 Gpa) and ultra-low temperature (300 mK) will be equipped.

E-mail for corresponding author: hbf@caep.cn
QP_01 A better view through new glasses: Developments at the Jülich Neutron Spin Echo Spectrometers

Olaf HOLDERER\textsuperscript{1}, Piotr ZOLNIERECZUK\textsuperscript{2}, Stefano PASINI\textsuperscript{3}, Laura STINGACIU\textsuperscript{3}, Michael MONKENBUSCH\textsuperscript{4}

\textsuperscript{1}Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany
\textsuperscript{2}Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Spallation Neutron Source, ORNL, Oak Ridge, USA
\textsuperscript{3}Oak Ridge National Laboratory, Spallation Neutron Source (SNS), Oak Ridge, USA
\textsuperscript{4}Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1), Jülich, Germany

Thermal fluctuations in soft matter systems take place on length- and time scales of nanometers and nanoseconds, accessible with neutron spin echo (NSE) spectroscopy. New developments in instrumentation as well as data treatment opened the door for new measurements with highest precision for subtle effects and gains in energy resolution. Superconducting main coils with optimized field shape have been installed at the J-NSE recently, providing better resolution and more flux for a given resolution. The magnetic shielding of the SNS-NSE provides unprecedented phase stability, which has been exploited for tiniest effects of additives to membrane fluctuations in microemulsions [1]. Both spectrometers work with superconducting and fringe field compensated coils, ensuring an excellent instrumental stability and the possibility to go to large scattering angles. New software for data evaluation, DrSPINE [2] provides the intermediate scattering function in an easy and robust way from the complex data structure of several angle (q) and Fourier time settings, both for reactor based and time of flight NSE instruments. Especially at the SNS-NSE the TOF structure of the data together with DrSPINE allows a flexible inspection of a quasicontinuous (Q,t) range with an “arbitrary” selection of binning of the data.

Domain motions in proteins under physiologically relevant conditions are an emerging topic for NSE spectroscopy, with the potential to link protein motion to function [3]. Optical components such as resonator structures and neutron prisms [4] improved the use and applicability of grazing incidence NSE experiments to study soft matter dynamics at the solid-liquid interface as a dynamic extension to GISANS. Phospholipid bilayers at the interface showed membrane motion with not overdamped modes [5].

E-mail for corresponding author: o.holderer@fz-juelich.de
Deep eutectic solvents (DES) are multi-component mixtures that have freezing point lower than their individual components [1, 2]. Mixture of alkylamide with lithium salts in a particular molar ratio form deep eutectic solvents with melting point lower than room temperature [3]. DES are novel class of solvents analogous in their physiochemical properties to ionic liquids. Some advantages like, biodegradability, low cost, extended moisture stability, etc. make them industrially viable solvents [1].

Over the last decade, there has been growing interest in understanding the structure and dynamics of these systems in order to prepare DES with tailor-made physical and chemical properties [1-3]. Here, we report for the first time, quasielastic neutron scattering (QENS) measurements on alkylamide based DES. QENS experiments have been carried out on DESs made form mixtures of alkylamide (RCONH$_2$, R=CH$_3$) and lithium salts (Li$^+X^-$; $X$= NO$_3^-$, ClO$_4^-$, Br$^-$), using IRIS spectrometer at ISIS facility, Rutherford Appleton Laboratory, UK.

It is found that the dynamics of DES is significantly constrained compared to the molten alkylamide as shown in Fig. 1 (upper panel). Detailed data analysis indicates presence of two distinct motions: (i) translation motion of whole alkylamide and (ii) localized internal motion. Translational motion of alkylamide is found to follow jump diffusion whereas internal motion can be described as localized translation motion. Effects of various anions, chain length of alkylamide and temperature on the microscopic dynamics of alkylamide have also been investigated. As shown in Fig. 1 the dynamics is found to be strongly dependent on the anion of the lithium salt, Br$^-$ effects the maximum and ClO$_4^-$ the least which is consistent with the viscosity data. There exist many reports based on MD simulation studies [3] which relate the observed effect towards hydrogen bond breaking ability of the anions. Our results are more or less in consistent with the MD simulations studies.

E-mail for corresponding author: sharmavk@barc.gov.in
Dynamics in lipid membrane play a vital role in various processes such as membrane protein interaction, cell signaling, drug delivery, cell division, bilayer permeability etc. Dioctadecyldimethylammonium bromide (DODAB), a potential candidate for applications in drug transport or DNA transfection, forms bilayer in aqueous media exhibiting a rich phase behavior. The detailed dynamical and phase behavior of pure DODAB bilayers are investigated by us earlier [1]. Despite of well known side effects, nonsteroidal anti-inflammatory drugs (NSAIDs) are one of the most prescribed drugs worldwide for their anti-inflammatory and antipyretic properties. Here, we report the effects of two NSAIDs, aspirin and indomethacin, on the thermotropic phase behaviour and the dynamics of DODAB lipid bilayer as studied using quasielastic neutron scattering techniques. Fixed elastic window scan (FEWS) (shown in Fig.1) showed that the addition of aspirin and indomethacin, profoundly affects the phase behaviour of DODAB bilayer in heating as well as in cooling cycles. It is observed that coagel to fluid phase transition takes place at lower temperatures with addition of aspirin and indomethacin compared to pure DODAB. It is found that while cooling, addition of the NSAIDs, inhibits the formation of the gel phase and directly go to the coagel phase.

Quasielastic neutron scattering (QENS) data are recorded with IRIS spectrometer, ISIS pulsed Neutron and Muon source at the Rutherford Appleton Laboratory, UK. Data analysis showed that only internal motion exists in the coagel phase, whereas in the fluid phase, lateral motion of the DODAB molecules is also observed in addition to internal motion. In the coagel phase, although the rotational diffusion coefficient of DODAB is found to be almost twice with the addition of the drugs, the mobility fraction did not change for indomethacin but becomes twice for aspirin. In the fluid phase, the diffusivity corresponding to lateral motion is reduced due to addition of indomethacin but almost no change is observed for aspirin.
the internal motion, while indomethacin does not show any significant effect, addition of aspirin leads to enhancement of internal motion. The different responses of DODAB bilayer to the aspirin and indomethacin provide a relevance to the study of affect of NSAID on dynamical characteristics of biomembrane mimetic systems.


E-mail for corresponding author: smitra@barc.gov.in
QP_04 Proton diffusion in the protic ionic liquid 2-Aminoethanaminium Triflate: A computational approach

Juan F. MORA CARDOZO¹, Pietro BALLONE², Jan P. EMBS¹

¹Paul Scherrer Institute, Laboratory for Neutron Scattering and Imaging, 5232 Villigen PSI, Switzerland.

²Italian Institute of Technology, Via Morego 30, Genova, Italy.

