# LILIN HE

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#### **EDUCATION**

- Ph.D. Polymer Physics, Clemson University, August, 2008
- M. S. Physical Chemistry, Institute of Chemistry, Chinese Academy of Sciences, July, 2001
- B.S. Environmental Science, Southwest University, China, July, 1998

#### **PROFESSIONAL EXPERIENCE**

Neutron Scattering Scientist	General Purpose Small Angle Neutron Scattering	(GP-SANS),Oak
	Ridge National Laboratory	2012-Present
Postdoctoral Research Associate	Oak Ridge National Laboratory	2008-2012

#### **RESEARCH INTERESTS**

- Applications of neutron and X-ray scattering techniques including small-angle scattering and reflectometry in understanding the structure and dynamics of polymer solutions, blends and gels;
- Structure-property relationships of innovative materials for supercapacitors, batteries and fuel cells;
- Behaviors of small molecules confined in porous media for carbon dioxide sequestration and hydrogen storage;
- Structure and dynamics of biological systems under near physiological conditions; interactions of DNA and protein within complexes and conformational changes in response to stimuli.

#### GRANTS

PI: Mid-Scale Level Investment proposal "A Controlled Atmosphere Heating/Freezing Stage for the GP-SANS" 2020 (\$26,741)

PI: Mid-Scale Level Investment proposal "An in situ high pressure cell for simultaneous SANS and Raman measurements" 2018 (\$120,000)

PI: Laboratory Directed Research and Development (LDRD) funding of the Oak Ridge National Laboratory, 2017-2019. *"Taking N^2 to N: Developing a Highly Efficient, Multiscale Modeling Framework for Hierarchical Materials"* (\$712,600)

Co-PI: Seed Money Fund of the Oak Ridge National Laboratory LDRD program, 2012-2013. "Detection and characterization of meso- and nanoscopic bubbles on the patterned and native metal surfaces using small-angle neutron scattering and reflectivity techniques" PI: Dr. Yuri B. Melnichenko (\$190,000)

Co-PI: Seed Money Fund of the Oak Ridge National Laboratory LDRD program, 2014-2015. "Developing Hydroxide Fuel Cells Based on Novel Polymers with Improved Stability and Higher Ionic Conductivity" PI: Dr. Xiaoguang Sun (\$190,000) Co-PI: Laboratory Directed Research and Development (LDRD) fund of the Oak Ridge National Laboratory, "*Designing polymers with excessive free volume for enhanced molecular and ion transport*" PI: Dr. Vera Bocharova (\$2,720,000)

Co-PI: Laboratory Directed Research and Development (LDRD) fund of the Oak Ridge National Laboratory, "Developing Hydroxide Fuel Cells Based on Novel Polymers with Improved Stability and Higher Ionic Conductivity" PI: Dr. Tomonori Saito (\$800,000)

# HONORS & AWARDS

- 2013 Dal Swaine Award by the Society for Organic Petrology
- 2012 Travel Award for the 2012 Symposium/Workshop "Carbons for Energy Applications" Organized by the American Carbon Society with support from Elsevier
- 2010 Best Poster Award for Laboratory Directed R&D projects, ORNL
- 1998 Graduation with honors, the top 3% students of a graduating class receives at Southwest University, China

# **RESEARCH EXPERIENCE**

# 1. In situ characterization of structure and dynamics of small molecules and ions under confinement

- Ion transport in electrodes made of carbonaceous materials and Metal-Organic Frameworks
- Microstructure of coals, shale and phase behaviors of greenhouse gases confined in the geological materials
- Phase behaviors of hydrogen confined in carbon nanopores
- 2. Solution structures of biological materials
  - Protein solution structure characterization using contrast variation small angle neutron scattering
- 3. Structure and transport characteristics of polymers

