

# MONDAY ORAL PRESENTATIONS

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\* Invited Paper

## Plenary and Prize Session

SESSION II.01: Plenary and Prize Session  
Session Chairs: Peter Gehring, Young Lee, Katie Weigandt and Stephen Wilson  
Monday Morning, June 6, 2022  
UMC Conference Room 235

## 8:00 AM WELCOME AND INSTRUCTIONS

**8:15 AM \*II.01.01**  
**CLIFFORD G. SHULL PRIZE WINNER: Tailoring Instruments to the Science and the Source: 35 Years at the NCNR** [Dan A. Neumann](#); National Institute of Standards and Technology, United States

**9:10 AM \*II.01.02**  
**PLENARY: The Dark Energy of Quantum Materials** [Laura Greene](#); Florida State University, United States

**9:45 AM BREAK**

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A1.01: Facilities  
Session Chair: John Ankner  
Monday Morning, June 6, 2022  
UMC West Ballroom 208

**10:15 AM A1.01.01**  
**Development of Neutron Scattering Facilities at the McMaster Nuclear Reactor** [Patrick Clancy](#); McMaster University, Canada

**10:45 AM A1.01.02**  
**Reactor Institute Delft 2.0** [Jeroen Plomp](#); Delft University of Technology, Netherlands

**11:00 AM A1.01.03**  
**New Guide System and Upgraded Instrument Suite at HFIR after Beryllium Reflector Change** [Georg Ehlers](#), Amy Jones, Michael C. Hoffmann, Lowell Crow, Franz X. Gallmeier, Thomas Huegle, Matthew J. Frost, Cassie S. Sabens, Kenneth C. Littrell, Richard M. Ibberson, Lisa DeBeer-Schmitt, Garrett E. Granroth, Sai Venkatesh Pingali, Hassina Z. Bilheux, Yuxuan Zhang, Andrii Y. Kovalevskiy, Travis J. Williams, Adam Aczel and Matthias D. Frontzek; Oak Ridge National Laboratory, United States

**11:15 AM A1.01.04**  
**Neutron Beamline Shielding Studies for the HFIR Beryllium Reflector Replacement Project** [Kyle Grammer](#) and Wei Lu; Oak Ridge National Laboratory, United States

**11:30 AM A1.01.05**  
**Future of Development Beamlines at the High Flux Isotope Reactor after the upcoming HFIR Beryllium Reflector Replacement** [Lowell Crow](#); Oak Ridge National Laboratory, United States

**11:45 AM A1.01.06**  
**The Cold Source Upgrade Project at the NIST Center for Neutron Research** [Rodrigo Vilaseca](#), Daniel Adler, Donald Pierce, Brian J. Kirby and Dan A. Neumann; NIST, United States

**12:00 PM A1.01.07**  
**Preliminary Neutronics Design of a Second Target Station at the ORNL's SNS** [Igor Remec](#), Franz X. Gallmeier, Kristel Ghoos, Tucker McClanahan, Thomas Miller, Kumar Mohindroo, Wouter de Wet and Lukas Zavorka; Oak Ridge National Laboratory, United States

**12:15 PM A1.01.08**  
**Development of Polarized Neutron at the China Spallation Neutron Source** [Tianhao R. Wang](#)<sup>1,2</sup> and Xin Tong<sup>1,2</sup>; <sup>1</sup>China Spallation Neutron Source, China; <sup>2</sup>Institute of high energy physics, China

## Hard Condensed Matter

SESSION B1.01: Magnetism and Topological Band Structures  
Session Chair: Martin Greven  
Monday Morning, June 6, 2022  
UMC East Ballroom 212

**10:15 AM \*B1.01.01**  
**Neutron Diffraction Studies on the Magnetic Properties of  $YMn_6Sn_6-xGe_x$**  [Rebecca L. Dally](#)<sup>1</sup>, Peter Siegfried<sup>2,2</sup>, Hari Bhandari<sup>2</sup>, David Jones<sup>2</sup>, Dina Michel<sup>2,2</sup>, Madhav Ghimire<sup>3</sup>, Lekhanath Poudel<sup>1</sup>, Markus Bleuel<sup>1</sup>, Jeffrey W. Lynn<sup>1</sup>, Igor Mazin<sup>2,2</sup> and Nirmal Ghimire<sup>2,2</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>George Mason University, United States; <sup>3</sup>Tribhuvan University, Nepal

**10:45 AM B1.01.02**  
**Weyl Mediated Helical Magnetism in NdAlSi and NdAlGe** [Jonathan Gaudet](#)<sup>1,2,3</sup>, Hung-Yu Yang<sup>4</sup>, Santu Baidya<sup>5</sup>, Baozhu Lu<sup>6</sup>, Guangyong Xu<sup>1</sup>, Yang Zhao<sup>1,2</sup>, Jose A. Rodriguez-Rivera<sup>1,2</sup>, Christina Hoffmann<sup>7</sup>, Lisa DeBeer-Schmitt<sup>7</sup>, Adam Aczel<sup>7</sup>, David Graf<sup>8</sup>, Darius Torchinsky<sup>6</sup>, Predrag Nikolic<sup>9,3</sup>, David Vanderbilt<sup>5</sup>, Tafti Fazel<sup>4</sup> and Collin Broholm<sup>3,1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States; <sup>3</sup>Johns Hopkins University, United States; <sup>4</sup>Boston College, United States; <sup>5</sup>Rutgers University, United States; <sup>6</sup>Temple University, United States; <sup>7</sup>Oak Ridge National Laboratory, United States; <sup>8</sup>National High Magnetic Field Laboratory, United States; <sup>9</sup>George Mason University, United States

**11:00 AM B1.01.03**  
**Field-Induced Fan-like Magnetic Orders in Topological  $EuIn_2As_2$  Studied by Single-Crystal Neutron Diffraction** [Simon X. Riberolles](#)<sup>1</sup>, Thais Victa Trevisan<sup>1,2</sup>, Brinda Kuthanazhi<sup>1,2</sup>, Feng Ye<sup>3</sup>, D. C. Johnston<sup>1,2</sup>, Sergey L. Bud'ko<sup>1,2</sup>, Paul C. Canfield<sup>1,2</sup>, R. J. McQueeney<sup>1,2</sup>, Peter P. Orth<sup>1,2</sup> and Benjamin G. Ueland<sup>1</sup>; <sup>1</sup>Ames Laboratory, United States; <sup>2</sup>Iowa State University of Science and Technology, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

11:15 AM B1.01.04

**Single Pair of Weyl Points in a Time-Reversal Symmetry Broken Semi-Metal** Keith Taddei<sup>1</sup>, Li Yin<sup>1</sup>, Duminda Sanjeeva<sup>2</sup>, Yu Li<sup>3</sup>, Jie Xing<sup>4</sup>, Clarina dela Cruz<sup>1</sup>, Daniel Phelan<sup>3</sup>, Athena Sefat<sup>1</sup> and David Parker<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>MURR, United States; <sup>3</sup>Argonne National Laboratory, United States; <sup>4</sup>University of South Carolina, United States

11:30 AM B1.01.05

**Spin Dynamics in the Antiferromagnetic Topological Insulator MnBi<sub>2</sub>Te<sub>7</sub>** Bing Li<sup>1,2</sup>, Simon X. Riberolles<sup>1,2</sup>, Daniel M. Pajerowski<sup>3</sup>, J.-Q. Yan<sup>3</sup> and R. J. McQueeney<sup>1,2</sup>; <sup>1</sup>Ames Laboratory, United States; <sup>2</sup>Iowa State University of Science and Technology, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

11:45 AM B1.01.06

**Topological Magnons in a Honeycomb Lattice Magnet CoTiO<sub>3</sub>** Bo Yuan<sup>1,2</sup>, Matthew Stone<sup>3</sup>, Guo-Jiun Shu<sup>4</sup>, Fangcheng Chou<sup>5</sup>, Patrick Clancy<sup>6</sup> and Young-June Kim<sup>1</sup>; <sup>1</sup>University of Toronto, Canada; <sup>2</sup>Max Planck Institute for the Structure and Dynamics of Matter, Germany; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>National Taipei University of Technology, Taiwan; <sup>5</sup>National Taiwan University, Taiwan; <sup>6</sup>McMaster University, Canada

12:00 PM B1.01.07

**Gapless Dirac magnons in CrCl<sub>3</sub>** Despina Louca<sup>1</sup>, John Schneeloch<sup>1</sup>, Yu Tao<sup>1</sup>, Yongqiang Cheng<sup>2</sup> and Luke Daemen<sup>2</sup>; <sup>1</sup>University of Virginia, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

12:15 PM B1.01.08

**Spin Excitations in Co-doped FeSn** Tao Xie<sup>1</sup>, Qiangwei Yin<sup>2</sup>, Qi Wang<sup>2</sup>, Alexander I. Kolesnikov<sup>1</sup>, Garrett E. Granroth<sup>1</sup>, Douglas L. Abernathy<sup>1</sup>, Dongliang Gong<sup>3</sup>, Zhiping Yin<sup>4</sup>, Hechang Lei<sup>2</sup> and Andrey Podlesnyak<sup>1</sup>; <sup>1</sup>Neutron Scattering Division, Oak Ridge National Laboratory, United States; <sup>2</sup>Department of Physics and Beijing Key Laboratory of Opto-Electronic Functional Materials & Micro-Nano Devices, Renmin University of China, China; <sup>3</sup>Department of Physics and Astronomy, University of Tennessee, United States; <sup>4</sup>Center for Advanced Quantum Studies and Department of Physics, Beijing Normal University, China

## Soft Matter

SESSION C1.01: Field-Driven Structures in Soft Matter  
Session Chair: Xiaodan Gu  
Monday Morning, June 6, 2022  
UMC Conference Room 235

10:15 AM \*C1.01.01

**Altering Block Copolymer (BCP) Self-Assembly and Phase Behavior via Magnetic Field Processing** Grace V. Kresge, Karthika Suresh and Michelle A. Calabrese; University of Minnesota Twin Cities, United States

10:45 AM C1.01.02

**Measuring and Modeling Interactions Between Orientable Nanoparticles in Flow** Patrick T. Corona, Jiamin Zhang, L. Gary Leal and Matthew Helgeson; University of California Santa Barbara, United States

11:00 AM C1.01.03

**Simultaneous Measurement of Structure and Rheology of Rod like Systems at High Shear Rates** Katie M. Weigandt, Ryan P. Murphy, Steve Kuei, Paul Salipante and Steven D. Hudson; National Institute of Standards and Technology, United States

11:15 AM C1.01.04

**Rheo-Small Angle Neutron Scattering Measurements of Shear-Thickening Colloidal Suspensions with Varying Interparticle Friction** Yu-Fan J. Lee<sup>1</sup>, Scott Brown<sup>2</sup> and Norman Wagner<sup>1</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>The Chemours Company, United States

11:30 AM C1.01.05

**An Analytical Method for Reconstructing the Orientation Ordering of Soft Matter Constituents from Their Scattering Anisotropy** Guan-Rong Huang<sup>1</sup>, Jan Michael Carrillo<sup>1</sup>, Yangyang Wang<sup>1</sup>, Changwoo Do<sup>1</sup>, Yuya Shinohara<sup>1</sup>, Takeshi Egami<sup>1</sup>, Lionel Porcar<sup>2</sup>, Yun Liu<sup>3</sup>, Bobby G. Sumpter<sup>1</sup> and Wei-Ren Chen<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Institut Laue-Langevin, France; <sup>3</sup>National Institute of Standards and Technology, United States

11:45 AM C1.01.06

**Extracting Meaning from Alignment Factor** Peter Gilbert<sup>1</sup>, Yun Liu<sup>1,2</sup> and Paul D. Butler<sup>1</sup>; <sup>1</sup>NIST Center for Neutron Research, United States; <sup>2</sup>University of Delaware, United States

12:00 PM C1.01.07

**Probing Topological Transitions of Inverse Worm-like Micelles Subject to Transient Shear Flow using Dielectric RheoSANS** Noah J. Cho<sup>1</sup> and Jeffrey J. Richards<sup>2</sup>; <sup>1</sup>Corning Korea, Korea (the Republic of); <sup>2</sup>Northwestern University, United States

## Neutron Physics

SESSION G1.01: Neutron Physics I  
Session Chair: Dusan Sarenac  
Monday Morning, June 6, 2022  
UMC Aspen Room 285, 287, 289

10:15 AM \*G1.01.01

**Pendellösung Interferometry Measurement of the Neutron Charge Radius and Constraints on New Physics** Benjamin Heacock<sup>1</sup>, Fujiie Takuhiro<sup>2</sup>, Robert W. Haun<sup>3</sup>, Albert Henins<sup>1</sup>, Katsuya Hirota<sup>2</sup>, Takuya Hosobata<sup>4</sup>, Michael G. Huber<sup>1</sup>, Masaaki Kitaguchi<sup>2</sup>, Dmitry Pushin<sup>5</sup>, Hirohiko Shimizu<sup>2</sup>, Masahiro Takeda<sup>4</sup>, Robert Valdillez<sup>6</sup>, Yutaka Yamagata<sup>4</sup> and Albert Young<sup>6</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>Nagoya University, Japan; <sup>3</sup>Tulane University, United States; <sup>4</sup>RIKEN, Japan; <sup>5</sup>University of Waterloo, Canada; <sup>6</sup>North Carolina State University, United States

10:45 AM G1.01.02

**Measuring Higher Order Neutron-Silicon Structure Factors with Pendellösung Interferometry Using a Pulsed Beam** Robert Valdillez<sup>1</sup>, Leah Broussard<sup>2</sup>, Matthew J. Frost<sup>2</sup>, Robert W. Haun<sup>3</sup>, Benjamin Heacock<sup>4</sup>, Colin Heikes<sup>5</sup>, Albert Henins<sup>4</sup>, Katsuya Hirota<sup>6</sup>, Shannon F. Hoogerheide<sup>4</sup>, Takuya Hosobata<sup>7</sup>, Michael G. Huber<sup>4</sup>, Masaaki Kitaguchi<sup>6</sup>, Dmitry Pushin<sup>8</sup>, Hirohiko Shimizu<sup>6</sup>, Masahiro Takeda<sup>7</sup>, Fujiie Takuhiro<sup>6</sup>, Yutaka Yamagata<sup>7</sup> and Albert Young<sup>1</sup>; <sup>1</sup>North Carolina State University, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>University of Colorado Boulder, United States; <sup>4</sup>National Institute of Standards and Technology, United States; <sup>5</sup>Northrop Grumman, United States; <sup>6</sup>Nagoya University, Japan; <sup>7</sup>RIKEN, Japan; <sup>8</sup>University of Waterloo, Canada

