Initial Breakout Session Topics
November 27, 2019

- **Biology**
  - Session 1: time-resolved proton transfer in biology, biochemistry, and medicine
  - Session 2: cell signaling at membranes
  - Session 3: macromolecular complex formation
  - Session 4: bioinspired materials and technology
  - Science sub-topics to consider include
    - Enzymatic reaction mechanisms (how can seeing all the protons help us understand enzymology)
    - Metalloproteins (Neutrons, unlike X-rays, do not damage metal centers what unique information can neutrons give on metalloproteins?)
    - Membrane Proteins: (Membrane proteins are typically difficult to crystallize what systems and science might STS instruments be able to study?)
    - Nucleic acids and ribozymes
    - Structures of complexes (drugs, protein-protein, protein-DNA/RNA)
  - Technical sub-topics to consider include
    - Time-resolved Experiments: How can neutron structures be generated along a timeline of the reaction: activation, inhibition & cryotrapping
    - Instrumentation needs (beamline, single-crystal spectroscopy, cryo [helium or N_2], humidity control)
    - Sample preparation needs (perdeuteration, deuterated reagents and crystal growth)
- **Engineering Materials and Industrial Applications**
  - Session 1: imaging and tomography science
  - Session 2: advanced engineering materials (aerospace & structures)
  - Session 3: energetic and nuclear materials/systems
  - Session 4: soft engineering materials and others
- **Environmental Science**
  - Session 1: Carbon Capture, Utilization and Storage (CCUS)
    - CO_2 adsorption and absorption processes in the vicinity of other gases requires a deep understanding of the capture mechanisms and associated structures at play. As do the chemical reactions responsible for CO_2 utilization (conversion to fuels, chemicals and materials), and those occurring during sequestration underground. The involvement of water in some of these processes together with a variety of light elements mean that neutrons are an ideal probe for discovery of processes and structures. Additional topics include carbon storage in soils.
  - Session 2: Clean water
    - Access to clean drinking water around the world is becoming an increasing challenge, where new membranes, adsorbents, ion-exchange systems and other approaches are needed to tackle this grand challenge. Given that H_2O molecules are integral to these processes, and the need for quantitative data across length scales (molecular level to macroscale), neutrons are well-suited to this research domain. Other aspects relating to water include energy generation from wastewaters and brackish water treatment.
  - Session 3: Environmental Materials and Processes
    - Materials for pollution remediation

        - Recycling plastics
        - Sustainable materials for industry (e.g., materials from waste streams, sustainable construction materials, renewable chemicals and fuels)
        - Materials degradation
    - Session 4: Open discussion and summary
- **Fundamental Physics**
    - Session 1: fundamental symmetries with CN/UCN (cold neutrons/ultra-cold neutrons)
    - Session 2: applications for fundamental physics (e.g. nuclear astrophysics and quantum information science with neutrons)
    - Session 3: neutrinos and dark matter
    - Session 4: open discussion/summary
- **Materials Discovery and Characterization**
    - Session 1: mastering hierarchical assembly and crystallization from complex solutions
    - Session 2: in situ examination of dynamic interfaces in energy storage and conversion materials
    - Session 3: discovery and synthesis of functional materials via high pressure
    - Session 4: detection and manipulation of defects and disorders beyond ideal equilibrium systems
- **Quantum Materials**
    - Session 1: fundamental interactions in quantum disordered systems
    - Session 2: structure and dynamics of topological quantum matter
    - Session 3: engineering and controlling emergent quantum states of matter
    - Session 4: open discussion of the future of neutron scattering in quantum materials
- **Soft Matter**
    - Science topics
        - I. Hierarchical self-assembly of soft matter
            - Directed assembly
            - Kinetics of self-assembly
            - Non-equilibrium, and far from equilibrium states
            - Crystallization, phase transformation
            - Polymer processing, transformations under large stress
            - In-situ techniques
        - II. Dynamics
            - Collective dynamics, coherent scattering
            - Dynamic heterogeneities, characteristic lengths scales in dynamics
            - Transport
            - Correlated dynamics
            - Aging
            - Non-linear rheology,
        - III. Active and stimuli-responsive matter
            - Dynamics and kinetics in stimuli responsive materials
            - Self-healing materials
            - Systems with dynamic bonds, polymer upcycling
            - Structure and dynamics of associating systems
        - IV. Surfaces and interfaces
            - Structure and dynamics in thin polymer films?
            - Interfacial properties in multicomponent systems (polymer nanocomposites, block copolymers, polymer blends)

- Session 1: general discussion, including all 4 topic areas above and any new ideas
- Session 2: discussion of topics I and IV
- Session 3: discussion of topics II and III
- Session 4: final discussion of all topics