# PROFESSIONAL ACTIVITIES

### 1. Session Chair and Review Committee:

- Coordinator of Soft Matter and Polymers Initiative, Neutron Scattering Division, ORNL
- Coordinator of Large Scale Structures group (now section) seminar
- Organized and chaired the session (2019 American Crystallographic Association annual conference): Morphological Characterization of porous Materials
- Review committee of APS SAXS proposals, 2016- present
- Selected Secretary 2016-2017, Small Angle Scattering SIG, American Crystallographic Association
- Selected session chair (2016 American Physical Society March Meeting): Polymer Dynamics -Insight from In-Situ Scattering
- Selected session chair (2012 American Conference on Neutron Scattering): Polymers and Films
- Selected session chair (2013 American Physical Society March Meeting): Charged and Ion Containing Polymers
- Co-organize and co-chair session of Scattering and Energy Storage Materials, ACA 2014, Albuquerque, NM

### 2. Referee of Peer Reviewed Journals:

- Soft Matter (Published by Royal Society of Chemistry, U.K.)
- Journal of Physical Chemistry Letters (Published by American Chemical Society, U.S.)
- Journal of Physics and Chemistry of Solids (Published by Elsevier Group, U.S.A. and Netherlands)

- Langmuir (Published by American Chemical Society, U.S.)
- Microporous and Mesoporous Materials (Published by Elsevier Group, U.S.A. and Netherlands)
- Journal of Applied Crystallography (Published by International Union of Crystallography, U.K.)
- Current Nanoscience
- European Polymer Journal
- Fibers and Polymers
- Industrial & Engineering Chemistry Research
- Journal of Materials Chemistry
- Macromolecular Chemistry & Physics
- Nanoscience & Nanotechnology
- Polymer International
- Carbon
- Proposals for beam time on the neutron scattering instruments at the NIST Center for Neutron Research
- Technical reviewer of ORNL publication tracking system
- Fuel
- Technical reviewer for the proposals submitted to NIST NCNR neutron source and APS Xray source

# 3. Workshop/Summer School:

- Organizing committee: the Workshop "SANS for geology", ORNL June, 2010.
- National Summer School on Neutron and X-ray Scattering, sponsored by Argonne National Lab and ORNL of U.S. Department of Energy
- Panel member, 3<sup>rd</sup> Annual Neutron Scattering for Novices Workshop, responsible for discussing experimental capabilities using ORNL SANS instruments for structural characterization (June 17-18, 2013)
- Organzing Committee, International Workshop "Structure and Dynamics of Confined and interfacial Fluids: Blending Scattering, Spectroscopy and Computer Modeling Techniques", July 16-18, 2014, Oak Ridge, Tennessee, US.
- Mantid Scientific Steering committee

# 4. Member of Professional Organization:

- Member, American Physics Society
- Member, Neutron Scattering Society of America

### WORKSHOPS

- 2003 National Summer School on Neutron and X-ray Scattering, sponsored by Argonne National Lab and Department of Energy, Chicago, USA, Certificate
- 2009 Workshop on Neutron Spin Echo Spectroscopy, ORNL, TN
- 2010 Workshop on the characterization of porous materials sponsored by Porous Materials Inc, Ithaca, NY. Certificate
- 2010 Workshop on Neutron & Catalysis, ORNL, TN
- 2010 Workshop on Solar Energy and Energy Storage, ORNL, TN
- 2011 Workshop on the Rheo-Neutron Scattering, Anton-Paar, ORNL, TN

# PEER REVIEWED PUBLICATIONS

1. Y. Yao et al. "A Unified User-Friendly Instrument Control and Data Acquisition System for the ORNL SANS Instrument Suite" (Accpeted in *Applied Sciences*)