11:00 AM G1.01.03

**Quantum Information Model for Neutron Diffraction Shows Promise for Neutron Optics Design** Olivier Nahman-Lévesque<sup>1</sup>, Dusan Sarenac<sup>1</sup>, David Cory<sup>1</sup>, Benjamin Heacock<sup>2</sup>, Michael G. Huber<sup>2</sup> and Dmitry Pushin<sup>1</sup>; <sup>1</sup>University of Waterloo, Canada; <sup>2</sup>National Institute of Standards and Technology, United States

### 11:15 AM G1.01.04

**Neutron Interferometry and Current Advances** Dmitry Pushin<sup>1</sup>, Benjamin Heacock<sup>2</sup>, Michael G. Huber<sup>2</sup>, Dusan Sarenac<sup>1</sup>, Chandra B. Shahi<sup>3</sup>, Ivar Taminiua<sup>1</sup> and David Cory<sup>1,1</sup>; <sup>1</sup>University of Waterloo, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>University of Maryland, United States

### 11:30 AM G1.01.05

**Generation and Detection of Structured Waves of Neutrons and Light** Charles W. Clark<sup>1</sup>, Dusan Sarenac<sup>2</sup>, Melissa E. Henderson<sup>2</sup>, Huseyin Ekinci<sup>2</sup>, Chandra B. Shahi<sup>1</sup>, David Cory<sup>2</sup>, Lisa DeBeer-Schmitt<sup>3</sup>, Michael G. Huber<sup>1</sup>, Connor L. Kapahi<sup>2</sup> and Dmitry Pushin<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Waterloo, Canada; <sup>3</sup>Oak Ridge National Laboratory, United States

### 11:45 AM G1.01.06

**Spin-Orbit Correlations in Neutron Beams** Dusan Sarenac<sup>1</sup>, Connor L. Kapahi<sup>1</sup>, Wangchun Chen<sup>2</sup>, Charles W. Clark<sup>3</sup>, David Cory<sup>1</sup>, Michael G. Huber<sup>2</sup>, Ivar Taminiua<sup>1</sup>, Kirill Zhernenkov<sup>4</sup> and Dmitry Pushin<sup>1</sup>; <sup>1</sup>University of Waterloo, Canada; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, United States; <sup>4</sup>Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Germany

### 12:00 PM G1.01.07

**Measurements of the Neutron's Charge Distribution; a History** Michael G. Huber<sup>1</sup>, Benjamin Heacock<sup>1</sup>, Robert Valdillez<sup>2</sup>, Fujiie Takuhiro<sup>3</sup>, Masaaki Kitaguchi<sup>3</sup>, Hirohiko Shimizu<sup>3</sup>, Katsuya Hirota<sup>4</sup>, Masahiro Takeda<sup>4</sup>, Yutaka Yamagata<sup>4</sup>, Dmitry Pushin<sup>5,6</sup> and Albert Young<sup>2</sup>; <sup>1</sup>NIST, United States; <sup>2</sup>North Carolina State University, United States; <sup>3</sup>Nagoya University, Japan; <sup>4</sup>RIKEN, Japan; <sup>5</sup>University of Waterloo, Canada; <sup>6</sup>Institute for Quantum Computing, Canada

### 12:15 PM G1.01.08

**Precision Measurement of the Gravitational Constant via Three-Phase Grating Neutron Interferometry** Connor L. Kapahi<sup>1,2</sup>, Dusan Sarenac<sup>2</sup>, Charles W. Clark<sup>3</sup>, David Cory<sup>1,2</sup>, Benjamin Heacock<sup>3</sup>, Michael G. Huber<sup>3</sup>, Youngju Kim<sup>3</sup> and Dmitry Pushin<sup>1,2</sup>; <sup>1</sup>University of Waterloo, Canada; <sup>2</sup>Institute for Quantum Computing, Canada; <sup>3</sup>National Institute of Standards and Technology, United States

## Hard Condensed Matter

SESSION B1.02: Disorder Inhomogeneity and Strong Correlations  
Session Chair: Olivier Delaire  
Monday Afternoon, June 6, 2022  
UMC East Ballroom 212

### 1:45 PM \*B1.02.01

**Correlated Structural Inhomogeneity in Oxide Superconductors** Martin Greven; University of Minnesota, United States

### 2:15 PM B1.02.02

**Large Change of Interlayer Vibrational Coupling with Stacking in  $\text{Mo}_{1-x}\text{W}_x\text{Te}_2$**  John Schneeloch<sup>1</sup>, Yu Tao<sup>1</sup>, Jaime A. Fernandez-Baca<sup>2</sup>, Guangyong Xu<sup>3</sup> and Despina Louca<sup>1</sup>; <sup>1</sup>University of Virginia, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>National Institute of Standards and Technology, United States

### 2:30 PM B1.02.03

**Role of Magnetic Defects and Defect-Engineering of Magnetic Topological Insulators** Farhan Islam<sup>1,2</sup>, Daniel M. Pajerowski<sup>3</sup>, jiaqiang yan<sup>3</sup>, R. J. McQueeney<sup>1,2</sup> and David Vaknin<sup>1,2</sup>; <sup>1</sup>Iowa State University of Science and Technology, United States; <sup>2</sup>Ames Laboratory, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

### 2:45 PM B1.02.04

**Diffuse Neutron and X-Ray Scattering from Inorganic Halide Perovskites** Matthew Krogstad<sup>1</sup>, Alex Rettie<sup>2</sup>, Stephan Rosenkranz<sup>1</sup>, Duck Young Chung<sup>1</sup>, Mercuri Kanatzidis<sup>3</sup>, Feng Ye<sup>4</sup>, Yaohua Liu<sup>4</sup>, Xing He<sup>5</sup>, Tyson L. Lanigan-Atkins<sup>5</sup>, Olivier Delaire<sup>5</sup> and Raymond Osborn<sup>1</sup>; <sup>1</sup>Argonne National Laboratory, United States; <sup>2</sup>University College London, United Kingdom; <sup>3</sup>Northwestern University, United States; <sup>4</sup>Oak Ridge National Laboratory, United States; <sup>5</sup>Duke University, United States

### 3:00 PM B1.02.05

**Impact of Site-Specific Cation Disorder on the Magnetic Structure Formation and Evolution in Entropy-Stabilized Perovskite Oxides** Nathan D. Arndt<sup>1</sup>, Brianna Musico<sup>2</sup>, Keon Sahebkar<sup>1</sup>, Qiang Zhang<sup>3</sup>, Alessandro Mazza<sup>3</sup>, Veerle Keppens<sup>2</sup>, T. Z. Ward<sup>3</sup> and Ryan Need<sup>1</sup>; <sup>1</sup>University of Florida, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

### 3:15 PM B1.02.06

**Cubic on the Streets, Tetragonal in the Sheets: the Nature of Local Dynamic Order in  $\text{CH}_3\text{NH}_3\text{PbI}_3$**  Tyler C. Sterling<sup>1</sup>, Nicholas Weadock<sup>2,2</sup>, Ballal Ahammed<sup>3</sup>, Elif Ertekin<sup>3</sup>, Michael Toney<sup>2,2</sup> and Dmitry Reznik<sup>1,2</sup>; <sup>1</sup>University of Colorado, Boulder, United States; <sup>2</sup>University of Colorado Boulder, United States; <sup>3</sup>University of Illinois at Urbana-Champaign, United States

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A1.02: Software: Instrumentation  
Session Chair: Paul Butler  
Monday Afternoon, June 6, 2022  
UMC West Ballroom 208

### 2:00 PM A1.02.01

**Material Decomposition for Hyperspectral Neutron Tomography** Charles A. Bouman<sup>1</sup>, Gregory Buzzard, T<sup>1</sup>, Mohammad Samin Nur Chowdhury<sup>1</sup>, Singanallur Venkatakrishnan<sup>2</sup> and Hassina Z. Bilheux<sup>2</sup>; <sup>1</sup>Purdue University, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

### 2:30 PM A1.02.02

**McStas2CAD: A Python-based Software Package for Scattering Instrument Concept Geometry Conversion** Matthew J. Frost and Lee Robertson; Oak Ridge National Laboratory, United States

### 2:45 PM A1.02.03

**Towards a User-friendly Workflow for Monte Carlo Neutron Scattering Simulations** Fahima Islam, Garrett E. Granroth, Jiao Lin and Thomas Huegle; Neutron Scattering Division, United States

### 3:00 PM A1.02.04

**Tally Components in McStas** Thomas Huegle, Matthew J. Frost, Garrett E. Granroth and Lee Robertson; Oak Ridge National Laboratory, United States

### 3:15 PM A1.02.05

**Neutron Velocity Selector Design and Impact on Simulation** William T. Higgins, Thomas Huegle, Kenneth C. Littrell, Franz X. Gallmeier and Georg Ehlers; Oak Ridge National Laboratory, United States

## Soft Matter

SESSION C1.02: Conjugated Polymers  
Session Chair: Megan Robertson  
Monday Afternoon, June 6, 2022  
UMC Conference Room 235

### 2:00 PM \*C1.02.01

**Analysis of the Structure and Dynamics of Conjugated Polymers via Combined Neutron Scattering and Molecular Simulations** Caitlyn M. Wolf<sup>1</sup> and [Lilo D. Pozzo](#)<sup>2,2</sup>; <sup>1</sup>NIST, United States; <sup>2</sup>University of Washington, United States

### 2:30 PM C1.02.02

**Unraveling the Side Chain Effects on Solution Structure of Donor-Acceptor Conjugated Polymers** [Zhiqiang Cao](#)<sup>1</sup>, Zhaofan Li<sup>2</sup>, Miao Xiong<sup>3</sup>, Guorong Ma<sup>1</sup>, Luke Galuska<sup>1</sup>, Song Zhang<sup>1</sup>, Michael Ocheje<sup>4</sup>, Gage Mason<sup>4</sup>, Changwoo Do<sup>3</sup>, Kunlun Hong<sup>5</sup>, Ting Lei<sup>3</sup>, Simon Rondeau-Gagné<sup>4</sup>, Wenjie Xia<sup>2</sup> and Xiaodan Gu<sup>1</sup>; <sup>1</sup>University of Southern Mississippi, United States; <sup>2</sup>North Dakota State University, United States; <sup>3</sup>Peking University, China; <sup>4</sup>University of Windsor, Canada; <sup>5</sup>Oak Ridge National Laboratory, United States

### 2:45 PM C1.02.03

**Effect of Polystyrene Additives and Solvent Quality on the Conformation and Self-Assembly of Conjugated Polymers in Mixed Solutions** [Sage Scheiwiler](#), Lilo D. Pozzo and Lorenzo Guio; University of Washington, United States

### 3:00 PM C1.02.04

**Chain Growth Kinetics of Conjugated Polymers on Ferromagnetic Nanoparticles Investigated by SANS** [Lilin He](#); Oak Ridge National Laboratory, United States

### 3:15 PM C1.02.05

**Combining Inelastic Neutron Scattering and Molecular Dynamics Simulation to Probe Conjugated Polymer Dynamics** [Xiaodan Gu](#)<sup>1</sup>, Zhiqiang Cao<sup>1</sup>, Wenjie Xia<sup>2</sup> and Amirhadi Alesadi<sup>2</sup>; <sup>1</sup>University of Southern Mississippi, United States; <sup>2</sup>North Dakota State University, United States

## Structural Materials and Engineering

SESSION F1.01: Using Neutrons for Advanced Manufacturing Characterization  
Session Chair: Zhenzhen Yu  
Monday Afternoon, June 6, 2022  
UMC Aspen Room 285, 287, 289

### 2:00 PM \*F1.01.01

**Determining Residual Stress in Weldments and Additively Manufactured Parts by Neutron Diffraction** [Hamid Eisazadeh](#); Old Dominion University, United States

### 2:30 PM F1.01.02

**Application of Neutron Grating Interferometry in Metal Additive Manufacturing** [Youngju Kim](#)<sup>1</sup>, Caitlyn M. Wolf<sup>2</sup>, Sarah M. Robinson<sup>2</sup>, Michael Cyrus Daugherty<sup>2</sup>, Jacob M. LaManna<sup>2</sup>, David Jacobson<sup>2</sup>, Eli Baltic<sup>2</sup>, Paul A. Kienzle<sup>2</sup>, Katie M. Weigand<sup>2</sup>, Nikolai N. Klimov<sup>2</sup>, Michael G. Huber<sup>2</sup>, Peter N. Bajcsy<sup>2</sup>, Ryan P. Murphy<sup>2</sup>, Jongyul Kim<sup>3</sup>, Wook Jin Lee<sup>4</sup>, Seung Wook Lee<sup>4</sup> and Daniel S. Hussey<sup>2</sup>; <sup>1</sup>University of Maryland, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>Korea Atomic Energy Research Institute, Korea (the Republic of); <sup>4</sup>Pusan National University, Korea (the Republic of)

### 2:45 PM F1.01.03

**Stresses Due to Friction Stir Weld Repair of Simulated Cracks in 304L Stainless Steel Plates** [Thomas Gnaupel-Herold](#)<sup>1</sup>, Madhumanti Bhattacharyya<sup>2</sup>, Indrajit Charit<sup>2</sup>, Krishnan Raja<sup>2</sup>, Jens Darsell<sup>3</sup> and Saumyadeep Jana<sup>3</sup>; <sup>1</sup>NIST, United States; <sup>2</sup>University of Idaho, United States; <sup>3</sup>PNNL, United States

### 3:00 PM F1.01.04

**Implications of Machining on Residual Stresses and Mechanical Properties of 316L Walls fabricated via Hybrid Additive Manufacturing** [Christopher Fancher](#), Rangasayee Kannan, Kyle Saleeby, Thomas Feldhausen and Peeyush Nandwana; Oak Ridge National Laboratory, United States

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A1.03: Software: Data Analysis and Modeling  
Session Chair: Charles Bouman  
Monday Afternoon, June 6, 2022  
UMC West Ballroom 208