Room temperature ionic liquids (RTILs) with melting temperatures below 100 °C are already used in different advanced chemical processes, in nanotechnology, catalysis, biomedicine, lubrication and in many more applications. Thanks to their ionic character, RTIL are electrolytes suitable for electrochemical applications. Tunable ionic charge density, high thermal and electrochemical stability are just some of the attractive properties of such liquids. Due to the high hydrogen content of the cation and the possibility of having H-free anions, protic and aprotic ionic liquids (PILs, APILs) are ideal for being studied by QENS experiments [1,2,3]. Electrical conductivity in PILs occurs via a bi-stable proton hopping between two (or more) complementary and competing donor/acceptor sites, located in the anion and cation, respectively. (Proton transport can then be followed in QENS using partial deuteration of non-acidic hydrogens.) Molecular dynamics (MD) simulations are a perfect tool to complement neutron experiments. MD basically operates on the same time and space scale as neutron scattering techniques and thus allows to obtain S(Q,ω) that can be compared to data from scattering experiments [4]. In this work, we show how to construct a reactive force field (FF) that is both capable to describe proton-like conductivity and also easy to implement. The selected system is the diamine-based PIL 2-Aminoethanaminium Triflate (DAEt-TF), which shows non-vehicular proton transport mechanisms, i.e. the main transport mechanism is based on proton-hopping events [5]; the figure shows a computed hydrogen-bond geometry (hydrogen bonds between selected protons in the cation and O-atoms in the anion are indicated by dashed lines). We used the empirical valence bond matrix method to implement proton-hopping dynamics in our simulations [6]. The force field has the functional form of the optimized potential for liquids simulations (OPLS), which is supported by most of the molecular dynamics software packages and then can be integrated to them. The FF was optimized with the help of density functional calculations in the Kohn-Sham formulation using plane waves and pseudopotentials. We will present simulation results and show implications for upcoming neutron scattering experiments on the simulated system.

E-mail for corresponding author: juan.mora@psi.ch
QP_05  In situ Quasi Elastic Neutron Scattering of Nafion Membrane with Water Vapor Pressure Control System

Takeshi YAMADA, Taiki TOMINAGA

CROSS, Neutron Science and Technology Center, Tokai, Japan

In situ measurement combining with the high flux neutron beam of MLF, J-PARC is adaptable for observing vapor adsorption, charge and discharge and deforming among other kinetics. We have developed in-situ water vapor pressure control system, for QENS, which controls absolute water vapor pressure. Here, the design and specification of the system is represented with results of in situ QENS measurement of Nafion® membrane.

In situ QENS measurement was performed at BL02 DNA near back scattering spectrometer installed at MLF, J-PARC with 3.6 μeV energy resolution [1]. The sample was Nafion® purchased from Alfa Aesar and was dried before the experiment under vacuum. The sample was loaded into the cylindrical cell and attached on the sample stick of the water vapor pressure control system. The sample stick was mounted on the top-loading cryo-furnace of BL02 DNA. The measurements were performed from dried state to $p/p_0 = 0.8$ for 42 h at 300 K.

The obtained integrated QENS intensity between 10 and 40 μeV in energy transfer and water vapor pressure was shown in Figure 1. The QENS intensity increased with increase of water vapor pressure. Further analysis is shown in the presentation.
Figure 1. Plot of integrated QENS intensity between 10 and 40 μeV in energy transfer (open circle) and water vapor pressure (solid line) as a function of time.


E-mail for corresponding author: t_yamada@cross.or.jp
The discovery of the stable i-Cd–Yb binary icosahedral phase and the isostructural i-Zn–Mg–Sc has allowed a deep understanding of quasicrystal atomic structure. Therefore, periodic approximants to quasicrystals offer a unique opportunity to better understand the structure, physical properties and stabilizing mechanisms of their quasicrystal counterparts. In the case of the 1/1 cubic Zn₆Sc approximant to the icosahedral quasicrystal i-MgZnSc, the structure of low temperature phase have been showing the tetrahedron ordering antiparallel along the [110] direction of high temperature phase.

We present a detailed study of Quasielastic Neutron Scattering (QENS) due to the tetrahedron dynamic among the order–disorder phase transition occurring at about $T_c = 160$ K. The QENS measurements have been performed at around $Q = 2.67 \, \text{Å}^{-1}$ near the $(1/2, 11/2, 2)$ superstructure reflection and for temperatures ranging from 100 K (i.e. below $T_c$) to 400 K.

The QENS experiments were conducted on the DNA time-of-flight type Si analyzer near backscattering spectrometer installed at the MLF, J-PARC. The spectrometer was operated in high-resolution $\Delta E$ mode and at high momentum transfer Q mode, with an instrumental resolution of $\Delta E = 12$ micro eV using Si311 analyzer. The measurements were carried out on a polycrystalline sample of about 18.5 gram.

In the measured QENS spectrum, we observed two relaxation processes, not only the fast process which is characterized several 100 micro eV at the full width at half maximum (FWHM), but also the slow process which is characterized several 10 micro eV at FWHM. In the previous paper [1], it was observed the fast process, on the other hand, not observed the slow process. We will report the detailed characters of not only slow process, but also the fast process.


E-mail for corresponding author: shibata.kaoru@jaea.go.jp
Deep eutectics (DEs) are novel class of solvents analogous in their physiochemical properties to ionic liquids. Some advantages like, biodegradability, cheaper preparation methods, extended moisture stability, etc. make them industrially viable solvents. Over the last decade, there has been growing interest in understanding the structure and dynamics of these systems in order to prepare DEs with tailor-made physical and chemical properties [1, 2]. Unlike in ionic liquids, DEs do not have discrete ions but are made of mixtures of metal salt and hydrogen bond donor [1]. It is to be noted that the charge delocalization due to hydrogen-bonding is responsible for the decrease in the melting point of the mixture relative to melting points of individual components. A mixture of acetamide and lithium nitrate in the molar ratio of 80:20 is observed to form a DE with freezing point below room temperature [3]. Here we report the combined results of Quasielastic Neutron Scattering (QENS) and MD simulation of this mixture at 300K. QENS experiments on DE were carried out at IRIS spectrometer, ISIS pulsed Neutron and Muon source at the Rutherford Appleton Laboratory, UK. The molecular dynamics of acetamide is modeled based on the assumption that the acetamide molecule is hydrogen-bonded to its neighbouring set of molecules forming a transient cage. The molecules rattle in a cage for some time, without breaking the hydrogen bond with their neighbours, as hydrogen-bond breaks, the acetamide molecules leave the cage and jump to the next site, reforming the hydrogen bond with a different set of neighbouring molecules. Quasielastic part of the QENS spectra is modeled with Fourier-transform of stretched exponential function. Incoherent intermediate scattering function (IISF) calculated from MD simulation, showed the existence of two different time scales. Fig. 1 shows the average timescales obtained from the QENS spectra and IISF from MD simulation. It is found that one of the time scale (slower one) obtained from MD simulation matches quite well with the timescale obtained from QENS spectra. This can be associated to the motion of acetamide centre of mass (COM) from one site to another. On the other hand, the faster timescale obtained from MD simulation, which is not observable in QENS spectra due to limited energy transfer window of the spectrometer, can be ascribed to the motion of the acetamide inside the relaxing cage.

Fig. 1. Average time obtained from QENS experiment and MD simulation.