### 3:45 PM A1.03.01

**Browser Based Visualization of Large 3D Datasets using NVIDIA IndeX** [Evan Carlin](#)<sup>1</sup>, Kevin Bruhwiler<sup>1</sup>, Robert Nagler<sup>1</sup>, David Bruhwiler<sup>1</sup>, Christina Hoffmann<sup>2</sup>, Andrei T. Savici<sup>2</sup>, Zachary Morgan<sup>2</sup>, Matthew Tucker<sup>2</sup>, Alexander Kuhn<sup>3</sup>, Jörg Mensmann<sup>3</sup>, Peter Messmer<sup>3</sup>, Marc Nienhaus<sup>3</sup>, Steffen Roemer<sup>3</sup> and Dragos Tatulea<sup>3</sup>; <sup>1</sup>RadiaSoft LLC, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>NVIDIA, Germany

### 4:00 PM A1.03.02

**Addressing the Resource Problem Through Community. SasView: An "Open, Collaborative, Community Development" Platform for Small Angle Scattering** [Paul D. Butler](#)<sup>1,2,3</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Delaware, United States; <sup>3</sup>The University of Tennessee, Knoxville, United States

### 4:15 PM A1.03.03

**Event Based Data Analysis and Visualization in Neutron Spectroscopy** [Andrei T. Savici](#)<sup>1</sup>, Igor Zaliznyak<sup>2</sup>, Garrett E. Granroth<sup>1</sup> and Ovidiu Garlea<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Brookhaven National Laboratory, United States

### 4:30 PM A1.03.04

**Do We Need an ISO Standard for the Reduction of Time-of-Flight Powder Diffraction Data?** [Malcolm Guthrie](#); Oak Ridge National Laboratory, United States

### 4:45 PM A1.03.05

**Hyperspectral Neutron CT with Material Decomposition** [Thilo Balke](#)<sup>1,2</sup>, Alexander Long<sup>1</sup>, Sven C. Vogel<sup>1</sup>, Brendt Wohlberg<sup>1</sup> and Charles Bouman<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory, United States; <sup>2</sup>Purdue University, United States

### 5:00 PM A1.03.06

**Simulation of Inelastic Neutron Scattering Spectra for Direct and Indirect-Geometry Instruments with AbINS** [Adam Jackson](#) and Sanghamitra Mukhopadhyay; Science and Technology Facilities Council, UK, United Kingdom

### 5:15 PM A1.03.07

**Generic Calibration Workflow for Time-of-Flight Instruments** [Yuanpeng Zhang](#); Oak Ridge National Laboratory, United States

## Materials Chemistry and Energy

SESSION E1.01: Materials Chemistry and Energy I

Session Chair: Graeme Luke  
Monday Afternoon, June 6, 2022  
UMC Aspen Room 285, 287, 289

### 3:45 PM \*E4.04.01

**Excess Vibrational Entropy in Metallic and Molecular Glasses** [Hillary Smith](#)<sup>1</sup>, Claire N. Saunders<sup>2</sup>, Camille Bernal<sup>2</sup>, Stefan H. Lohaus<sup>2</sup>, Douglas L. Abernathy<sup>3</sup>, Jiao Lin<sup>3</sup>, Marios Demetriou<sup>4</sup> and Brent Fultz<sup>2</sup>; <sup>1</sup>Swarthmore College, United States; <sup>2</sup>Caltech, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>Glassmetal, United States

### 4:15 PM E4.04.02

**The Two-Dimensional Nature of Dynamic Disorder in Hybrid Metal Halide Perovskite Semiconductors** [Nicholas Weadock](#)<sup>1</sup>, Tyler C. Sterling<sup>1</sup>, Matthew Krogstad<sup>2</sup>, Feng Ye<sup>3</sup>, David Vonshen<sup>4</sup>, Julian Vigi<sup>5</sup>, Ballal Ahammed<sup>6</sup>, Peter Gehring<sup>7</sup>, Hans-Georg Steinrueck<sup>8</sup>, Elif Ertekin<sup>6</sup>, Hemamala Karunadasa<sup>5</sup>, Dmitry Reznik<sup>1</sup> and Michael Toney<sup>1</sup>; <sup>1</sup>University of Colorado Boulder, United States; <sup>2</sup>Argonne National Laboratory, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>Rutherford Appleton Laboratory, United Kingdom; <sup>5</sup>Stanford University, United States; <sup>6</sup>University of Illinois at Urbana-Champaign, United States; <sup>7</sup>National Institute of Standards and Technology, United States; <sup>8</sup>Universität Paderborn, Germany

### 4:30 PM E4.04.03

**Neutron Scattering to Characterize Adsorbents and Their Hosts** [Craig M. Brown](#)<sup>1</sup>, Ryan Klein<sup>2</sup>, Benjamin A. Trump<sup>1</sup> and Hayden A. Evans<sup>1</sup>; <sup>1</sup>NIST Center for Neutron Research, United States; <sup>2</sup>National Renewable Energy Laboratory, United States

### 4:45 PM E4.04.04

**Neutron Scattering Kernels for Methane I & II and Ethane III J. R. Granada**<sup>1</sup>, J.I. Márquez Damián<sup>2</sup>, S. Rudic<sup>3</sup> and G. Skoro<sup>3</sup>; <sup>1</sup>Argentine Atomic Energy Commission, Argentina; <sup>2</sup>European Spallation Source ERIC, Sweden; <sup>3</sup>ISIS Facility, United Kingdom

### 5:00 PM E4.04.05

**Structure Modulation of LnMnFeO<sub>4</sub> upon Oxidation into LnMnFeO<sub>4.5</sub> (Ln=Y, Yb, Lu)** [Tianyu Li](#) and Efrain E. Rodriguez; University of Maryland, United States

### 5:15 PM E4.04.06

**Diffusion Dynamics of FLiNaK Molten Salt Characterized with Quasi-Elastic Neutron Scattering** [Brent J. Heuser](#), Golam Rakib and Yang Zhang; University of Illinois, United States

## Hard Condensed Matter

SESSION B1.03: Novel Magnetic Structures and Excitations

Session Chair: Rebecca Dally  
Monday Afternoon, June 6, 2022  
UMC East Ballroom 212

### 4:00 PM \*B1.03.01

**Coexisting Singlet and Ordered Spins in a Complex Quasi-2D magnet Cu<sub>3</sub>B<sub>2</sub>O<sub>6</sub>** [Bo Yuan](#)<sup>1</sup>, [Kemp Plumb](#)<sup>2</sup>, [Matthew Stone](#)<sup>3</sup>, [Yiming Qiu](#)<sup>4</sup>, [Nicholas Butch](#)<sup>4</sup>, [Guangyong Xu](#)<sup>4</sup>, [Patrick Clancy](#)<sup>5</sup> and [Young-June Kim](#)<sup>6</sup>; <sup>1</sup>Max Planck Institute for the Structure and Dynamics of Matter, Germany; <sup>2</sup>Brown University, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>National Institute of Standards and Technology, United States; <sup>5</sup>McMaster University, Canada; <sup>6</sup>University of Toronto, Canada

### 4:30 PM B1.03.02

**Longitudinal Magnon Decay and Renormalization in Ba<sub>2</sub>FeSi<sub>2</sub>O<sub>7</sub>** [Seunghwan Do](#)<sup>1</sup>, [Hao Zhang](#)<sup>2</sup>, [Travis J. Williams](#)<sup>1</sup>, [Tao Hong](#)<sup>1</sup>, [Ovidiu Garlea](#)<sup>1</sup>, [Jose A. Rodriguez-Rivera](#)<sup>3</sup>, [Tae-Hwan Jang](#)<sup>4</sup>, [Sang-Wook Cheong](#)<sup>5</sup>, [Jae-Hoon Park](#)<sup>4</sup>, [Cristian Batista](#)<sup>2</sup> and [Andrew D. Christianson](#)<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States; <sup>3</sup>NIST Center For Neutron Research, United States; <sup>4</sup>MPPHC-CPM, Max Planck POSTECH/Korea Research Initiative, Korea (the Republic of); <sup>5</sup>Rutgers, The State University of New Jersey, United States

### 4:45 PM B1.03.03

**Magnetic Structures and Dynamics in CuMnAs and Related Cu<sub>2</sub>Sb-type Antiferromagnets** [Daniel Shoemaker](#); University of Illinois at Urbana-Champaign, United States

### 5:00 PM B1.03.04

**Bootstrapped Dimensional Crossover of a Spin Density Wave in Layered Nickelate** [Anjana M. Samarakoon](#)<sup>1</sup>, [Joerg Strempler](#)<sup>1</sup>, [Feng Ye](#)<sup>2</sup>, [Yiming Qiu](#)<sup>3</sup>, [Stephan Rosenkranz](#)<sup>1</sup>, [Michael Norman](#)<sup>1</sup>, [John Mitchell](#)<sup>1</sup> and [Daniel Phelan](#)<sup>1</sup>; <sup>1</sup>Argonne National Laboratory, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>National Institute of Standards and Technology, United States

### 5:15 PM B1.03.05

**Chemically-Induced Magnetic Dead Shells in Superparamagnetic Ni Nanoparticles from Polarized Small-Angle Neutron Scattering** [Bhaskar Das](#)<sup>1</sup>, [Joseph Batley](#)<sup>1</sup>, [Kathryn L. Krycka](#)<sup>2</sup>, [Julie A. Borchers](#)<sup>2</sup>, [Patrick Quarterman](#)<sup>2</sup>, [Caroline Korostynski](#)<sup>1</sup>, [My Nguyen](#)<sup>1</sup>, [Ishita Kamboj](#)<sup>1</sup>, [Eray Aydil](#)<sup>3</sup> and [Chris Leighton](#)<sup>1</sup>; <sup>1</sup>University of Minnesota, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>New York University, United States

## Biology, Biophysics and Biotechnology

SESSION D1.01: Structure and Dynamics of Proteins and Peptide Assemblies

Session Chairs: Elizabeth Kelley and Haden Scott  
Monday Afternoon, June 6, 2022  
UMC Conference Room 235

### 4:00 PM \*D1.01.01

**Supramolecular Self-Assembly of Computationally Designed Coiled Coil Building Blocks** [Nairiti J. Sinha](#); University of California, Santa Barbara, United States

### 4:30 PM D1.01.02

**Studying Internal Dynamics of the Monoclonal Antibody with SANS and NSE** [Roisin Donnelly](#)<sup>1,2</sup>, [Yun Liu](#)<sup>2,1</sup> and [Norman Wagner](#)<sup>1,2</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>NIST Center for Neutron Scattering, United States

### 4:45 PM D1.01.03

**Small-Angle Scattering to Understand Preservative-Induced Aggregation of Poloxamer 188 in Pharmaceutical Formulations** [Rachel R. Ford](#)<sup>1</sup>, [Peter Gilbert](#)<sup>1</sup>, [Ken Qian](#)<sup>2</sup>, [Norman Wagner](#)<sup>3</sup> and [Yun Liu](#)<sup>1</sup>; <sup>1</sup>NIST Center for Neutron Research, United States; <sup>2</sup>Eli Lilly & Company, United States; <sup>3</sup>University of Delaware, United States

### 5:00 PM D1.01.04

**Investigating Aggregation Surfaces In Thawed Bispecific Antibody Fragments** [Julia Greenfield](#); National Institute of Standards and Technology, United States

5:15 PM D1.01.05

Characterize Conformational Flexibility of Monoclonal Antibodies using Small-Angle Scattering Amy Xu; Louisiana State University, United States

# TUESDAY ORAL PRESENTATIONS

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\* Invited Paper

## Plenary and Prize Session

SESSION I2.01: Plenary and Prize Session  
Session Chairs: Peter Gehring, Young Lee, Katie Weigandt and Stephen Wilson  
Tuesday Morning, June 7, 2022  
UMC Conference Room 235

### 8:15 AM FELLOWS ANNOUNCEMENT

#### 8:30 AM \*I2.01.01

**SCIENCE PRIZE WINNER: Magnons are not Forever** Martin Mourigal; Georgia Institute of Technology, United States

#### 9:10 AM \*I2.01.02

**PLENARY: SANS Contrast Variation Experiments on Multi-Component Biological Complexes: What's the Big Deal?** Susan Krueger; National Institute of Standards and Technology, United States

### 9:45 AM BREAK

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A2.05: Instrumentation: Hard Matter  
Session Chair: Ken Herwig  
Tuesday Morning, June 7, 2022  
UMC West Ballroom 208

#### 10:15 AM \*A2.05.01

**BIFROST: A Multiplexing Indirect Geometry Time-of-Flight Spectrometer for Extreme Environments** Rasmus Toft-Petersen<sup>1,2</sup>, Liam Whitelegg<sup>2</sup>, Bjørn C. Hauback<sup>3</sup>, Philippe Bourges<sup>4</sup>, Christof Niedermayer<sup>5</sup>, Henrik M. Ronnow<sup>6</sup>, Kim Lefmann<sup>7</sup> and Niels B. Christensen<sup>1</sup>; <sup>1</sup>Technical University of Denmark, Denmark; <sup>2</sup>European Spallation Source, Sweden; <sup>3</sup>Institute for Energy Technology, Norway; <sup>4</sup>Laboratoire Léon Brillouin, France; <sup>5</sup>Paul Scherrer Institut, Switzerland; <sup>6</sup>Swiss Federal Institute of Technology Lausanne, Switzerland; <sup>7</sup>Niels Bohr Institute, Denmark

#### 10:45 AM A2.05.02

**Update on the Cold Spectrometer Project, PoLAR, at the NCNR** Leland W. Harriger<sup>1</sup>, Stephen D. Wilson<sup>2</sup>, Jeffrey Lynn<sup>1</sup>, Dan A. Neumann<sup>1</sup>, Jeremy Cook<sup>1</sup>, Donald Pierce<sup>1</sup> and Nancy Hadad<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of California, Santa Barbara, United States

11:00 AM A2.05.03

**Progress on the Design of Centaur, the Small- and Wide-Angle Neutron Scattering Diffractometer/Spectrometer at the Second Target Station of SNS** Shuo Qian; Oak Ridge National Laboratory, United States

11:15 AM A2.05.04

**An Update on PIONEER, a Single-Crystal Neutron Diffractometer at the Second Target Station** Yaohua Liu and Peter Torres; Oak Ridge National Laboratory, United States

11:30 AM A2.05.05

**Development of the Multi-Analyzer Neutron Triple Axis (MANTA) Spectrometer at ORNL** Travis J. Williams<sup>1</sup>, Garrett E. Granroth<sup>1</sup>, Adam Aczel<sup>1</sup>, Barry Winn<sup>1</sup>, Adit Desai<sup>2</sup>, Marcus Daum<sup>2</sup> and Martin Mourigal<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Georgia Institute of Technology, United States

11:45 AM A2.05.06

**Upgrade of the BT-8 Diffractometer for Stress and Texture** Thomas Gnaupel-Herold<sup>1</sup>, Justin Milner<sup>2</sup> and Ed Binkley<sup>1</sup>; <sup>1</sup>NIST, United States; <sup>2</sup>NASA GRC, United States

12:00 PM A2.05.07

**Polychromatic Multiplexing Stress-Strain Diffractometer** Sean Fayfar<sup>1</sup>, Jay T. Cremer<sup>2</sup> and Boris Khaykovich<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology, United States; <sup>2</sup>Adelphi Technology, Inc., United States

12:15 PM A2.05.08

**Concept for a Hybrid Neutron Diffraction/ Small Angle Scattering Instrument for Nuclear Energy Applications** Kenneth C. Littrell and Georg Ehlers; Oak Ridge National Laboratory, United States

## Hard Condensed Matter

SESSION B2.04: Frustrated Magnetism  
Session Chair: Kemp Plumb  
Tuesday Morning, June 7, 2022  
UMC East Ballroom 212

10:15 AM \*B2.04.01

**Neutron Scattering Studies of Rare-earth-based Quantum Spin Liquid Candidates** Sara Haravifard; Duke University, United States

10:45 AM B2.04.02

**Evolution of Field-Induced and Impurity-Induced Magnetic Order in the Quantum Spin Liquid Candidate NaYbSe<sub>2</sub>** Ganesh Pokharel, Soren Bear and Stephen D. Wilson; University of California, Santa Barbara, United States

11:00 AM B2.04.03

**Anomalous Crystalline Electric Field Excitation in Triangular Lattice Cerium Materials** Mitchell Bordelon<sup>1,2</sup>, Brenden Ortiz<sup>2</sup>, Pritam Bhattacharyya<sup>3</sup>, Lorenzo Posthuma<sup>2</sup>, Ganesh Pokharel<sup>2</sup>, Paul Sarte<sup>2</sup>, Thorben Petersen<sup>3</sup>, Mohamed Eldeeb<sup>3</sup>, Garrett E. Granroth<sup>4</sup>, Xiaoling Wang<sup>2</sup>, Mark Sherwin<sup>2</sup>, Clarina dela Cruz<sup>4</sup>, Ulrich Roessler<sup>3</sup>, Livi Hozoi<sup>3</sup>, Martin Mourigal<sup>5</sup>, Stuart Calder<sup>4</sup>, Craig M. Brown<sup>6</sup>, Daniel M. Pajerowski<sup>4</sup>, Arnab Banerjee<sup>4</sup>, Douglas L. Abernathy<sup>4</sup>, Eric Bauer<sup>1</sup>, Priscila Rosa<sup>1</sup> and Stephen D. Wilson<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory, United States; <sup>2</sup>University of California, Santa Barbara, United States; <sup>3</sup>Institute for Theoretical Solid State Physics, Germany; <sup>4</sup>Oak Ridge National Laboratory, United States; <sup>5</sup>Georgia Institute of Technology, United States; <sup>6</sup>National Institute of Standards and Technology, United States

11:15 AM \*B2.04.04

**Relaxation Dynamics in Spin Ice Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>** Yishu Wang<sup>1</sup>, Timothy R. Reeder<sup>1</sup>, Yoshitomo Karaki<sup>2</sup>, Jonas Kindervater<sup>1</sup>, Thomas Halloran<sup>1</sup>, Nicholas C. Maliszewskyj<sup>3</sup>, Yiming Qiu<sup>3</sup>, Jose A. Rodriguez-Rivera<sup>3</sup>, Sergiy Gladchenko<sup>3</sup>, Seyed Koohpayeh<sup>1</sup>, Satoru Nakatsuji<sup>4</sup> and Collin Broholm<sup>1</sup>; <sup>1</sup>Johns Hopkins University, United States; <sup>2</sup>University of Ryukyus, Japan; <sup>3</sup>NIST Center for Neutron Research, United States; <sup>4</sup>The University of Tokyo, Japan

11:45 AM B2.04.05

**Real Space and Time Dynamics of Heisenberg Antiferromagnet KCuF<sub>3</sub> Measured by Neutron Scattering** Allen Scheie<sup>1</sup>, Pontus Laurell<sup>2</sup>, Bella Lake<sup>3</sup>, Stephen Nagler<sup>1</sup>, Matthew Stone<sup>1</sup>, Jean-Sebastian Caux<sup>4</sup> and Alan Tennant<sup>2,1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States; <sup>3</sup>Helmholtz-Zentrum Berlin, Germany; <sup>4</sup>University of Amsterdam, Netherlands

12:00 PM B2.04.06

**Magnetic Structure of Single Crystalline Barlowite in an Applied Magnetic Field** Aaron T. Breidenbach<sup>1,2</sup>, Rebecca Smaha<sup>1,2</sup>, Wei He<sup>1,2</sup>, Adam Aczel<sup>3</sup>, Jeffrey Lynn<sup>4,5</sup> and Young Lee<sup>1,1,2</sup>; <sup>1</sup>Stanford University, United States; <sup>2</sup>SLAC National Accelerator Laboratory, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>NIST Center for Neutron Research, United States; <sup>5</sup>The University of Tennessee, Knoxville, United States

12:15 PM B2.04.07

**Dynamical Ground State in the XY Pyrochlore Yb<sub>2</sub>Ga<sub>5</sub>Bo<sub>7</sub>** Adam Aczel<sup>1</sup>, Paul Sarte<sup>2</sup>, Joe Paddison<sup>1</sup>, Christopher Wiebe<sup>3</sup>, Brenden Ortiz<sup>2</sup>, K.H. Hong<sup>4</sup>, Mitchell Bordelon<sup>2</sup>, Dalmau Reig-i-Plessis<sup>5</sup>, Matthew Stone<sup>1</sup>, Stuart Calder<sup>1</sup>, Daniel M. Pajerowski<sup>1</sup>, Lucile Mangin-Thro<sup>6</sup>, Yiming Qiu<sup>7</sup>, Paul Attfield<sup>4</sup>, Stephen D. Wilson<sup>2</sup>, Christopher Stock<sup>4</sup>, Haidong Zhou<sup>8</sup>, Alannah Hallas<sup>5</sup>, Eun Sang Choi<sup>9</sup> and Minseong Lee<sup>10</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>University of California, Santa Barbara, United States; <sup>3</sup>University of Winnipeg, Canada; <sup>4</sup>University of Edinburgh, United Kingdom; <sup>5</sup>University of British Columbia, Canada; <sup>6</sup>ILL, France; <sup>7</sup>National Institute of Standards and Technology, United States; <sup>8</sup>The University of Tennessee, Knoxville, United States; <sup>9</sup>National High Magnetic Field Laboratory, United States; <sup>10</sup>Los Alamos National Laboratory, United States

## Soft Matter

SESSION C2.04: Grafted Polymers and Nanocomposites  
Session Chair: John Riley  
Tuesday Morning, June 7, 2022  
UMC Conference Room 235

10:15 AM \*C2.04.01

**Molecular Bottlebrushes: Scattering Measurements and Simulations** Michael J. Hore and Raj Mukkamala; Case Western Reserve University, United States

10:45 AM C2.04.02

**Vanadium Ion Dynamics of Ionomer Nanocomposites** Xueting Wang<sup>1</sup>, Apoorva Balwani<sup>1</sup>, Mayura S. Silva<sup>1</sup>, Madhusudan Tyagi<sup>2</sup>, Stephen Creager<sup>1</sup> and Eric M. Davis<sup>1</sup>; <sup>1</sup>Clemson University, United States; <sup>2</sup>National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR), United States

11:00 AM C2.04.03

**Dynamically Tunable Structural Color from Micrometer-domains** Yuyin Xi<sup>1,2</sup> and Yun Liu<sup>1,2</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Delaware, United States

11:15 AM C2.04.04

**The Microscopic Structure and Dynamics of PEO-Silica Nanocomposite: Effect of Nanoparticle Size on Short-Time Polymer Dynamics** [Jihyuk Kim](#)<sup>1</sup>, Antonio Faraone<sup>2</sup>, Orsolya Czakkel<sup>3</sup>, Michael Ohl<sup>4</sup>, Stephan Forster<sup>4</sup> and Norman Wagner<sup>1</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>Institut Laue-Langevin, France; <sup>4</sup>Research Center Juelich GmbH, Germany

11:30 AM C2.04.05

**The Impact of Graft Type on the Assembly of Nanoscale Organic Hybrid Materials in Solution using Small Angle Neutron Scattering** [Md Ashraful Haque](#)<sup>1</sup>, Tony G. Feric<sup>2</sup>, Sara T. Hamilton<sup>2</sup>, Ah-Hyung Park<sup>2</sup> and Mark Dadmun<sup>1,3</sup>; <sup>1</sup>University of Tennessee, Knoxville, United States; <sup>2</sup>Columbia University, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

11:45 AM C2.04.06

**Study of Interdiffusion of Bilayer Polymer Grafted Nanoparticle Films at Interfaces by Neutron Reflectivity** Wenjie Wu<sup>1</sup>, Kshitij Sharma<sup>1</sup>, John F. Ankner<sup>2</sup>, Jack Douglas<sup>3</sup> and [Alamgir Karim](#)<sup>1</sup>; <sup>1</sup>University of Houston, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>National Institute of Standards and Technology, United States

12:00 PM C2.04.07

**A New Computational Method (CREASE) to Analyze and Interpret Small Angle Scattering Profiles from Assembled Structure in Polymer Solutions** [Zijie Wu](#) and Arthi Jayaraman; University of Delaware, United States

12:15 PM C2.04.08

**SESANS and SANS Studies to Understand the Presence of an Initial Opaque Phase in the Self-Assembly of Di-Block Copolymers** [Antonia Denkova](#); Delft University of Technology, Netherlands

## Emerging Applications of Neutron Scattering in Engineering, Arts and Sciences

SESSION H2.01: Emerging ML Applications—Neutrons and Beyond  
Session Chairs: Tyler Martin and Alan Tennant  
Tuesday Morning, June 7, 2022  
UMC Aspen Room 285, 287, 289

10:15 AM \*H2.01.01

**Machine Learning: A Data-Driven Spectrometer for Neutron Scattering** [Mingda Li](#); Massachusetts Institute of Technology, United States

10:45 AM \*H2.01.02

**Accelerate Discovery of New Chemical Synthesis Pathways using Autonomous Experiments Combined with AI Agents** [Kristin Schmidt](#), Dmitry Zubarev, Sarath swaminathan, Renato Fontoura de Gusmao Cerqueira, Nathaniel Park, Tim Erdmann, Daniel Sanders and Jed Pitera; IBM Research, United States

11:15 AM \*H2.01.03

**Autonomous Control at X-Ray Sources from Accelerator to Detector** [Daniel Ratner](#); SLAC, United States

## Soft Matter

SESSION C2.05: Surfactants and Emulsions  
Session Chair: John Riley  
Tuesday Afternoon, June 7, 2022  
UMC Conference Room 235

1:45 PM \*C2.05.01

**Using Neutrons to Probe the Structure of PFAS Surfactant Micelles** [Marina Tsianou](#); University at Buffalo, The State University of New York, United States

2:15 PM C2.05.02

**Controllable Nanostructures via a Bicellar Template – Characterized by Contrast-Variation SANS** [Chung-Hao Liu](#) and Mu-Ping Nieh; University of Connecticut, United States

2:30 PM C2.05.03

**Chemical and Physical Control on the Nanostructures of Ionic Amphiphilic Oligomer Assemblies: Elucidated by Spectroscopy and Neutron Reflectivity** [Zening Liu](#), Hanyu Wang, Tianyu Li, Lu Lin, John Katsaras, Kunlun Hong, Jim Browning, Benjamin Doughty and Charles P. Collier; Oak Ridge National Laboratory, United States

2:45 PM C2.05.04

**Self-Association in Pluronic®-Cationic Surfactant Mixed System: A Scattering and Molecular Dynamics Approach** [Ketan C. Kuperkar](#)<sup>1</sup>, German Perez-Sanchez<sup>2</sup> and Pratap Bahadur<sup>1</sup>; <sup>1</sup>Veer Narmad South Gujarat University (VNSGU), Surat, India; <sup>2</sup>Campus Universitario de Santiago, Portugal

3:00 PM C2.05.05

**Variation of Bicontinuous Microemulsion Surface Structures on Hydrophilic and Amphiphilic Substrates** [Luke Heroux](#)<sup>1,2</sup>, Adam Imel<sup>2</sup>, Brian Barth<sup>2</sup>, Thomas Zawodzinski<sup>2</sup> and Mark Dadmun<sup>2,1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States

3:15 PM C2.05.06

**Measuring Co-surfactant Demixing Across Internal Nanodroplet Interfaces by SANS** [Tanvi Sheth](#), Nairiti Sinha and Matthew Helgeson; University of California, Santa Barbara, United States

## Hard Condensed Matter

SESSION B2.05: Spin Glass and Complex Magnetic Structures  
Session Chair: Martin Mourigal  
Tuesday Afternoon, June 7, 2022  
UMC East Ballroom 212

2:00 PM B2.05.01

**Highly Tunable Magnetic Phases in Transition Metal Dichalcogenide Fe<sub>1/3+δ</sub>NbS<sub>2</sub>** [Shan Wu](#)<sup>1,2</sup>, Zhijun Xu<sup>3</sup>, Shannon Haley<sup>2,1</sup>, Sophie Weber<sup>2,1</sup>, Eran Maniv<sup>2,1</sup>, Yiming Qiu<sup>3</sup>, Adam Aczel<sup>4</sup>, Jeffrey Neaton<sup>2,1</sup>, James Analytis<sup>1,2</sup> and Robert Birgeneau<sup>1,2</sup>; <sup>1</sup>University of California, Berkeley, United States; <sup>2</sup>Lawrence Berkeley National Laboratory, United States; <sup>3</sup>NIST Center for Neutron Research, United States; <sup>4</sup>Oak Ridge National Laboratory, United States



2:30 PM B2.05.02

**Inelastic Neutron Scattering Study of the Anisotropic Spin Glass Fe<sub>2</sub>TiO<sub>5</sub>** Yu Li<sup>1</sup>, P. G. LaBarre<sup>2</sup>, Daniel M. Pajerowski<sup>3</sup>, A. P. Ramirez<sup>2</sup>, Stephan Rosenkranz<sup>1</sup> and Daniel Phelan<sup>1</sup>; <sup>1</sup>Argonne National Laboratory, United States; <sup>2</sup>Univ. California Santa Cruz, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