E-mail for corresponding author: harishlgk1992@gmail.com
Protons are essential charge carriers for the scheme of hydrogen fuel economy. Proton conducting metal oxides are of growing interest for their potential use as electrolyte materials in solid oxide fuel cells and electrolysers at intermediate temperature. To further improve the proton conductivity in order to compete with the conventional oxygen ion conducting electrolytes, we seek to understand the physical and chemical mechanisms for proton transport. Our study on the proton conductivity in barium cerate and barium zirconate based perovskites by applying high pressure shows that compressive strain eliminates the proton conductivity by increasing its activation energy. The proton conducting mechanism was investigated by impedance spectroscopy, quasielastic neutron scattering, x-ray diffraction, and Raman spectroscopy at high temperature and high pressure, suggesting that the proton conductivity is correlated with the phonon hardening in crystal structure. Quantitative analysis of the proton jumping frequencies showed that the Ce-O stretching mode effectively promote the proton transport. Temperature dependence of the proton jump frequency satisfies the Holstein polaron model [1]. The results from this work are expected to help lead our way for rational choice of materials and device design for solid oxide fuel cells operating at intermediate temperatures.


E-mail for corresponding author: qianli.chen@sjtu.edu.cn
Further understanding of better thermoelectric properties of BiCuTeO compared to BiCuSeO

Shuhua YAO¹, Dajun Lin¹, Dehong YU²

¹National Laboratory of Solid State Microstructures & Department of Materials Science and Engineering, Nanjing University, Nanjing, 210093, China
²Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia

Thermoelectric (TE) energy conversion is a promising technology for both electrical power generation in harvesting waste heat and electronic cooling. The conversion efficiency of a TE device is characterized by the dimensionless figure of merit ($ZT$) as $ZT = S^2\sigma/k$. Generally, these parameters cannot be optimized simultaneously in conventional compounds. Different from this conventional wisdom, oxide-based compounds with natural super-lattice structure can possess metallic conductivity and moderate Seebeck coefficient. This behavior has been demonstrated in metal oxides BiCuSeO-based oxychalcogenides. BiCuSeO, with alternate stacking of $(\text{Cu}_2\text{Se}_2)^2\text{−}$ and $(\text{Bi}_2\text{O}_2)^2\text{+}$ layer along c-axis, has intrinsically low thermal conductivity (~1W/m·K). Thus extensive studies have focused on increasing $S$ and $\sigma$ to improve the TE performance of BiCuSeO.

In this work, to achieve a better understanding of the thermal electrical properties of this group of materials, we perform a systematical investigation on the thermoelectric properties of BiCuSeO and BiCuTeO in the temperature range from 300 to 400 K. It is found that the figure of merit of BiCuTeO is almost one order of magnitude higher than that of BiCuSeO at room temperature, due to the much higher electrical conductivity and lower thermal conductivity. First-principles calculations shows that the electron band gap of BiCuTeO is much smaller than that of BiCuSeO and this leads to the better electrical conductivity of the BiCuTeO. Combining theoretical calculations and experimental measurements, the red-shift of phonon density of states and larger anharmonic vibrational properties of BiCuTeO, compared to BiCuSeO, have been observed. This contributes to the low thermal conductivities of the BiCuTeO. The study indicates that BiCuTeO is a promising thermoelectric material potentially having much better performance than BiCuSeO which has been reported to have ZT value of 1.4 at 923 K after Ba doping [1].


E-mail for corresponding author: shyao@nju.edu.cn
QP_10  Slowing down of dynamics with less dense packing in metallic glass-forming liquids modulated by alloying Al element

Chenchen YUAN, Fan YANG, Florian KARGL, Dirk HOLLAND-MORITZ, Giovanna G SIMEONI, and Andreas MEYER

1 School of Material Science & Engineering, Southeast University, Nanjing 211189, P. R. China
2 Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany
3 Heinz Maier-Leibnitz Zentrum (MLZ) and Physics Department, Technische Universität München, 85748 Garching, Germany

Addition of a third component to a binary metallic glass forming melt can significantly improves its glass forming ability. In some cases only a very small amount of such elements is necessarily. The underlying mechanism is so far not very well understood. Particularly, very little attention has been paid to the change of melt properties in this respect. We thus studied the microscopic mass transport and the macroscopic flow behavior of the Zr-(Co,Ni)-(Al,Pd,Ti) melt with a systematic variation of the third component. Utilizing the containerless processing technique of electrostatic levitation allows us to obtain precise data on diffusion coefficient and melt viscosity over a wide temperature range, without artifacts caused by container-melt reactions. We shows that the addition of the of Al to the binary Zr-(Co,Ni) melt leads to an increase of the melt viscosity of system accompanied by a remarkable decrease of the Co, Ni self-diffusion coefficient [1]. In contrast, upon alloying of Ti and Pd the effect of slowing-down of the liquid dynamics is much weaker. However, the average packing fraction of the Al contained melt derived from the measured macroscopic density is smaller than that of the corresponding binary alloys. This indicates that apparently such slowing down of the liquid dynamics cannot be explained a hard-sphere like model of packing, although metallic glass-forming melts in which is absent are often considered to be most closed to a hard-sphere like system [2]. Instead, the chemical interactions of Al with transition metal atoms should play an important role here, which also contribute to their improved glass-forming ability. Our studies indicate, even in metallic glass-forming melts which can be simply described under hard-sphere model assumption for lacking directional bonding, the average packing fraction is not a suitable parameter for predicting liquid dynamics.


E-mail for corresponding author: yuancc@seu.edu.cn
Molecular rings have attracted on-going attention for their remarkable spin dynamic properties at the crossover between classical and quantum regimes. A new cyclic complex \([\text{Cr}_8\text{Y}_8(\text{mda})_{16}(\text{CH}_3\text{COO})_8(\text{NO}_3)_8] \cdot 3\text{CH}_3\text{CN}, \{\text{Cr}_8\text{Y}_8\}\) for short, has been synthesized and studied. The magnetic susceptibility study suggested ferromagnetic (FM) coupling between \(\text{Cr}^{\text{III}}\) moments [1]. Thus \{\text{Cr}_8\text{Y}_8\} represents a rare FM example of the chromium rings. In order to confirm the nature of this ferromagnetic coupling by a direct measurement of \(J\), we performed low-temperature specific heat and inelastic neutron scattering (INS) experiments. The low-lying magnetic excitations obtained by evaluating the Schottky anomalies in the specific-heat data are consistent with those measured directly in INS experiment. A single \(J\)-value of \(~0.1\ \text{meV}\) has been determined. The zero-field splitting of ground-state level has been tentatively attributed to the anisotropy mechanism of the coordination environment of the \(\text{Cr}^\text{III}\) ions.


E-mail for corresponding author: zdfu@hotmail.com
Role of iron doping in short range antiferromagnetic NiO nanoparticles

Tai-Yue Li, Ashish C. Gandhi, Chun-Ming Wu, Jen-Chih Peng, Sheng Yun Wu

1 Department of Physics, National Dong Hwa University, Hualien 97401, Taiwan
2 Synchrotron radiation research center, Hsinchu 300, Taiwan