2:45 PM B2.05.03

**Freezing of a Disorder Induced Spin Liquid with Strong Quantum Fluctuations** Xiao Hu<sup>1</sup>, Daniel M. Pajerowski<sup>2</sup>, Depei Zhang<sup>2</sup>, Andrey Podlesnyak<sup>2</sup>, Yiming Qiu<sup>3</sup>, Qing Huang<sup>4</sup>, Haidong Zhou<sup>4</sup>, Israel Klich<sup>1</sup>, Alexander I. Kolesnikov<sup>2</sup>, Matthew Stone<sup>2</sup> and Seung-Hun Lee<sup>1</sup>; <sup>1</sup>University of Virginia, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>National Institute of Standards and Technology, United States; <sup>4</sup>The University of Tennessee, Knoxville, United States

3:00 PM B2.05.05

**Competing Magnetic Ground States of NaCo<sub>2</sub>(SeO<sub>3</sub>)<sub>2</sub>(OH): A New Sawtooth Structure with Co<sup>2+</sup> S = 3/2** Duminda Sanjeeva<sup>1</sup>, Ovidiu Garlea<sup>2</sup> and Keith Taddei<sup>2</sup>; <sup>1</sup>University of Missouri, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

## Neutron Physics

SESSION G2.02: Neutron Physics II  
Session Chair: Leah Broussard  
Tuesday Afternoon, June 7, 2022  
UMC Aspen Room 285, 287, 289

2:00 PM \*G2.02.01

**Fundamentals of Entangled Neutron Beams** Gerardo Ortiz<sup>1,2</sup>; <sup>1</sup>Indiana University, United States; <sup>2</sup>Indiana University Quantum Science and Engineering Center, United States

2:30 PM G2.02.02

**How Entangled Neutron Beams Unveil Chiral Spin Orders** Abu Ashik Md Irfan and Gerardo Ortiz; Indiana University, United States

2:45 PM G2.02.03

**Spin-textured Neutron Beams and Orbital Angular Momentum** Sam McKay<sup>1,1,1</sup>, Quan Le Thien<sup>1,1</sup>, Fankang Li<sup>2</sup>, Abu Irfan<sup>1,1</sup>, Jiazhou Shen<sup>1,1,1</sup>, Eric B. Dees<sup>1,1,1</sup>, Stephen J. Kuhn<sup>1,1,1</sup>, David V. Baxter<sup>1,1,1</sup>, Gerardo Ortiz<sup>1,1</sup> and Roger Pynn<sup>1,1,1</sup>; <sup>1</sup>Indiana University, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

3:00 PM G2.02.04

**New Determination of the <sup>3</sup>He Neutron Incoherent Scattering Length Δb'** Earl Babcock; Juelich Centre for Neutron Science, Germany

## Emerging Applications of Neutron Scattering in Engineering, Arts and Sciences

SESSION H2.02: Emerging ML Applications—Diffraction to Dynamics

Session Chair: Alan Tennant  
Tuesday Afternoon, June 7, 2022  
UMC West Ballroom 208

2:00 PM H2.02.01

**Using AI to Determine Space Group from Neutron Powder Diffraction Data** William Ratcliff<sup>1,2</sup>, Haotong Liang<sup>2</sup>, Aaron G. Kusne<sup>1,2</sup> and Ichiro Takeuchi<sup>2</sup>; <sup>1</sup>NIST, United States; <sup>2</sup>University of Maryland, United States

2:15 PM H2.02.02

**Super-resolution Dispersions Measured by Direct Geometry Spectrometers** Jiao Lin<sup>1</sup>, Gabriele Sala<sup>1</sup>, Matthew Stone<sup>2</sup> and Andrew D. Christianson<sup>2</sup>; <sup>1</sup>Oak Ridge National Lab, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

2:30 PM H2.02.03

**A Method for Determining Mid-Range Order in Semi-Crystalline Materials using Inelastic Neutron Scattering and Density Functional Theory** Makena Dettmann<sup>1</sup>, Lucas S. Cavalcante<sup>1</sup>, John Anthony<sup>2</sup> and Adam Moule<sup>1</sup>; <sup>1</sup>University of California, Davis, United States; <sup>2</sup>University of Kentucky, United States

2:45 PM H2.02.04

**Machine Learning for Sample Alignment in Neutron Scattering Experiments** Abdourahmane Diaw<sup>1</sup>, Kevin Bruhwiler<sup>1</sup>, Chris Hall<sup>1</sup>, Jonathan Edelen<sup>1</sup>, Stuart Calder<sup>2</sup> and Christina Hoffmann<sup>2</sup>; <sup>1</sup>RadiaSoft LLC, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

3:00 PM H2.02.05

**Autonomous Discovery of the Magnetic Order Parameter with ANDIE, the Autonomous Neutron Diffraction Explorer** Austin McDannald<sup>1</sup>, Matthias D. Frontzek<sup>2</sup>, Andrei T. Savici<sup>2</sup>, Mathieu Doucet<sup>2</sup>, Efrain E. Rodriguez<sup>3,4</sup>, Kate Meuse<sup>5</sup>, Jessica Opsahl-Ong<sup>6</sup>, Daniel Samarov<sup>1</sup>, Ichiro Takeuchi<sup>3,4</sup>, William Ratcliff<sup>1,3</sup> and Aaron G. Kusne<sup>1,3</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>University of Maryland, United States; <sup>4</sup>Maryland Quantum Materials Center, United States; <sup>5</sup>Cornell University, United States; <sup>6</sup>Rice University, United States

3:15 PM H2.02.06

**Modeling Multi-Crystalline and Amorphous INS Spectra: Simulation Methods, Accuracy, and Expence** Makena Dettmann<sup>1</sup>, Lucas S. Cavalcante<sup>1</sup>, Daniel Vong<sup>1</sup>, Nir Goldman<sup>2</sup> and Adam Moule<sup>1</sup>; <sup>1</sup>UC Davis, United States; <sup>2</sup>Lawrence Livermore National Laboratory, United States

# WEDNESDAY ORAL PRESENTATIONS

\* Invited Paper

## Plenary and Prize Session

SESSION I3.01: Plenary and Prize Session  
Session Chairs: Peter Gehring, Young Lee, Katie Weigandt and  
Stephen Wilson  
Wednesday Morning, June 8, 2022  
UMC Conference Room 235

**8:30 AM \*I3.01.01**  
**SUSTAINED RESEARCH PRIZE WINNER: Neutrons, Biological Membranes, and Future Directions** John Katsaras; Oak Ridge National Laboratory, United States

**9:10 AM \*I3.01.02**  
**PLENARY: Neutron Scattering from Exotic Magnetic Ground States** Bruce D. Gaulin; McMaster University, Canada

**9:45 AM BREAK**

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A3.06: Instrumentation: Soft Matter and Imaging  
Session Chair: John Barker  
Wednesday Morning, June 8, 2022  
UMC West Ballroom 208

**10:15 AM \*A3.06.01**  
**Performance Upgrades to the BT-2 Neutron Imaging Facility** Jacob M. LaManna<sup>1</sup>, Michael Cyrus Daugherty<sup>1,2</sup>, Youngju Kim<sup>1,2</sup>, Eli Baltic<sup>1</sup>, Daniel S. Hussey<sup>1</sup> and David Jacobson<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States

**10:45 AM A3.06.02**  
**INFER: Dark-field Tomography of Hierarchical Structures** Daniel S. Hussey<sup>1</sup>, Caitlyn M. Wolf<sup>1</sup>, Youngju Kim<sup>2</sup>, Sarah M. Robinson<sup>1</sup>, Michael Cyrus Daugherty<sup>2</sup>, Ryan P. Murphy<sup>1</sup>, Paul A. Kienzle<sup>1</sup>, Nikolai N. Klimov<sup>1</sup>, Michael G. Huber<sup>1</sup>, Peter N. Bajcsy<sup>1</sup>, David Jacobson<sup>1</sup>, Jacob M. LaManna<sup>1</sup> and Katie M. Weigandt<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States

**11:00 AM A3.06.03**  
**Upgrade of the Neutron Spin Echo Spectrometer at the NIST Center for Neutron Research** Antonio Faraone<sup>1</sup>, Norman Wagner<sup>2</sup>, Michihiro Nagao<sup>1,3,2</sup>, Christoph Brocker<sup>1,3</sup>, Nicholas C. Maliszewskyj<sup>1</sup>, Michael Monkenbusch<sup>4</sup>, Olaf Holderer<sup>4</sup>, Tadeusz Kozielski<sup>4</sup> and Dan A. Neumann<sup>1</sup>; <sup>1</sup>NIST Center for Neutron Research, United States; <sup>2</sup>University of Delaware, United States; <sup>3</sup>University of Maryland, United States; <sup>4</sup>Jülich Centre for Neutron Science, Germany

**11:15 AM A3.06.04**

**The Quite Intense Kinetics Reflectometer (QIKR) at the Spallation Neutron Source (SNS) Second Target Station (STS)** John F. Ankner, Danielle Wilson, Rudy Thermer, Scott Dixon and Zeke Salazar; Oak Ridge National Laboratory, United States

**11:30 AM A3.06.05**

**Recent Advances at the Cold Neutron Imaging Instrument at High Flux Isotope Reactor** Yuxuan Zhang<sup>1</sup>, Hassina Z. Bilheux<sup>1</sup>, Erik Stringfellow<sup>1</sup>, Jean Bilheux<sup>1</sup>, Jonathan Smith<sup>1</sup>, Les Butler<sup>2</sup>, Kyungmin Ham<sup>2</sup>, Wieslaw Stryjewski<sup>2</sup> and Michael Vincent<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Louisiana State University, United States

**11:45 AM A3.06.06**

**Angle-encoding Radiography with Neutrons** Sam McKay<sup>1,1,1</sup>, Fankang Li<sup>2</sup>, David V. Baxter<sup>1,1,1</sup> and Roger Pynn<sup>1,1,1</sup>; <sup>1</sup>Indiana University, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

**12:00 PM A3.06.07**

**Dynamic Microfluidic Modulation of Neutrons and x-rays** Ryan P. Murphy, Sarah M. Robinson, Jacob M. LaManna, Caitlyn M. Wolf, Youngju Kim, Michael Cyrus Daugherty, Michael G. Huber, Peter N. Bajcsy, David Jacobson, Paul A. Kienzle, Katie M. Weigandt, Daniel S. Hussey and Nikolai N. Klimov; National Institute of Standards and Technology, United States

**12:15 PM A3.06.08**

**The VENUS iMaging Beamline Construction Project at the Spallation Neutron Source** Hassina Z. Bilheux, Tommy Thomasson, Aaron Hanks, Amy Byrd, Amy Jones, Harley Skorpenske, Erik Stringfellow, Bill McHargue, Irina Popova, Franz X. Gallmeier, Jean Bilheux, Ryan Mangus, Scott Keener and George Rennich; Oak Ridge National Laboratory, United States

## Hard Condensed Matter

SESSION B3.06: Phonons and Lattice Dynamics  
Session Chair: Dmitry Reznik  
Wednesday Morning, June 8, 2022  
UMC East Ballroom 212

**10:15 AM B3.06.01**

**Inelastic Neutron Scattering Measurements of New Spectral Features from Nonlinear Phonon Interactions** Brent Fultz<sup>1</sup>, Yang Shen<sup>1</sup>, Claire N. Saunders<sup>1</sup>, Camille Bernal<sup>1</sup>, Michael E. Manley<sup>2</sup> and Vladimir Ladygin<sup>1</sup>; <sup>1</sup>California Institute of Technology, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

**10:30 AM B3.06.02**

**Structural Fluctuations, Complex Ground-States and Strongly Anharmonic Phonons in Metal Halide Perovskites** Olivier Delaire<sup>1</sup>, Xing He<sup>1</sup>, Tyson L. Lanigan-Atkins<sup>1</sup>, Matthew Krogstad<sup>2</sup>, Mayanak K. Gupta<sup>1</sup>, Chengjie Mao<sup>1</sup>, Daniel M. Pajerowski<sup>3</sup>, Douglas L. Abernathy<sup>3</sup>, Feng Ye<sup>3</sup>, Tao Hong<sup>3</sup>, Songxue Chi<sup>3</sup>, Yaohua Liu<sup>3</sup>, Guangyong Xu<sup>4</sup>, Zhijun Xu<sup>4</sup>, Stephan Rosenkranz<sup>2</sup> and Raymond Osborn<sup>2</sup>; <sup>1</sup>Duke University, United States; <sup>2</sup>Argonne National Laboratory, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>National Institute of Standards and Technology, United States

**10:45 AM B3.06.03**

**Mutual Spin-Phonon Driving Effects and Phonon Eigenvector Renormalization in NiO** Qiyang Sun<sup>1</sup>, Bin Wei<sup>1,2</sup>, Yaokun Su<sup>1</sup>, Hillary Smith<sup>3</sup>, Jiao Lin<sup>4</sup>, Douglas L. Abernathy<sup>4</sup> and Chen Li<sup>1,1</sup>; <sup>1</sup>University of California, Riverside, United States; <sup>2</sup>Henan Key Laboratory of Materials on Deep-Earth Engineering, School of Materials Science and Engineering, China; <sup>3</sup>Swarthmore College, United States; <sup>4</sup>Oak Ridge National Laboratory, United States

**11:00 AM B3.06.04**

**Role of Anharmonicity in the High-temperature Thermodynamics of Chromium** Camille Bernal<sup>1</sup>, Hillary Smith<sup>2</sup>, Claire N. Saunders<sup>1</sup>, Dennis S. Kim<sup>3</sup>, Douglas L. Abernathy<sup>4</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology, United States; <sup>2</sup>Swarthmore College, United States; <sup>3</sup>Massachusetts Institute of Technology, United States; <sup>4</sup>Oak Ridge National Laboratory, United States

**11:15 AM B3.06.05**

**Flattening of the Acoustic Phonon Branches in the Clathrate Ba<sub>8</sub>Ga<sub>16</sub>Ge<sub>30</sub>** Susmita Roy<sup>1</sup>, Tyler C. Sterling<sup>1</sup>, Dan Parshall<sup>1</sup>, Eric Toberer<sup>2</sup>, Mogens Christensen<sup>3</sup>, Devashibhai T. Adroja<sup>4</sup> and Dmitry Reznik<sup>1,5</sup>; <sup>1</sup>UNIVERSITY OF COLORADO BOULDER, United States; <sup>2</sup>Colorado School of Mines, United States; <sup>3</sup>University of Aarhus, Denmark; <sup>4</sup>ISIS Facility, STFC, Rutherford Appleton Laboratory, United Kingdom; <sup>5</sup>Center for Experiments on Quantum Materials, University of Colorado Boulder, United States

**11:30 AM B3.06.06**

**Atomic Tunneling in BaTiS<sub>3</sub>** Raphael P. Hermann, Michael E. Manley, Duncan H. Moseley, Daniel M. Pajeroski, Barry Winn and Eugene Mamontov; Oak Ridge National Laboratory, United States

**11:45 AM B3.06.07**

**Investigation of the Thermophysical Properties of Cuprite by Inelastic Neutron Scattering and Machine Learning Calculations** Claire N. Saunders<sup>1</sup>, Vladimir Ladygin<sup>1</sup>, Dennis S. Kim<sup>1</sup>, Olle Hellman<sup>2</sup>, Hillary Smith<sup>3</sup>, Camille Bernal<sup>1</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology, United States; <sup>2</sup>Linköping University, Sweden; <sup>3</sup>Swarthmore College, United States

**12:00 PM B3.06.08**

**Phason Dominated Thermal Transport in Fresnoite** Michael E. Manley<sup>1</sup>, Andrew May<sup>1</sup>, Barry Winn<sup>1</sup>, Douglas L. Abernathy<sup>1</sup>, Raffi Sahul<sup>2</sup> and Raphael P. Hermann<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Amphenol Corporation, United States

## Biology, Biophysics and Biotechnology

SESSION D3.02: Insights into Lipid Membrane Properties and Protein-Lipid Interactions

Session Chairs: Roisin Donnelly and Nairiti Sinha  
Wednesday Morning, June 8, 2022  
UMC Conference Room 235

**10:15 AM \*D3.02.01**

**The Orientation of KRAS at the Plasma Membrane Helps Recruit RAF Kinase** Andrew Stephen; Frederick National Laboratory for Cancer Research, United States

**10:45 AM D3.02.02**

**Characterization of Structurally Disordered Peripheral Membrane Proteins with Neutron Reflectometry** Frank Heinrich<sup>1,2</sup>; <sup>1</sup>Carnegie Mellon University, United States; <sup>2</sup>National Institute of Standards and Technology, United States

**11:00 AM D3.02.04**

**The Transmembrane Helix of pHLIP Slows Down Membrane Thickness Fluctuations and Translational Diffusion** Haden L. Scott<sup>1</sup>, Violeta Burns-Casamayor<sup>2</sup>, Andrew Dixon<sup>3</sup>, Robert Standaert<sup>4</sup>, Christopher B. Stanley<sup>1</sup>, Laura Stingaciu<sup>1</sup>, Jan Michael Carrillo<sup>1</sup>, Bobby G. Sumpter<sup>1</sup>, John Katsaras<sup>1</sup>, Wei Qiang<sup>5</sup>, Frederick Heberle<sup>3</sup>, Blake Mertz<sup>2</sup>, Rana Ashkar<sup>6</sup> and Francisco Barrera<sup>3</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>West Virginia University, United States; <sup>3</sup>The University of Tennessee, Knoxville, United States; <sup>4</sup>East Tennessee State University, United States; <sup>5</sup>Binghamton University, The State University of New York, United States; <sup>6</sup>Virginia Tech, United States

**11:15 AM D3.02.05**

**Relationship between Viscosity and Acyl Tail Dynamics in Lipid Bilayers** Michihiro Nagao<sup>1,2,3</sup>, Elizabeth Kelley<sup>1</sup>, Antonio Faraone<sup>1</sup>, Makina Saito<sup>4</sup>, Yoshitaka Yoda<sup>5</sup>, Masayuki Kurokuzu<sup>6</sup>, Shinichi Takata<sup>7</sup>, Makoto Seto<sup>6</sup> and Paul D. Butler<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States; <sup>3</sup>University of Delaware, United States; <sup>4</sup>Tohoku University, Japan; <sup>5</sup>Japan Synchrotron Radiation Research Institute, Japan; <sup>6</sup>Kyoto University, Japan; <sup>7</sup>J-PARC, Japan

**11:30 AM D3.02.06**

**The Structural Origins of Lipid Bilayer Dynamic Response** James E. Fitzgerald<sup>1</sup>, Elizabeth Kelley<sup>2</sup>, Norman Wagner<sup>1</sup>, Michihiro Nagao<sup>2</sup> and Edward Lyman<sup>1,1</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>National Institute of Standards and Technology, United States

**11:45 AM D3.02.07**

**Determination of Sphingomyelin Molecular Structure using SANS, SAXS, NMR, and Molecular Dynamics** Jacob J. Kinnun<sup>1,1</sup>, Milka Doktorova<sup>2</sup>, Norbert Kučerka<sup>3,4</sup>, Jianjun Pan<sup>5</sup>, Drew Marquardt<sup>6</sup>, Haden L. Scott<sup>1,1</sup>, Richard Venable<sup>7</sup>, Richard Pastor<sup>7</sup>, Stephen Wassall<sup>8</sup>, Frederick Heberle<sup>9</sup> and John Katsaras<sup>1,9,1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>University of Texas Health Science Center, United States; <sup>3</sup>Joint Institute for Nuclear Research, Russian Federation; <sup>4</sup>Comenius University, Slovakia; <sup>5</sup>University of South Florida, United States; <sup>6</sup>University of Windsor, Canada; <sup>7</sup>National Institutes of Health, United States; <sup>8</sup>Indiana University-Purdue University Indianapolis, United States; <sup>9</sup>University of Tennessee, United States

**12:00 PM D3.02.08**

**Structural Studies of mRNA Vaccines using Combined SANS/SAXS and CryoEM** Thomas E. Cleveland<sup>1,2</sup>, Manuel Carrasco<sup>3</sup>, Lacey Wright<sup>3</sup> and Michael Buschmann<sup>3</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States; <sup>3</sup>George Mason University, United States

## Materials Chemistry and Energy

SESSION E3.02: Materials Chemistry and Energy II

Session Chair: Graeme Luke  
Wednesday Morning, June 8, 2022  
UMC Aspen Room 285, 287, 289

**10:15 AM \*E3.01.01**

**Search for Broken Symmetries in Kagome Lattice Superconductor CsV<sub>3</sub>Sb<sub>5</sub>** Graeme Luke<sup>1,2</sup>, Jonah Gautreau<sup>1</sup>, Sudarshan Sharma<sup>1</sup>, Mathew Pula<sup>1</sup>, Yasutomo Uemura<sup>3</sup>, Stephen D. Wilson<sup>4</sup>, Brenden Ortiz<sup>4</sup> and Yuzki Oey<sup>4</sup>; <sup>1</sup>McMaster University, Canada; <sup>2</sup>TRIUMF, Canada; <sup>3</sup>Columbia University, United States; <sup>4</sup>University of California, Santa Barbara, United States

**10:45 AM E3.01.02**

**Phonon Dynamics and Thermal Transport in Ti<sub>3</sub>VSe<sub>4</sub>** Yoel F. Lencina Wendt<sup>1</sup>, Qingan Cai<sup>1</sup>, Brian Sales<sup>2</sup>, Ayman Said<sup>3</sup> and Chen Li<sup>2,1,1</sup>; <sup>1</sup>University of California, Riverside, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>Argonne National Laboratory, United States

**11:00 AM E3.01.03**

**High Throughput Operando Neutron Diffraction at the Nanoscale Ordered Materials Diffractometer (NOMAD)** Jue Liu, Zhijia Du, Xianyang Wu and Michelle Everett; Oak Ridge National Laboratory, United States

11:15 AM E3.01.04

**In Situ Observation of Dynamic Electrode-Electrolyte Interfaces under Li-Mediated Electrochemical N<sub>2</sub> Reduction Conditions** Sarah J. Blair<sup>1,2</sup>, Mathieu Doucet<sup>3</sup>, Jim Browning<sup>3</sup>, Adam C. Nielander<sup>2</sup>, Alessandro Gallo<sup>2</sup> and Thomas F. Jaramillo<sup>1,2</sup>; <sup>1</sup>Stanford University, United States; <sup>2</sup>SLAC National Accelerator Laboratory, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

11:30 AM E3.01.05

**Lithium-Polymer Batteries—A Microscopic View!** Michael Ohl<sup>1,2</sup>, Juergen Allgaier<sup>1</sup>, Marcella Cabrera-Berg<sup>1</sup>, Changwoo Do<sup>3</sup>, Yuya Doi<sup>4</sup>, Rene Halver<sup>1</sup>, Eugene Mamontov<sup>3</sup>, Ridhima Nain<sup>3</sup>, Naresh C. Osti<sup>3</sup>, Godehard Sutmann<sup>1,6</sup>, Hui Wang<sup>7</sup>, Stephan Forster<sup>1</sup> and Takeshi Egami<sup>3,2</sup>; <sup>1</sup>Forschungszentrum Jülich GmbH, Germany; <sup>2</sup>Univ. Tennessee, United States; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>Nagoya University, Japan; <sup>5</sup>Indian Institute of Technology Delhi, India; <sup>6</sup>Ruhr-University Bochum, Germany; <sup>7</sup>Stanford Linear Accelerator Center, United States

11:45 AM E3.01.06

**Tuning Chemical Short-Range Order in Complex High-Entropy Oxides** Katharine Page<sup>1,2</sup>, Xin Wang<sup>1</sup> and Bo Jiang<sup>2</sup>; <sup>1</sup>The University of Tennessee, Knoxville, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A3.07: Instrumentation: Sample Environment  
Session Chair: Sergiy Gladchenko  
Wednesday Afternoon, June 8, 2022  
UMC West Ballroom 208

2:00 PM \*A3.07.01

**Advances in High-Pressure Neutron Scattering at Oak Ridge National Laboratory** Mary-Ellen Donnelly; Oak Ridge National Laboratory, United States

2:30 PM A3.07.02

**A Pre-Conceptual Design of a 20 – 25 T Vertical-Field Split Magnet for Neutron Scattering** Mark Bird<sup>1</sup>, Scott Bole<sup>1</sup>, Ken Herwig<sup>2</sup>, Dylan Kolb-Bond<sup>1</sup> and Jack Toth<sup>1</sup>; <sup>1</sup>NHMFL - FSU, United States; <sup>2</sup>ORNL, United States

2:45 PM A3.07.03

**RheoSurfR – Neutron Reflectivity-Rheology Sample Environment for Studying Soft Matter, Biology, and Materials Processing at Air-Liquid and Liquid-Liquid Interfaces** Benjamin R. Thompson<sup>1</sup>, Mason Keresty<sup>2</sup>, Hannah Nevel<sup>2</sup>, Richard Dombrowski<sup>2</sup> and Norman Wagner<sup>1,2</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>STF Technologies LLC, United States

3:00 PM A3.07.04

**4D Rheo-SANS: A Novel Sample Environment for Measuring Structure-Property Relationships in Soft Matter and Biological Materials** Nathan Alexander<sup>1</sup>, Jonathan Kopf<sup>2</sup>, Benjamin R. Thompson<sup>1</sup>, Richard Dombrowski<sup>2</sup> and Norman Wagner<sup>1,2</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>STF Technologies LLC, United States

3:15 PM A3.07.05

**Rapid and Controllable Cooling of High-Temperature Neutron Furnace** Yue Xiao<sup>1</sup>, Chien-Hua Chen<sup>1</sup>, Patryk Radyjowski<sup>1</sup>, Max Demydovych<sup>1</sup>, Chad Burkholder<sup>1</sup> and Rebecca A. Mills<sup>2</sup>; <sup>1</sup>Advanced Cooling Technologies, Inc, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

## Hard Condensed Matter

SESSION B3.07: Orbital Physics and Beyond Dipolar Magnetism  
Session Chair: Benjamin Ueland  
Wednesday Afternoon, June 8, 2022  
UMC East Ballroom 212

2:00 PM B3.07.01

**Anisotropic Spin Wave Excitations in a Multiferroic BiFeO<sub>3</sub>** Masaaki Matsuda<sup>1</sup>, Depei Zhang<sup>1</sup>, Sachith Dissanayake<sup>1</sup>, Barry Winn<sup>1</sup>, Toshimitsu Ito<sup>2</sup> and Randy Fishman<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>AIST, Japan

2:15 PM B3.07.02

**Magnetism and Symmetry Lowering in the 5d<sup>1</sup> Double Perovskite Ba<sub>2</sub>NaOsO<sub>6</sub> Probed with Polarized Neutron Diffraction and Total Scattering** Stuart Calder, Yan Wu, Jue Liu and Jiaqiang Yan; Oak Ridge National Laboratory, United States

2:30 PM B3.07.03

**Dual Orbital Degeneracy Lifting in a Strongly Correlated Electron System** Emil Bozin<sup>1</sup>, Robert J. Koch<sup>1</sup>, Ryan Sinclair<sup>2</sup>, Marshall McDonnell<sup>3</sup>, Runze Yu<sup>1</sup>, Milinda Abeykoon<sup>1</sup>, Simon Billinge<sup>1</sup>, Alexei Tsvelik<sup>1</sup>, Matthew Tucker<sup>3</sup>, Haidong Zhou<sup>2</sup> and Weiguo Yin<sup>1</sup>; <sup>1</sup>Brookhaven National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

2:45 PM B3.07.04

**Lattice and Magnetic Dynamics in YVO<sub>3</sub> Mott Insulator Studied by Neutron Scattering and First-Principles Calculations** Yu Tao<sup>1</sup>, Douglas L. Abernathy<sup>2</sup>, Tianran Chen<sup>3</sup>, Taner Yildirim<sup>3,4</sup>, Jiaqiang Yan<sup>2,5</sup>, Jianshi Zhou<sup>6</sup>, John Goodenough<sup>6</sup> and Despina Louca<sup>1</sup>; <sup>1</sup>University of Virginia, United States; <sup>2</sup>Oak Ridge National Laboratory, United States; <sup>3</sup>National Institute of Standards and Technology, United States; <sup>4</sup>University of Pennsylvania, United States; <sup>5</sup>The University of Tennessee, Knoxville, United States; <sup>6</sup>The University of Texas at Austin, United States