Bulk NiO is antiferromagnetic below $T_N \approx 523$ K and was one of the first magnetic materials studied by neutron scattering in the pioneering work of Shull et al. [1]. These early neutron scattering experiments confirmed the existence of antiferromagnetic ordering as postulated by Néel. The relatively high Néel temperature of NiO makes it a promising material for applications. Since the work of Shull et al., the magnetic structure of NiO is antiferromagnetic with the antiferromagnetic modulation in one of the cubic \((111)\) directions \((1\ 1\ 1)-\text{type modulation vector}\) and with the spins oriented close to the corresponding \((111)\) plane. The spin orientation in NiO is difficult to determine, in particular for nanoscale samples, and in most investigations it is not determined with any appreciable accuracy. The low-symmetry surroundings of surface atoms and the large surface contribution to the magnetic anisotropy mean that the spin structure in nanoparticles may be different from that of the bulk material [2]. This could also be the case for nanoparticles of NiO, and the spin configuration at the surface of the NiO nanoparticles will certainly be of importance for their exchange coupling to other particles or surfaces [3]. Neutron diffraction [4] is one of the few methods that can be used to determine the magnetic structure of antiferromagnetic materials. The conventional method of unpolarized neutron powder diffraction can be used on nanoparticle samples [4] and in fact Cooper et al. recently used this method on 7-nm NiO particles to compare the magnetic and nuclear correlation lengths, showing that a layer with spin disorder exists at the particle surfaces [5]. Here, we report the investigation on the magnetic spin structure induced by Fe-doped and anisotropic energy in Fe-doped NiO nanoparticles. The relation of the temperature dependence of the magnetic inter- or intra coupling effect, anisotropy energy, and magnetic ordering can be understood through high resolution cold neutron measurements. The Fe doping and nanosized effect induced crystal distortion and short range magnetic correlation can be investigated in the NiO system, implying that the magnetic spin structure of NiO nanocrystals is complicated, but neutron scattering can be used to solve this problem.


E-mail for corresponding author: sywu@gms.ndhu.edu.tw(SYWu)
The occurrence of large natural clathrate hydrate deposits on the oceanic sea floors and the possibility that these gas hydrates could be mined as an energy source of hydrocarbon gas or used to sequester CO\textsubscript{2} gas are still attracting considerable interest.

Gas hydrates form clathrate structures consisting of hydrocarbon molecules within "cages" of water molecules. There are two clathrates of practical interest, the sI and sII structures. The sII structure can accommodate propane molecules, which is not possible for the smaller cages of the sI structure. Alternatively, the sII structure will not form in pure methane gas, except at exceptional pressures. For a complex mixture of hydrocarbons in natural gas, both sI and sII structures are formed.

To effectively sequester CO\textsubscript{2} gas by replacing CH\textsubscript{4} from deep water gas hydrates instantaneously would greatly benefit of a fundamental understanding of the diffusion process of exchanging gases within the hydrate structure. Several recent studies [1-4] have already shown that diffusion must occur between the cages. Also the use of double clathrate hydrates as an effective method of storing/transporting natural gas has been studied. To describe the underlying gas fractionation effect within the various cages of hydrate structures the knowledge of the dynamics of the guest molecules is vital.

We present our first inelastic neutron scattering experiments on pure methane sI and methane-propane sII hydrates using PELICAN, the time-of-flight spectrometer, at ANSTO at a wavelength of 6 Å (2.25 meV neutrons) and an energy resolution of 65 µeV. The samples were prepared ex-situ from deuterated ice powder via gas absorption. D\textsubscript{2}O was used to prevent inelastic scattering from the water framework. We used various hydrogenated and deuterated mixtures of methane and propane gas so as the motion of the gases in different cages of the clathrate structure could be studied in a temperature range of 1.5 – 70K in steps of 15K at ambient pressure. The interactions between propane and methane in adjacent cages mediated through water molecules shared between the cages at various temperatures were also studied. The cage structures of our samples were preliminary characterised using high resolution neutron powder diffraction. Only sI-, sII hydrates and remaining ice were found. No solidified methane or propane was detected.

Inelastic neutron scattering provides a new opportunity for the study of cage occupancy in mixed gas hydrates.


E-mail for corresponding author: akl@ansto.gov.au
QP_14 QENS data analysis on Mantid: A modern approach

Brandon HEWER, Spencer HOWELLS, Anders MARKVARDSEN, Sanghamitra MUKHOPADHYAY

ISIS Neutron and Muon Facility, Rutherford Appleton Laboratory, STFC, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX, United Kingdom

Data analysis of Quasi-elastic Neutron Scattering (QENS) experiments often requires multiple steps involving fitting the spectra with several empirical functions based on analytical models [1-2]. Parameters of those models can be interdependent and dependent also on the momentum transfer vector Q. With the increase of the capability of neutron scattering instruments and sophisticated sample environment facilities, modern QENS experiments are performed on complex chemical systems in those challenging situations. The applicability of QENS experiments thus has broadened its horizon from traditional liquid, biological and soft matter systems to the investigations of materials for solving global challenges, such as solar cell materials [3], fuel cell materials [4] or movements of molecules on catalytic surfaces [5]. More sophisticated models are required to analyse those data which are beyond the capability of the existing analysis software available for QENS.

To bridge the gap of the capability of traditionally used software for QENS data analysis, a modern data analysis interface dedicated for this technique has been implemented in Mantid. Since Mantid is an open source software and many of the neutron and muon facilities across the world have already agreed to adopt it as the tool for their data reduction and analysis, it is the right platform to implement this analysis interface there for the benefit of users across facilities. This interface provides a user friendly Graphical User's Interface (GUI) with options to fit both, scattering function, S(Q,W), and intermediate scattering function, I(Q,t), with several analytical models. A sequential as well as simultaneous fitting option across spectrum making possible to do a local-global fitting with choice of constrain and correlate spectra across Q values. This multi-dimensional (MD) data analysis interface also provides options for fitting with several models of jump diffusions and analysis of elastic incoherent structure factor (EISF).

In this presentation we will discuss implementation and different features of QENS data analysis interface on Mantid along with few examples [6] relevant to the science program on IRIS and OSIRIS spectrometers at ISIS, UK. Since the work on this software is on-going, its scope and future outlook of designing a comprehensive QENS MD fitting GUI will also be discussed.

E-mail for corresponding author: Sanghamitra.mukhopadhay@stfc.ac.uk
The design of T-REX, a bi-spectral chopper spectrometer for the ESS

Nicolò VIOLINI, Jörg VOIGT, Andrea ORECCHINI, Pietro TOZZI, Hans KÄMMERLING, Mario KOENEN, Anton KHAPLANOV, Thomas BRUCKEL

Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Università degli Studi di Perugia, I-06123 Perugia, Italy

CNR-IOM Unità di Perugia c/o Dipartimento di Fisica e Geologia, Università degli Studi di Perugia, I-06123 Perugia, Italy

European Spallation Source, SE-22100 Lund, Sweden

T-REX is a bispectral direct-geometry chopper spectrometer accepted for construction at the European Spallation Source (ESS). Currently the project is in the engineering design phase. Here we will show technical solutions for various instrument components, with a focus on the secondary spectrometer and the strategy to achieve neutron polarization and analysis over the wide energy band covered by the instrument.

T-REX will be equipped with PSD detectors based on the $^{10}$B multigrid technology [1] to cover the large area (20 m$^2$ in the full scope) with minimal gaps and a high detection efficiency for neutrons of energy up to 200 meV. We will show the design of the mechanical integration and the vacuum interface.

T-REX features XYZ neutron spin polarization analysis. Neutron polarization is achieved with the SEOP setup [2]. Neutron spin analysis in XYZ is performed with the magic PASTIS setup [3]. Specific investigations of high quality $^3$He cells are required [4], to achieve a long decay time of the polarization of the gas, which is a crucial for long lasting inelastic scattering experiments. We will show the status of the design of various technical solutions.