3:00 PM B3.07.05

**The Detection of Magneto-Electric Multipoles with Spherical Neutron Polarimetry: CuO and LiMnPO<sub>4</sub>** Jian Rui Soh<sup>1,2</sup>, Andrea Urru<sup>3</sup>, Paola Forino<sup>1</sup>, Rasmus Toft-Petersen<sup>2</sup>, NICOLA SPALDIN<sup>3</sup> and Henrik M. Ronnow<sup>1</sup>; <sup>1</sup>EPFL, Switzerland; <sup>2</sup>Technical University of Denmark, Denmark; <sup>3</sup>ETH Zurich, Switzerland

## Soft Matter

SESSION C3.06: Bio-Inspired Soft Matter  
Session Chair: Javen Weston  
Wednesday Afternoon, June 8, 2022  
UMC Conference Room 235

2:00 PM \*C3.06.01

**Understanding and Controlling the Solution Self-Assembly of Amphiphilic Polypeptoid Block Copolymers** Donghui Zhang; Louisiana State University, United States

### 2:30 PM C3.06.02

**Phase Morphology of Amorphous Solid Dispersions using Small-Angle Neutron Scattering and Neutron Interferometry** Caitlyn M. Wolf<sup>1</sup>, Youngju Kim<sup>2,1</sup>, Sarah M. Robinson<sup>1</sup>, Michael Cyrus Daugherty<sup>2,1</sup>, Ryan P. Murphy<sup>1</sup>, Nikolai N. Klimov<sup>1</sup>, Michael G. Huber<sup>1</sup>, Peter N. Bajcsy<sup>1</sup>, David Jacobson<sup>1</sup>, Jacob M. LaManna<sup>1</sup>, Paul A. Kienzle<sup>1</sup>, Daniel S. Hussey<sup>1</sup> and Katie M. Weigandt<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States

### 2:45 PM C3.06.03

**Microstructures of Starch Granules as Revealed by Scattering Techniques** Yimin Mao<sup>1,2</sup> and Yong-Cheng Shi<sup>3</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>University of Maryland, United States; <sup>3</sup>Kansas State University, United States

### 3:00 PM C3.06.04

**Glucose Induced Self-Assembly and Phase Separation in Hydrophilic Triblock Copolymer Solution and its Governing Mechanism** Divya K. Patel<sup>1</sup>, Ketan C. Kuperkar<sup>1</sup> and Pratap Bahadur<sup>2</sup>; <sup>1</sup>Sardar Vallabhbhai National Institute of Technology (SVNIT), India; <sup>2</sup>Veer Narmad South Gujarat University (VNSGU), India

### 3:15 PM C3.06.05

**Diffusion Coefficients of Anisotropic Particles Measured by NSE: A Case Study Using Monoclonal Antibody** Yanqin Zhai<sup>1</sup>, Nicos Martys<sup>2</sup>, William L. George<sup>2</sup>, Joseph E. Curtis<sup>2</sup>, Jannatun Nayem<sup>3</sup>, Yang Zhang<sup>1</sup> and Yun Liu<sup>2,3</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>University of Delaware, United States

### 3:30 PM C3.06.06

**Understanding the Microscopic Mechanism Behind the Dielectric Relaxation in Water using Inelastic Neutron Scattering** Yadu Krishnan Sarathchandran<sup>1</sup>, Yuya Shinohara<sup>2</sup>, Wojciech Dmowski<sup>1</sup>, Eugene Mamontov<sup>2</sup>, Daniel M. Pajerowski<sup>2</sup> and Takeshi Egami<sup>1,2</sup>; <sup>1</sup>University of Tennessee, Knoxville, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

## Structural Materials and Engineering

SESSION F3.02: Using Neutrons for Large Scale Engineering Applications  
Session Chair: Jeffrey Bunn  
Wednesday Afternoon, June 8, 2022  
UMC Aspen Room 285, 287, 289

### 2:00 PM \*F1.02.01

**Application of Neutron Diffraction for Industrial Materials & Manufacturing Development** Shenyang Huang; GE Research, United States

### 2:30 PM F1.02.02

**Effects of Mechanical Deformation on Dislocation Density, Phase Separation and Hydrogen Diffusion in Pipeline Steel** Zachary Buck<sup>1</sup>, Matthew Connolly<sup>1</sup>, May Martin<sup>1</sup>, Damian Lauria<sup>1</sup>, Peter Bradley<sup>1</sup>, Andrew Slifka<sup>1</sup>, Ke An<sup>2</sup>, Yan Chen<sup>2</sup> and Naresh C. Osti<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

### 2:45 PM F1.02.03

**Damage Modes in Hydrogen-Assisted Fatigue Probed by Neutron and X-Ray Scattering** Matthew Connolly<sup>1</sup>, Zack Buck<sup>1</sup>, May Martin<sup>1</sup>, Robert Amaro<sup>2</sup>, Peter Bradley<sup>1</sup>, Damian Lauria<sup>1</sup>, Jun-Sang Park<sup>3</sup> and Andrew Slifka<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>AMTT, United States; <sup>3</sup>Argonne National Laboratory, United States

### 3:00 PM F1.02.04

**Elevated Temperature Dislocation Density Reductions in Cold-Worked ASTM A586 High-Strength Steel Wire** Jumari A. Robinson, Adrian Brugger and Raimondo Betti; Columbia University, United States

## Biology, Biophysics and Biotechnology

SESSION D3.03: New Tools and Methods for Biological Scattering Experiments  
Session Chairs: Rachel Ford and Jacob Kinnun  
Wednesday Afternoon, June 8, 2022  
UMC Conference Room 235

### 3:45 PM D3.03.01

**Time-Resolved In-Situ Reaction SANS Study Details Structural Changes to Noncellulosic Biopolymer in Switchgrass Plant Cell Wall** Sai Venkatesh Pingali<sup>1</sup>, Zhi Yang<sup>2</sup>, Marcus Foston<sup>3</sup>, Hugh O'Neill<sup>1</sup>, Volker S. Urban<sup>1</sup>, Arthur Ragauskas<sup>4</sup>, Barbara Evans<sup>1</sup> and Brian Davison<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Massey University, New Zealand; <sup>3</sup>Washington University in St. Louis, United States; <sup>4</sup>The University of Tennessee, Knoxville, United States

### 4:00 PM D3.03.02

**Developing DENSS for Neutron Contrast Variation Data -- DENSS Multiple** Shuo Qian; Oak Ridge National Laboratory, United States

### 4:15 PM D3.03.03

**Structure-Based Calculation of Biomolecular Neutron Scattering Contrast Match Points with Explicit Deuteration** Alan Hicks<sup>1</sup>, Paul Abraham<sup>1</sup>, Qiu Zhang<sup>1</sup>, Jeremy Smith<sup>2,1</sup>, Hugh O'Neill<sup>1</sup> and Loukas Petridis<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States

### 4:30 PM D3.03.04

**Applying New Models to Describe Biomembrane Structure and Solvent Partitioning in Living Cell Membranes and Membrane Mimics** Luoxi Tan<sup>1</sup>, Nicholas Smith<sup>2,3</sup>, Haden L. Scott<sup>3</sup>, John Katsaras<sup>3</sup>, Sai Venkatesh Pingali<sup>3</sup>, Jeremy Smith<sup>2,3</sup>, Brian Davison<sup>3</sup>, James Elkins<sup>3</sup> and Jonathan Nickels<sup>1</sup>; <sup>1</sup>University of Cincinnati, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

### 4:45 PM D3.03.05

**Low-Background Neutron Reflectometry Measurement Strategies for Solid/Liquid Interfaces** David P. Hoogerheide<sup>1</sup>, Joe Dura<sup>1</sup>, Frank Heinrich<sup>1,2</sup>, Brian Maranville<sup>1</sup>, Paul A. Kienzle<sup>1</sup> and Charles F. Majkrzak<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, United States; <sup>2</sup>Carnegie Mellon University, United States

## Materials Chemistry and Energy

SESSION E3.03: Materials Chemistry and Energy III  
Wednesday Afternoon, June 8, 2022  
UMC Aspen Room 285, 287, 289

### 3:45 PM E3.02.01

**The Symmetry Relationship Between Magnetic Order and Toroidal Moments in  $\text{LiM}_2\text{Mn}_{1-x}\text{PO}_4$  ( $M = \text{Co}, \text{Fe}$ )** Stephanie Gnewuch and Efrain E. Rodriguez; University of Maryland, United States

#### 4:00 PM E3.02.02

**Electronic Conduction Induced Dendrite Formation in Solid Electrolytes** Fudong Han; Rensselaer Polytechnic Institute, United States

#### 4:15 PM E3.02.03

**Raising the Transition Temperature of Olivines  $\text{Li}_{1-x}\text{Fe}_x\text{Mn}_1-x\text{PO}_4$  Through Selective Li-Deintercalation** Timothy J. Diethrich and Efrain E. Rodriguez; University of Maryland, College Park, United States

#### 4:30 PM E3.02.04

**Van Hove Correlation Function of Magnesium Chloride Molten Salt** Yuya Shinohara<sup>1</sup>, Alexander S. Ivanov<sup>1</sup>, Garrett E. Granroth<sup>1</sup>, Douglas L. Abernathy<sup>1</sup> and Takeshi Egami<sup>2,1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>The University of Tennessee, Knoxville, United States

#### 4:45 PM E3.02.05

**Mapping the Light Elements in Complex Oxides for High-rate Lithium-ion Batteries** Kent Griffith and Kenneth R. Poeppelmeier; Northwestern University, United States

#### 5:00 PM \*E3.02.06

**Exploring Oxygen Motion Through Perovskites  $\text{La}_{0.9}\text{Sr}_{0.1}\text{Co}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$  with In Situ Diffraction** Allyson M. Fry-Petit<sup>1</sup>, Mara Milhander<sup>1,2</sup> and Jose Gonzalez Jimenez<sup>1,2</sup>; <sup>1</sup>California State University, Fullerton, United States; <sup>2</sup>Rutgers, The State University of New Jersey, United States

## Hard Condensed Matter

SESSION B3.08: Unconventional Superconductors and Related Materials

Session Chair: Shan Wu  
Wednesday Afternoon, June 8, 2022  
UMC East Ballroom 212

#### 4:00 PM \*B3.08.01

**Carrier Tuning of Stoner Ferromagnetism in  $\text{Ca}(\text{Co}_{1-x}\text{Fe}_x)_2\text{As}_2$**  Benjamin G. Ueland<sup>1,2</sup>, Santanu Pakhira<sup>1,2</sup>, Bing Li<sup>1,2</sup>, Aashish Sapkota<sup>1,2</sup>, N. S. Sangeetha<sup>1</sup>, Toby G. Perring<sup>3</sup>, Yongbin Lee<sup>1</sup>, Liqin Ke<sup>1</sup>, D. C. Johnston<sup>1,2</sup> and R. J. McQueeney<sup>1,2</sup>; <sup>1</sup>Ames Laboratory, United States; <sup>2</sup>Iowa State University of Science and Technology, United States; <sup>3</sup>STFC Rutherford Appleton Laboratory, United Kingdom

#### 4:30 PM B3.08.02

**Understanding Charge Density Wave superlattice structure and potential Quantum Spin Liquid behavior in 1T-TaS<sub>2</sub> and 1T-TaSe** Sharon S. Philip and Despina Louca; University of Virginia, United States

#### 4:45 PM B3.08.03

**Structural Correlations in the Hole-Doped Cuprate  $\text{HgBa}_2\text{CuO}_{4+\delta}$**  Zachary W. Anderson<sup>1</sup>, Damjan Pele<sup>2</sup>, Matthew Krogstad<sup>3</sup>, Nikolaos Biniskos<sup>4</sup>, Biqiong Yu<sup>1</sup>, Yaohua Liu<sup>5</sup>, Liam Thompson<sup>1</sup>, Jack Zwettler<sup>1</sup>, Richard Spieker<sup>1</sup>, Nina G. Bielinski<sup>1</sup>, Feng Ye<sup>5</sup>, Stephan Rosenkranz<sup>3</sup>, Raymond Osborn<sup>3</sup> and Martin Greven<sup>1</sup>; <sup>1</sup>University of Minnesota, United States; <sup>2</sup>University of Zagreb, Croatia; <sup>3</sup>Argonne National Laboratory, United States; <sup>4</sup>Forschungszentrum Jülich GmbH, Germany; <sup>5</sup>Oak Ridge National Laboratory, United States

#### 5:00 PM B3.08.04

**Magnetic Fluctuations in Superconducting and Non-Superconducting 11 Iron Chalcogenides** Igor Zaliznyak<sup>1</sup>, Yangmu Li<sup>2,1</sup>, Ovidiu Garlea<sup>3</sup>, Andrei T. Savici<sup>3</sup>, Zhijun Xu<sup>4,1</sup>, Gu Genda<sup>1</sup> and John Tranquada<sup>1</sup>; <sup>1</sup>Brookhaven National Laboratory, United States; <sup>2</sup>Institute of Physics, China; <sup>3</sup>Oak Ridge National Laboratory, United States; <sup>4</sup>National Institute of Standards and Technology, United States

#### 5:15 PM B3.08.05

**Nematic Correlation Length in Iron-Based Superconductors Probed by Inelastic X-Ray Scattering** Dmitry Reznik; University of Colorado-Boulder, United States

## Emerging Applications of Neutron Scattering in Engineering, Arts and Sciences

SESSION H3.03: Emerging ML Applications—Soft Matter and Chemistry

Session Chair: Tyler Martin  
Wednesday Afternoon, June 8, 2022  
UMC West Ballroom 208

#### 4:00 PM H3.03.01

**Machine Learning for Neutron Reflectometry** Mathieu Doucet, William Heller and Richard Archibald; Oak Ridge National Laboratory, United States

#### 4:15 PM H3.03.02

**Davis Computational Spectroscopy workflow - from structure to spectra** Lucas Samir Ramalho Cavalcante, Makena Dettmann, Ambarish Kulkarni and Adam Moule; UC Davis, Brazil

#### 4:30 PM H3.03.03

**Machine Learning-Enabled Inverse Analysis of Small Angle Scattering Data** Graham W. Roberts, Mu-Ping Nieh, Anson Ma and Qian Yang; University of Connecticut, United States

#### 4:45 PM H3.03.04

**Machine Learning Augmented Computational Reverse-Engineering Analysis for Scattering Experiments of Assembled Mixtures of Nanoparticles** Christian Heil and Arthi Jayaraman; University of Delaware, United States

#### 5:00 PM H3.03.05

**Designing an Active Learning Agent for Autonomous Small-Angle Scattering** Tyler B. Martin, Aaron G. Kusne, Austin McDannald and Peter A. Beaucage; National Institute of Standards and Technology, United States