E-mail for corresponding author: n.violini@fz-juelich.de
The recent upgrade of TOSCA (ISIS Neutron and Muon Source, UK), with the installation of a high \( m \)-value neutron guide [1], has opened up new opportunities for fast multi-parametric experiments or the reliable measurements of small specimens. For a broadband neutron spectrometer optimized for molecular spectroscopy such as TOSCA, a full characterization of the limits of detection and quantitation is fundamental to understand the new analytical performance of the upgraded instrument as well as for planning new experiments.

In order to accurately estimate the limit of detection (LOD) and the limit of quantitation (LOQ), we have used a set of different masses of three different samples, namely, zirconium hydride (ZrH\(_2\)), low density polyethylene (LDPE) and 2,5-diiodothiophene (C\(_4\)H\(_2\)I\(_2\)S). These three materials offer different insights, thanks to their specific properties: ZrH\(_2\) has a simple, reproducible, and well-known behaviour; LDPE can be obtained with precise thickness; and finally C\(_4\)H\(_2\)I\(_2\)S is the calibrant of choice for TOSCA since its spectrum contains plenty of well-defined peaks.

In this contribution, we report the LOD and the LOQ for different regions of the TOSCA spectrum. These data have been analyzed using a staged procedure that exploits a number of different techniques to determine instrument capability and limitations, while enforcing self-consistency checks. Due to the accurate selection of the standards, the adopted quantification allows us to obtain calibration curves for any analyte. This new quantitative and analytical procedure can be easily adopted to benchmark and evaluate other instruments of this kind such as VESPA, the vibrational spectrometer planned for the European Spallation Source.
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E-mail for corresponding author: claudia.scatigno@uniroma2.it
DNA is a TOF type Si crystal analyzer backscattering spectrometer installed at the Japan Proton Accelerator Research Complex (J-PARC) spallation source\cite{1}. DNA uses a pulse-shaping chopper to extract sharp pulsed neutron from strong but broad spectrum of coupled moderator, which achieves good energy resolution (~2.4\mu eV) and large neutron flux simultaneously. In addition, broad neutron pulse of coupled moderator allow us to go high energy transfers of ~1500 \mu eV. Thus, DNA gives wide dynamic range over three orders of magnitude from \mu eV to meV, which covers a variety of research fields. In average, 25 \% of proposals are about soft- and bio-matter including biomaterials, micelles, and polymers, 21\% are related to hard-matter physics including lattice dynamics and magnetism, and the third majority group is about liquid (18\%). Not only for basic research, DNA is devoted to industrial applications (17\%) including rubbers, battery, and functional polymers. Of course, DNA is used for the study of ion and proton dynamics (9\%). We also encourage the first-time user for neutron study (9\%). In this presentation, we will briefly introduce typical research conducted by using DNA.

\cite{1} K. Shitaba et al., JPS Conference Proceedings, 8, 030622 (2015).

E-mail for corresponding author: m_matsuura@cross.or.jp
WP_04  How we lost most of the flux on MAPS, and how we got it back again

Russell EWINGS¹, Ross STEWART², Toby PERRING¹, Rob BEWLEY¹, Rebecca RIEHL-SHAW¹, Davide RASPINO¹

¹ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, United Kingdom

After a long ISIS shutdown on target station 1 during 2016, it was found that the neutron flux on the MAPS spectrometer was substantially compromised, with an energy-dependent reduction of between two and five measured. To determine and remedy the cause of this problem, extensive investigations were performed, both on the instrument and involving neutronic and ray-tracing simulations. The key measurement that provided the most insight into the nature of the problem was to use a pinhole camera setup to obtain a spatially-resolved image of the neutron source as viewed from the sample. This revealed a highly inhomogeneous distribution of flux from the source, in contrast to a similar measurement performed on the adjacent VESUVIO beamline which views the same moderator face but showed no such inhomogeneity. The problem was eventually solved by replacing the MAPS beamline shutter, an expensive and difficult task.

E-mail for corresponding author: russell.ewings@stfc.ac.uk
WP_05   Completion of the MAPS time-of-flight spectrometer upgrade

Russell EWINGS¹, Ross STEWART¹, Toby PERRING¹, Rob BEWLEY¹, Simon WALLER¹

¹ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, United Kingdom

MAPS has been in operation since 2000 and was the first chopper spectrometer to employ a large array of position sensitive detectors, and also the first to be designed solely for the purpose of measuring excitations in single crystals. It was originally envisaged that MAPS would be used predominantly for studies of high-energy excitations, using neutrons with incident energies in the epithermal range. Its use evolved over time such that a significant proportion of the beam time was devoted to single crystal excitation experiments involving the use of thermal neutrons, measuring excitations with energies as low as a few meV.

MAPS continued to be world competitive at high energies (Ei >~ 100 meV), but was losing its advantage at thermal energies to newer instruments. A project to install a neutron guide, add an extra disk chopper, and redesign the moderator viewed by the instrument was initiated in 2014 in order to address this. The project was completed in December 2017.

Here we will summarize the characteristics of the guide and the new chopper system, and show results from the completed commissioning period that illustrate various aspects of the instrument’s performance. The flux gains from the guide agreed very closely with Monte-Carlo simulations. The new disk chopper allows a (planned) limited form of rep-rate-multiplication to be utilised, or a mode of running which suppresses the background for high-temperature measurements. We will show some early results from the user programme that already illustrate the benefits these improvements are having on the science that can be performed on MAPS.

E-mail for corresponding author: russell.ewings@stfc.ac.uk
The SNS-NSE instrument is an ultrahigh resolution neutron spectrometer for characterizing the slow dynamics of soft condensed matter. Due to a wavelength span of $2 \, \text{Å} < \lambda < 14 \, \text{Å}$ using a simultaneous wavelength frame of $3-3.6 \, \text{Å}$ high data collection efficiency is achieved allowing nearly gapless coverage of a broad wave-vector-time-range with only a few scattering angle settings.

The SNS-NSE instrument is particularly suitable to investigate slow dynamical processes and unravel molecular motions at nanoscopic and mesoscopic scale in a variety of disciplines like: soft–matter and polymer science, biophysics, biochemistry, and nanotechnology. Typical applications include the molecular rheology of polymer melts, relaxation phenomena in networks and rubbers, interface fluctuations in complex fluids [1], transport processes in polymeric electrolytes and gel systems, the domain dynamics of proteins [2] and enzyme’s, lipid systems and biological membranes [3], disruptive effects of anti-inflammatory medication on membrane cell organization [4]; transport process thru cell membranes and porous media. With proper adaptations the SNS-NSE instrument can also aid studies in condensed matter physics, materials science and magnetism.


E-mail for corresponding author: o.holderer@fz-juelich.de
Progress in High Resolution Chopper Spectrometer HRC by improving collimator and Fermi chopper

Shinichi ITOH1, Tetsuya YOKOO1, Takatsugu MASUDA2, Shinichiro ASAI2, Hiraku SAITO1, Daichi KAWANA2, Ryosuke SUGIURA2, Toshio ASAMI2, Yoshiaki IHATA3

1Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tsukuba, Japan
2The Institute for Solid State Physics, The University of Tokyo, Tokai, Japan
3Materials and Life Science Experimental Facility, J-PARC Center, Tokai, Japan

The High Resolution Chopper Spectrometer (HRC) is installed at MLF, J-PARC, for a wide range of dynamical studies of materials over a wide energy-momentum space with high resolution [1-3]. On the HRC, three types of inelastic neutron scattering experiments can be performed: high-resolution experiments in a conventional energy momentum space, neutron Brillouin scattering (NBS), and eV neutron spectroscopy. NBS, that is inelastic neutron scattering near to the forward direction, is effective for observing coherent excitations in non-single-crystal samples such as ferromagnetic spin waves in powder samples and acoustic phonons in liquids and polycrystalline samples. Owing to the kinematic constraints of neutron spectroscopy, incident neutron energy ($E_i$) in the sub-eV region with a high resolution is necessary, and the scattered neutrons need to be detected at very low scattering angles, for measuring NBS. On the HRC, NBS experiments became feasible by reducing background and increasing the neutron flux at low scattering angles [4]. The NBS option makes the HRC different from other chopper spectrometers. Because the solid angle of detecting area for NBS experiments is limited to very low scattering angles, improvement for gaining the neutron flux is essential. A collimator system installed just at the upper stream of the sample reduces background at low scattering angles. Needless to say, a Fermi chopper determines the resolution and the neutron flux. We made some efforts to gain the neutron flux by improving the collimator system as well as the Fermi chopper [5]. Recently, we made further improvements. At around $E_i = 100$ meV, the neutron flux was greatly gained for the energy resolution $\Delta E/E_i = 2\%$, and the best energy resolution was achieved to be 1% something with a reasonable neutron flux.


E-mail for corresponding author: shinichi.itoh@kek.jp
WP_08  Time-of-flight direct-geometry spectrometer 4SEASONS at J-PARC

Ryoichi KAJIMOTO\textsuperscript{1}, Mitsutaka NAKAMURA\textsuperscript{1}, Kazuya KAMAZAWA\textsuperscript{2}, Yasuhiro INAMURA\textsuperscript{1}, Kazuhiko IKEUCHI\textsuperscript{2}, Kazuki IIDA\textsuperscript{2}, Motoyuki ISHIKADO\textsuperscript{2}, Naoki MURAI\textsuperscript{1}

\textsuperscript{1}J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan
\textsuperscript{2}Comprehensive Research Organization for Science and Society, Tokai, Ibaraki, Japan

4SEASONS (aka SIKI) is a time-of-flight direct geometry chopper spectrometer in the Materials and Life Science Experimental Facility (MLF) at the Japan Proton Accelerator Research Complex (J-PARC). It is designed for measurements of dynamics in the $10^0$-$10^2$ meV energy range \cite{1}. The momentum-energy region for this spectrometer occupies the middle of the momentum-energy space covered by all MLF spectrometers \cite{2}. Reflecting the fact that 4SEASONS was originally designed to meet the requirements for studies of high-$T_c$ oxide superconductors, copper and iron-based high-$T_c$ superconductors are still major research targets for the instrument. Including these materials, strongly correlated electron systems and magnetism dominate 80% of the experiment proposals. On the other hand, a sizable number of proposals belong to other research fields such as thermoelectric materials and catalysts. In addition to these user programs, the upgrade of the instrument is continuously progressed. Recently, a part of the neutron guide tube was replaced, which led to an increase in the flux by 10-20%. The number of detectors has been increased and will be increased further, which will improve the ability for the study of lattice dynamics. Efforts have been paid to accommodate new sample environments, and we have successfully performed the first inelastic scattering experiment under magnetic fields very recently. In the presentation, we will show the specifications of the instrument, usage statistics, and recent examples of scientific outputs and instrument upgrades.


E-mail for corresponding author: ryoichi.kajimoto@j-parc.jp
Suite of the neutron spectrometers in J-PARC

Tetsuya YOKOO\textsuperscript{1,2}, Ryoichi KAJIMOTO\textsuperscript{1,3}, Mitsutaka NAKAMURA\textsuperscript{1,3}, Yukinobu KAWAKITA\textsuperscript{1,3}, Masato MATSUURA\textsuperscript{4}, Hitoshi ENDO\textsuperscript{1,2}, Hideki SETO\textsuperscript{1,2}, Shinichi ITOH\textsuperscript{1,2}, Kenji NAKAJIMA\textsuperscript{1,3}, Seiko OHIRA-KAWAMURA\textsuperscript{1,3}

\textsuperscript{1}J-PARC Center, Tokai, Japan
\textsuperscript{2}High Energy Accelerator Research Organization, Tsukuba, Japan
\textsuperscript{3}Japan Atomic Energy Agency, Tokai, Japan
\textsuperscript{4}Comprehensive Research Organization for Science and Society, Tokai, Japan

The spectroscopy for material science is one of powerful tools to investigate the mechanism of physical properties. For deep understanding of the dynamics in physical degrees of freedom, dynamical structures $S(q,E)$ should be measured in wide area of momentum and energy space. To realize the wide coverage of $q$ and $E$ space, six inelastic spectrometers with different concepts are now part of spectrometer suite in MLF \cite{1}. Three of them are direct geometry spectrometers, 4SEASONS, HRC and AMATERAS utilizing Fermi or disk choppers to select the neutron energy. The set of chopper spectrometers covering wide momentum and energy space enables us to realize various researches in diverse field. The other is DNA indirect geometry instrument. A very high energy resolution can be achieved with silicon perfect crystal analyzer and high speed pulse shaping disk choppers. This spectrometer is suitable to investigate dynamical behaviors of proteins, such as human $\alpha$-synuclein, which form amyloid fibrils. VIN ROSE and POLANO are younger generation of spectrometers in MLF. VIN ROSE is a neutron spin echo instrument with MIEZE- and NRSE-type just started user program. Spin echo spectrometer can be achieved the highest energy resolution for investigating slow dynamics in soft matter materials. POLANO is a chopper spectrometer with capability of polarization analysis. The main construction was completed and started unpolarized beam commissioning. Since higher energy polarized neutron experiments up to 100 meV is the interesting range of the research field in so-called strongly correlated electron systems, final goal of polarization energy is over 100 meV in POLANO. In the presentation, recent instrumental upgrade and development of devices will be reported as well as remarkable scientific outcomes.


E-mail for corresponding author: tetsuya.yokoo@kek.jp

Back to the program
Neutron scattering instrumentation has previously been designed with radial scattering assumed from the centre of the sample. Any deviation from this is then a source of error, contributing to the resolution characteristics of the instrument. This is an acceptable simplification where the sample is small relative to the distance between sample and detector. Changing the sample to detector distance ratio should offer possibilities to allow imaging through parallel beam collimation, which is illustrated in Figure 1.

Collimators that enforce the transport of parallel beams from the sample to a detector will define the spatial resolution of the proposed instrument. A detector array to determine $S(Q)$ for each collimator element will provide pixels matched to the geometry of the collimator. To gain energy resolution, a crystal monochromator after the collimator will disperse the parallel beams according to their energy. A second collimator will select a desired angle and define the final energy reaching the detector, thus creating a spatially resolved indirect geometry instrument. The concept for one detector array is shown in Figure 2.

A single array in transmission would give the greatest signal. Arrangement of multiple elements could however also be used to collect the scattered neutrons. If arranged in a cone symmetric around the beam, each imaging element will sample the same space in $Q$ and $\omega$. Any other geometry will collect images with different paths through $(Q,\omega)$ space. With appropriate care in design, an instrument could be developed suitable for both measurements, with arbitrary grouping of imaging elements in the data reduction stage. Pixel averaging could also provide greater signal at the expense of spatial resolution.