# THURSDAY ORAL PRESENTATIONS

\* Invited Paper

## Plenary and Prize Session

SESSION I4.01: Plenary and Prize Session  
Session Chairs: Peter Gehring, Young Lee, Katie Weigandt and  
Stephen Wilson  
Thursday Morning, June 9, 2022  
UMC Conference Room 235

8:15 AM \*I4.01.01

**OUTSTANDING STUDENT RESEARCH PRIZE WINNER:**  
**Magnetic Phase Transitions and Spin-Wave Dynamics in  $Y_{1-x}La_xTiO_3$  and  $Y_{1-x}Ca_xTiO_3$**  Sajna Hameed; University of Minnesota  
Twin Cities, United States

9:10 AM \*I4.01.02

**PLEANARY: Neutrons for Clean Bioenergy** Jeremy Smith;  
University of Tennessee/Oak Ridge National Laboratory, United States

9:40 AM POSTER AWARD ANNOUNCEMENT

9:45 AM BREAK

## Advances in Neutron Facilities, Instrumentation and Software

SESSION A4.09: Neutron Devices and Ancillary Equipment  
Session Chairs: Mary-ellen Donnelly and Fankang Li  
Thursday Morning, June 9, 2022  
UMC West Ballroom 208

10:15 AM \*A4.09.01

**Status of the Second Target Station Project** Ken Herwig; Oak Ridge  
National Laboratory, United States

10:45 AM A4.09.02

**Correcting Divergent Beam Aberrations in a Neutron Resonance  
Spin Echo (NRSE) instrument** Stephen J. Kuhn<sup>1</sup>, Sam McKay<sup>1</sup>,  
Fankang Li<sup>2</sup>, Eric B. Dees<sup>1</sup>, Jiazhou Shen<sup>1</sup> and Roger Pynn<sup>1,2</sup>; <sup>1</sup>Indiana  
University Bloomington, United States; <sup>2</sup>Oak Ridge National  
Laboratory, United States

11:00 AM A4.09.04

**The Strange Invisibility of Cold Neutrons in Highly Neutron  
Absorbing B4C—Towards a Novel Family of Neutron Optics** Malik  
Maaza<sup>1,2</sup>; <sup>1</sup>University of South Africa, South Africa; <sup>2</sup>iThemba LABS-  
National Research Foundation of South Africa, South Africa

11:15 AM A4.09.05

**Development of an Enhanced Solid-State Neutron Detector** Hank  
Thurston<sup>1,2,3</sup> and Elias Garratt<sup>1,1</sup>; <sup>1</sup>Michigan State University, United  
States; <sup>2</sup>Hillsdale College, United States; <sup>3</sup>Trinary Capital, LLC, United  
States

11:30 AM A4.09.06

**A Superconducting Device for Widening the Effective Angle in  
Quasi-Elastic Spin-Echo Neutron Scattering Experiments** Eric B.  
Dees<sup>1</sup>, Robert Dalglish<sup>2</sup>, Steven R. Parnell<sup>3</sup>, Stephen J. Kuhn<sup>1</sup>,  
Fankang Li<sup>4</sup>, Sam McKay<sup>1</sup>, Jiazhou Shen<sup>1</sup> and Roger Pynn<sup>1,4</sup>; <sup>1</sup>Indiana  
University, United States; <sup>2</sup>Rutherford Appleton Lab, United  
Kingdom; <sup>3</sup>TU Delft, Netherlands; <sup>4</sup>Oak Ridge National Laboratory,  
United States

11:45 AM A4.09.07

**Low Temperature Goniometer for Neutron Research.** Sergiy  
Gladchenko; National Institute of Standards and Technology, United  
States

12:00 PM A4.09.09

**High Resolution Larmor Diffraction at Oak Ridge National  
Laboratory** Kaleb Burrage<sup>1</sup>, Masaaki Matsuda<sup>1</sup>, Jaime A. Fernandez-  
Baca<sup>1</sup>, Chengjie Mao<sup>2</sup>, Olivier Delaire<sup>2</sup> and Fankang Li<sup>1</sup>; <sup>1</sup>Oak Ridge  
National Laboratory, United States; <sup>2</sup>Duke University, United States

12:15 PM A4.09.10

**In-Situ <sup>3</sup>He polarization for JCNS instrumentation** Earl Babcock;  
Juelich Centre for Neutron Science, Germany

## Hard Condensed Matter

SESSION B4.10: Spin Textures and Helimagnets  
Session Chair: Andrew Christianson  
Thursday Morning, June 9, 2022  
UMC East Ballroom 212

10:15 AM \*B4.10.01

**Skyrmion Lattice Manipulation with Electric and Thermal  
Currents** Morten R. Eskildsen; University of Notre Dame, United  
States

10:45 AM B4.10.02

**Neutron Diffraction Study of Complex Helical Magnetic Ordering  
in Ni-doped  $EuCo_2As_2$  Single Crystals** Tianxiong Han<sup>1,2</sup>, Simon X.  
Riberolles<sup>1</sup>, Benjamin G. Ueland<sup>1</sup>, R. J. McQueeney<sup>1,2</sup>, Yan Wu<sup>3</sup>,  
Santanu Pakhira<sup>1</sup> and D. C. Johnston<sup>1,2</sup>; <sup>1</sup>Ames Laboratory, United  
States; <sup>2</sup>Iowa State University of Science and Technology, United  
States; <sup>3</sup>Oak Ridge National Laboratory, United States

11:00 AM B4.10.03

**Three-Dimensional Neutron Tomography of a Bulk Skyrmion  
Lattice** Melissa E. Henderson<sup>1</sup>, Benjamin Heacock<sup>2</sup>, Markus Bleuel<sup>2</sup>,  
Colin Heikes<sup>2</sup>, Michael G. Huber<sup>2</sup>, Jeff Krzywon<sup>2</sup>, Olivier Nahman-  
Levesque<sup>1</sup>, Mathew Pula<sup>3</sup>, Dusan Sarenac<sup>1</sup>, Kirill Zhernenkov<sup>4</sup>, David  
Cory<sup>1</sup> and Dmitry Pushin<sup>1</sup>; <sup>1</sup>Institute for Quantum Computing,  
University of Waterloo, Canada; <sup>2</sup>NIST Center for Neutron Research,  
United States; <sup>3</sup>McMaster University, Canada; <sup>4</sup>Julich Centre for  
Neutron Science, Germany

11:15 AM B4.10.05

**Novel Magnetic Structures in  $M1/3TaS_2$**  Junjie Yang and Yunpeng  
Gao; New Jersey Institute of Technology, United States

### 11:30 AM B4.10.06

**Field-Tunable Toroidal Moment in a Chiral-Lattice Magnet** Huibo Cao<sup>1</sup>, Lei Ding<sup>1</sup>, Xianghan Xu<sup>2</sup>, Harald Jeschke<sup>3</sup>, Xiaojian Bai<sup>1</sup>, Erxi Feng<sup>1</sup>, Admasu Alemayehu<sup>2</sup>, Jaewook Kim<sup>2</sup>, Feiting Huang<sup>2</sup>, Qiang Zhang<sup>1</sup>, Xiabin Ding<sup>4</sup>, Neil Harrison<sup>4</sup>, Vivian Zapf<sup>4</sup>, Daniel Khomskii<sup>5</sup>, Igor Mazin<sup>6</sup> and Sang-Wook Cheong<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>Rutgers University, United States; <sup>3</sup>Okayama University, Japan; <sup>4</sup>Los Alamos National Laboratory, United States; <sup>5</sup>II. Physikalisches Institut, Universität zu Köln, Germany; <sup>6</sup>George Mason University, United States

### 11:45 AM B4.10.07

**Slow Relaxation with Signature of Glassiness in Non-Centrosymmetric Helimagnet** ScFeGe Sunil K. Karna<sup>1</sup>, John F. DiTusa<sup>2</sup>, David Young<sup>3</sup>, Wei Tian<sup>4</sup> and Adam Aczel<sup>4</sup>; <sup>1</sup>Norfolk State University, United States; <sup>2</sup>Indiana University-Purdue University Indianapolis, United States; <sup>3</sup>Louisiana State University, United States; <sup>4</sup>Oak Ridge National Laboratory, United States

### 12:00 PM B4.10.09

**Depth Profiles of Hybrid Magnetic Skyrmions Determined by Neutron Scattering** WLNC Liyanage<sup>1</sup>, Nan Tang<sup>1</sup>, Elizabeth Quigley<sup>1,2</sup>, Sergio Montoya<sup>3</sup>, Julie A. Borchers<sup>4</sup>, Alexander Grutter<sup>4</sup>, Sunil Sinha<sup>3</sup>, Brian Maranville<sup>4</sup>, Eric Fullerton<sup>3</sup>, Lisa DeBeer-Schmitt<sup>5</sup> and Dustin A. Gilbert<sup>1,1</sup>; <sup>1</sup>The University of Tennessee, Knoxville, United States; <sup>2</sup>Purdue, United States; <sup>3</sup>University of California, San Diego, United States; <sup>4</sup>National Institute of Standards and Technology, United States; <sup>5</sup>Oak Ridge National Laboratory, United States

### 12:15 PM B4.10.10

**Revisiting Static and Dynamic Magnetic Correlations in the Chiral Helimagnet** Cr1/3NbS2 Lisa DeBeer-Schmitt<sup>1</sup>, Lazar Kish<sup>2</sup>, Adam Aczel<sup>1</sup>, Travis J. Williams<sup>1</sup>, Huibo Cao<sup>1</sup>, Timothy Charlton<sup>1</sup>, Nirmal Ghimire<sup>3</sup>, Jacob Ruff<sup>4</sup>, Michael A. McGuire<sup>5</sup>, Stephen J. Kuhn<sup>6</sup>, Morten R. Eskildsen<sup>7</sup> and David Mandrus<sup>8</sup>; <sup>1</sup>ORNL, United States; <sup>2</sup>University of Illinois at Urbana-Champaign, United States; <sup>3</sup>George Mason University, United States; <sup>4</sup>Cornell University, United States; <sup>5</sup>Oak Ridge National Laboratory, United States; <sup>6</sup>Indiana University-Bloomington, United States; <sup>7</sup>University of Notre Dame, United States; <sup>8</sup>The University of Tennessee, Knoxville, United States

## Soft Matter

SESSION C4.07: Nanoparticles, Methods, and General Soft Matter  
Session Chair: Javen Weston  
Thursday Morning, June 9, 2022  
UMC Conference Room 235

### 10:15 AM \*C4.07.01

**Frustrated Coulombic and Cation Size Effects on Nanoscale Boehmite Aggregation: A Tumbler Small- and Ultra-Small-Angle Neutron Scattering Study** Lawrence M. Anovitz<sup>1</sup>, Patricia Huestis<sup>2</sup>, Nikhil Rampal<sup>1</sup>, Andrew G. Stack<sup>1</sup>, Jay A. LaVerne<sup>2</sup>, Xin Zhang<sup>3</sup>, Geregory K. Schenter<sup>3</sup>, Jaehun Chun<sup>3</sup>, Benjamin A. Legg<sup>3</sup>, Lili Liu<sup>3</sup>, Markus Bleuel<sup>4</sup>, Cedric Gagnon<sup>4</sup> and David F. Mildner<sup>4</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>University of Notre Dame, United States; <sup>3</sup>Physical Sciences Division, United States; <sup>4</sup>National Institute of Standards and Technology, United States

### 10:45 AM C4.07.02

**Investigating the Oxidation of Atmospheric Aerosols using Neutron Reflectometry** Rebecca Welbourn<sup>1</sup> and Martin King<sup>2</sup>; <sup>1</sup>ISIS Neutron & Muon Source, United Kingdom; <sup>2</sup>Royal Holloway University of London, United Kingdom

### 11:00 AM C4.07.03

**How Much Crosslinking Causes a Polymer Chain to Become a Nanoparticle?** Jacob Fischer<sup>1</sup>, Lu Han<sup>2</sup>, Tomonori Saito<sup>2</sup> and Mark Dadmun<sup>1,2</sup>; <sup>1</sup>The University of Tennessee, United States; <sup>2</sup>Oak Ridge National Laboratory, United States

### 11:15 AM C4.07.04

**Molecular Deformation and Relaxation Dynamics of Ionomers Revealed by Complementary Small-Angle Scattering Techniques** Christopher N. Lam, Wei-Ren Chen and Yangyang Wang; Oak Ridge National Laboratory, United States

### 11:30 AM C4.07.05

**Rapid Automated Morphology Identification and Parameter Determination from Small Angle Scattering Data via Machine Learning** Graham W. Roberts, Mu-Ping Nieh, Anson Ma and Qian Yang; University of Connecticut, United States

### 11:45 AM C4.07.06

**Automated SANS/SAXS Exploration of Soft Materials with the Autonomous Formulation Laboratory** Peter A. Beaucage and Tyler B. Martin; National Institute of Standards and Technology, United States

### 12:00 PM C4.07.07

**Measurement of Time-Resolved Adsorption Profiles in PMMA-Methanol System with Neutron Imaging** Martin Wissink<sup>1</sup>, Michael Kass<sup>1</sup>, Charles E. Finney<sup>1</sup>, Jacob M. LaManna<sup>2</sup>, David Jacobson<sup>2</sup> and Hassina Z. Bilheux<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, United States; <sup>2</sup>National Institute of Standards and Technology, United States

### 12:15 PM C4.07.08

**Studying Morphology Transitions on Sequential Annealing of Lamellar Block Copolymer Thin Films via Neutron Reflectivity** Kshiti Sharma<sup>1</sup>, Maninderjeet Singh<sup>1</sup>, Sushil K. Satija<sup>2</sup>, John F. Ankner<sup>3</sup>, Jack Douglas<sup>2</sup> and Alamgir Karim<sup>1</sup>; <sup>1</sup>University of Houston, United States; <sup>2</sup>National Institute of Standards and Technology, United States; <sup>3</sup>Oak Ridge National Laboratory, United States

### 12:30 PM C4.07.09

**Thermodynamic Interactions in Polydiene/Polyolefin Blends** Megan L. Robertson, Jialin Qiu and Ramanan Krishnamoorti; University of Houston, United States

### 12:45 PM C4.07.10

**Specific Salt Effects on Equilibrium and Flow Structure of Wormlike Micelles** Javen S. Weston<sup>1</sup>, Nour Alawami<sup>1</sup> and Katie M. Weigandt<sup>2</sup>; <sup>1</sup>The University of Tulsa, United States; <sup>2</sup>National Institute of Standards and Technology, United States