Obtaining images at multiple angles offers the opportunity for tomographic reconstruction with greatly reduced (or possibly eliminated) sample rotation. Investigation of heterogeneous samples in three dimensions, offers great opportunities for in-situ studies and samples that may be damaged or be impenetrable to x-rays.
Figure 1: Beam interaction with sample for radial approximation and parallel beams

Figure 2: Individual collimator element

E-mail for corresponding author: ian.silverwood@stfc.ac.uk
Sample environment commonly used at the chopper spectrometers in J-PARC MLF

Seiko OHIRA-KAWAMURA¹, Masao WATANABE¹, Ryuta TAKAHASHI¹,
Koji MUNAKA², Shinichi TAKATA¹, Yoshifumi SAKAGUCHI²,
Motoyuki ISHIKADO², Keichi OHUCHI², Hiroshi ARIMA², Takanori HATTORI¹,
Yasuhiro YAMAUCHI¹, Masatoshi NAKAMURA¹, Takayuki OKU¹

¹J-PARC Center, Tokai, Ibaraki, Japan
²Comprehensive Research Organization for Science and Society, Tokai, Ibaraki, Japan

At the Materials and Life Science Experimental Facility (MLF) in J-PARC, most of sample environment (SE) such as closed-cycle refrigerator (CCR) is prepared by the instruments individually as the standard SE equipment depending on the experiments carried out at the instrument. This system has advantages that the instrument group can directly contact the users and respond to their request and that the instrument can design its various components, such as the sample space and shielding materials, to adopt the instrument. On the other hand, several pieces of SE, which are not utilized so frequently but essential, are managed by the SE team. They are commonly used at several instruments in MLF [1,2]. In these SEs, three cryostats and a high-temperature furnace are available at direct geometry spectrometers (4SEASONS, HRC and AMATERAS) and a near-back scattering spectrometer (DNA), and a superconducting magnet is available at three these direct geometry spectrometers. Furthermore, a CCR for Paris-Edinburgh press is under commissioning aiming to realize the inelastic/quasielastic neutron scattering experiments at low temperatures under pressure. The SE team has prepared these SEs for user’s experiment and has supported their operation during the experiment.

In this presentation, we introduce the current situation of the SE commonly used at the instruments at MLF and activity of the SE team.


E-mail for corresponding author: seiko.kawamura@j-parc.jp
WP_12  Upgrade of TOF spectrometer NEAT at Helmholtz Zentrum Berlin

Gerrit GÜNTHER¹, Veronika GRZIMEK¹, Lars DRESCHER¹, Toralf Kaulich¹, Margarita RUSSINA²

¹Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Neutron time-of-flight spectrometer NEAT has a long history of successful application to the study of dynamics and function. It is best suited to probe dynamic phenomena directly in space and time in the large time domain $10^{-14} - 10^{-10}$ s and on the length scale ranging from 0.05 to about 5 nm. Recent upgrade of the instrument resulted in 300 fold higher count rate compare to predecessor placing NEAT on the level of the world best. The advanced features of the new instrument include novel integrated guide-chopper system which deliver neutron beam with variable characteristics and substantial increase of the detector angle coverage with simultaneous increase of angular resolution. New instrumental capabilities provide optimal experimental conditions for investigation of microscopic dynamics in soft and hard matter including excitations in single crystals, applications with high magnetic field up to 14 T or in-situ confinement of gasses and liquids in porous systems. High power of the instrument allows to substantially reduce the amount of materials needed for investigation. Novel data acquisition using event recording techniques provides an opportunity to follow the formation of the bonds in real time. Here we present details of the NEAT upgrade, measured instrument characteristics and show first experimental results.


E-mail for corresponding author: Margarita.Russina@helmholtz-berlin.de
A new era for the TOSCA vibrational spectrometer

Jeff Armstrong

ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell Oxford, Didcot OX110QX, UK

The TOSCA spectrometer at the ISIS Neutron and Muon Source (Rutherford Appleton Laboratory UK) has recently undergone a major upgrade of its primary flight path\[1\]. This has opened new avenues of vibrational spectroscopy for the instrument. The measurement times for samples have decreased by over an order of magnitude, opening the door for smaller sample sizes, in-situ temperature studies, in-situ reaction studies and parametric studies of materials which were simply not feasible before the upgrade. I catalog the depth and breadth of experiments which are now possible on TOSCA, and give predictions for the types of experiment which will occur in the future, and the infrastructure which will be required to support such experiments.


E-mail for corresponding author: jeff.armstrong@stfc.ac.uk
The three-axis spectrometer IN8 at ILL offers advanced conditions for studies of thermal excitations in single crystals and liquids. The instrument performance and flexibility are ensured by the use of large double-focusing monochromators and analysers providing high counting rate even for small and low scattering samples. The new monochromator unit has been recently commissioned which is the fruit of the experience accumulated in the former TAS-group at ILL in using Bragg-focusing beam optics with independently variable and remotely controlled horizontal and vertical focusing (bending) of the crystal reflecting planes. The new monochromator for the thermal neutron beam considerably outperforms the previously used one. It consists of 4 different exchangeable crystal planes. The two planes are built from mosaic crystals of pyrolytic graphite and copper with the principal reflections $PG002$ and $Cu200$ chosen to provide a broad range of monochromatic neutron wave vectors and energy resolution of the incident beam. The other two planes are assembled with elastically bent perfect silicon crystals set to make use of the reflections $Si111$ and $Si311$ with prohibited second-order diffraction harmonics. The mosaic crystal planes are used in experiments requesting maximum monochromatic intensity at the sample position and variable resolution. The silicon crystal planes, with similar to mosaic crystals available resolution range, provide particularly “clean” conditions for experiments with multi-analysrer configurations (such as FlatCone, for instance) at the expense of marginally lower monochromatic flux. The following step in the renovation of the spectrometer is the ongoing construction of the classical single-detector secondary spectrometer set-up called THERMES (THERMal Excitation Spectra). Further development of the specific sample environment for this spectrometer is under discussion.
WP_15  Applicability and limitations of $G(r,E)$ analysis transformed from the inelastic neutron scattering data

Mitsutaka NAKAMURA, Kazuya KAMAZAWA, Motoyuki ISHIKADO,
Tatsuya KIKUCHI, Yukinobu KAWAKITA

1Japan Atomic Energy Agency, J-PARC Center, Tokai, Japan
2Comprehensive Research Organization for Science and Society, Tokai, Japan
3Sumitomo Rubber Industries, LTD., Kobe, Japan

Recently, we reported the phonon dynamical study of a polycrystalline NaI by using the dynamical structure factor in real-space $G(r,E)$ transformed from the inelastic neutron scattering (INS) data [1]. Our study has shown that the INS experiments under the conventional condition $Q_{\text{max}} \sim 5 \text{ Å}^{-1}$ can provide us a meaningful information on the phonon dynamics at around the first nearest neighbor distance on accepting the worse real-space resolution. These results suggest the possibility that a large amount of $S(Q,E)$ data which were previously obtained can be effectively reused.

In this study, we will examine both the applicability and limitations of $G(r,E)$ analysis for various types of materials whose INS data were obtained at the Fermi chopper spectrometer 4SEASONS[2] in J-PARC.


E-mail for corresponding author: mitsutaka.nakamura@j-parc.jp
WP_16 The effect of putting a neutron velocity selector before the monochromator in the thermal neutron triple-axis spectrometer

Xiaoyan Ma¹², Huiqian Luo¹, and Shiliang Li¹²⁴

¹Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
²School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China
³Collaborative Innovation Center of Quantum Matter, Beijing 100190, China

A new triple-axis thermal neutron scattering instrument named ‘BAMBOO’ has been constructed by the Institute of Physics (IOP), Chinese Academy of Sciences, and installed at China Advanced Research Reactor (CARR). It is an international initiative to put a multiple-disc velocity selector before the pyrolytic graphite (PG) monochromator, which have many advantages such as remove the high-order neutrons efficiently, decrease incoherent scattering, and select the energy after scattering randomly which allows us to continuously fine tune the energy and momentum resolution in a simple manner. In addition, it provides much more choices in an experiment that may significantly improve the data quality. Here we show the eliminating efficiency of high order neutrons and the antiferromagnetic order measurement of BaFe₁ₓCr₀.₀₅(As₀.₇₂P₀.₂₈)₂ single crystal sample.

E-mail for corresponding author: slli@iphy.ac.cn
Inelastic neutron spectrometers at China Advanced Research Reactor (CARR)

Lijie HAO, Zhendong FU, Kai SUN, Dongfeng CHEN

China Institute of Atomic Energy, Neutron scattering laboratory, Beijing, China

China Advanced Research Reactor (CARR) locates at China Institute of Atomic Energy (CIAE) in Beijing. This reactor is a multi-purpose research reactor which is devoted to neutron scattering, neutron imaging, radioisotopes production, neutron transmutation doping silicon and neutron activation analysis. The full power of CARR is 60MW and the maximum thermal neutron flux is $8 \times 10^{14}$ (cm$^2$ . s). This reactor reached the first criticality in May 2010 and its first full power operation was in March 2012. There are 8 thermal neutron channels and 4 cold neutron channels installed in the experiment hall. By now, nine neutron scattering instruments have been completed including High Resolution Powder Diffractometer (HRPD), High Intensity Powder Diffractometer (HIPD), Residual Stress Diffractometer (RSD), Thermal Triple-Axis Spectrometer I (CIAE-JCNS-TAS), Triple-Axis Spectrometer II (IOP-CIAE-TAS), Four-Circle Diffractometer (FCD), Texture Diffractometer (TD), small-angle scattering instrument (SANS) and horizontal sample-geometry Neutron Reflectometer (NR). Other five instruments under construction are Thermal and Cold Neutron Radiography Facilities, Multi Axis Crystal Spectrometer, Cold Neutron Triple Axis and Industry and Engineering Application Diffractometer.

There are four inelastic neutron spectrometers at CARR. Thermal triple-axis spectrometer I was relocated from Forschungszentrum Jülich (FZJ). This instrument has a large double focusing monochromator and a double focusing analyzer which help to achieve high neutron flux in measurements. Thermal triple-axis spectrometer II was constructed jointly by CIAE and the Institute of Physics (IOP) of Chinese Academy of Sciences. A velocity selector was installed to remove the high-order neutrons. Cold neutron triple axis and multi axis crystal spectrometer was jointly constructed with Renmin University of China. The installation of cold neutron triple axis spectrometer was completed in 2018. A polarizing super mirror will be installed to provide polarized beam. Multi axis crystal spectrometer was designed with 34 detector channels to improve detection efficiency. It will be installed in 2019.

E-mail for corresponding author: haolijie2010@126.com
The time-of-flight direct-geometry neutron spectrometer, Pelican, has been in user program since 2014 at the OPAL research reactor, at the Australian Nuclear Science and Technology Organisation (ANSTO). The Pelican instrument was designed to meet the diverse requirements of the Australian scientific community from physics, chemistry, material science, to biology. A wide range of research fields is covered. These include crystal-field excitations, phonon densities of states, magnetic excitations for various multifunctional materials including high Tc superconductors, novel magnetic, thermoelectric, ferroelectric and piezoelectric materials; molecular dynamics in hydrogen-bonded and storage materials, catalytic materials, cements, soils and rocks; and water dynamics in proteins and ion diffusion in membranes. Polarized neutrons and polarisation analysis option makes the full use of the neutron spin to study magnetism and to separate the coherent and incoherent scatterings.

In this presentation, the performance and capabilities of the instrument will be demonstrated with several systems studied using quasi-elastic and inelastic neutron scatterings. These include water dynamics around amino acids, crystal field excitations in magnetic molecular crystals, low energy magnetic excitations in spin frustrated magnet, oxygen diffusion in solid oxide conductors and phonon density of states in thermoelectric materials.

E-mail for corresponding author: dyu@ansto.gov.au
WP_19  EMU – the high-resolution neutron spectrometer at the Australian Centre for Neutron Scattering

Nicolas R. DE SOUZA¹, Alice KLAPPROTH²

¹ANSTO, Australian Centre for Neutron Scattering, Lucas Heights N.S.W., Australia

ANSTO has recently brought into user operation a high-resolution neutron spectrometer, EMU, at its OPAL research reactor. The spectrometer is based on Si (111) crystal backscattering, thereby achieving a ~1.2 μeV energy transfer resolution over ±31 μeV and momentum transfers from 0.1 to 1.95 Å⁻¹.

Typical applications therefore include experimental characterization of the molecular dynamics at the nanosecond nanometre scale, via measurements of the quasielastic neutron scattering from hydrogenous (e.g. macromolecular, organic...) and other materials. Within the Australian research user community there is also substantial interest in resolving diffusion from ionic species in energy materials.

Examples from the first two years of operation of EMU will be shown, illustrating its capabilities so far, with most experiments were carried out with standard cryo-furnaces (2 to 800 K temperature range). Other experiments requiring other ancillary equipment such as controlled-gas delivery, pressure, applied fields, etc. are possible and welcome from the user community.

E-mail for corresponding author: nds@ansto.gov.au
Ray tracing (RT) is a widely-used technique for the simulation of neutron scattering instrumentation. Neutrons are represented as rays which are intersected with the geometry of a virtual instrument. Upon each intersection, a Monte Carlo (MC) choice is made as to how the ray propagates; by studying a large number of neutron rays, information is obtained about the performance of the instrument. This can be used for optimization of instrument geometry, carrying out virtual experiments, and verifying the viability of instrument designs.

The most commonly used package for carrying out such simulations is McStas, which provides an extremely mature tool set for carrying out MCRT. Despite its maturity, however, the performance of MCRT algorithms can be significantly improved by taking advantage of the fact that it is a 'massively parallelizable' problem. With the advent of libraries such as CUDA and OpenCL, it has become relatively simple to access the parallel computation ability of modern Graphical Processing Units (GPUs).

RAMP (Raytracing Achieved via Massive Parallelization) is a prototype MC ray-tracer implemented via OpenCL, in which instruments are represented as a set of components. Each component is comprised of two OpenCL kernels which handle ray-tracing and scattering for the component. Preliminary testing of instruments simulated in RAMP against analogous instruments simulated in McStas have shown factor 10-15 improvements in simulation time for the same number of simulated rays.

E-mail for corresponding author: goran.nilsen@stfc.ac.uk