- S Xie, B Zhang, Y Mao, L He, K Hong, FS Bates, TP Lodge "Influence of Added Salt on Chain Conformations in Poly (ethylene oxide) Melts: SANS Analysis with Complications" *Macromolecules* 53, 7141-7149, 2020.
- 3. Y Ma, Y Wu, JG Lee, **L He**, G Rother, AL Fameau, WA Shelton, B Bharti, "Adsorption of fatty acid molecules on amine functionalized silica nanoparticles: Surface organization and foam stability" *Langmuir*, 36, 3703-3712, 2020.
- L He, L Yang, M Dinca, R Zhang, J Li, "Observation of Ion Electrosorption in Metal Organic Framework Micropores with in operando Small - Angle Neutron Scattering" *Angewandte Chemie*, 132, 9860-9866, (2020)
  - ORNL Neutrons 2020 Top 10 scientific achievements
- 5. R Zhang, S Liu, **L He**, TP Blach, Y Wang "Characterizing anisotropic pore structure and its impact on gas storage and transport in coalbed methane and shale gas reservoirs" *Energy and Fuels*, 34, 3161-3172, (2020)
- 6. Rui Zhang, Xiaoxing Wang, Shimin Liu Lilin He, Chunshan Song, Xiao Jiang, Tomasz P. Blach "Discover inherent characteristics of polyethylenimine-functionalized porous materials for CO2 capture" *ACS Applied Materials & Interfaces*. 11, 36515-36524 (2019).
  - ORNL Neutrons 2019 Top 10 scientific achievements
- Wang J., Chen W., Nagao M., Shelat P., Hammer B.A., Tietjen G.T., Cao K.D., Henderson J.M., He L., Lin ., Akgun B., Meron M., Qian S., Ward S., Marks J.D., Emrick T., Lee K.Y., "Tailoring Biomimetic Phosphorylcholine-Containing Block Copolymers as Membrane-Targeting Cellular Rescue Agents", *Biomacromolecules* 20, 9, 3385-3391 (2019)
- 8. Wu Y., Ma Y., He L., Rother G., Shelton W.A., Bharti B., "Directed Pore-Uptake and Phase Separation of Surfactant Solutions Under Confinement", Journal of Physical Chemistry C, 123, 15, 9957-9966 (2019).
- 9. Genix A.C., Bocharova V., Carroll B., Lehmann M.L., Saito T., Krueger S., He L., Dieudonne-George P., Sokolov A.P., Oberdisse J., "Understanding the Static Interfacial Polymer Layer by Exploring the Dispersion States of Nanocomposites", ACS Applied Materials & Interfaces, 11, 17863-17872 (2019).
- L. He, C. Li, W. A. Hamilton, T. Hong, X. Tong, B. L. Winn, L. Crow, K. Bailey and N. C. Gallego. "Anomalous neutron scatteringhalo'observed in highly oriented pyrolytic graphite" Journal of Applied Crystallography 2019, 52 (2).
- 11. Abdoulaye Djirea, Priyank Pande, Aniruddha Deb, Jason B.Siegel, Olabode T. Ajenifujah, Lilin He, Alice E.Sleightholme, Paul G.Rasmussen, Levi T.Thompsonace "Unveiling the pseudocapacitive charge storage mechanisms of nanostructured vanadium nitrides using in-situ analyses" Nano Energy 2019, 60, 72-81.
- 12. Guijie Sang, Shimin Liu, Rui Zhang, Derek Elsworth, Lilin He, "Nanopore characterization of mine roof shales by SANS, nitrogen adsorption, and mercury intrusion: Impact on water adsorption/retention behavior" International Journal of Coal Geology 2018, 200, 173-185.

- Yang Wang, Yong Qin, Rui Zhang, Lilin He, Lawrence M. Anovitz, Markus Bleuel, David F. R. Mildner, Shimin Liu, and Yanming Zhu. "Evaluation of Nanoscale Accessible Pore Structures for Improved Prediction of Gas Production Potential in Chinese Marine Shales" Energy & Fuels 2018, 32 (12), 12447-12461.
- Abdoulaye Djire, Jason B.Siegel, Olabode Ajenifujah, Lilin He, Levi T.Thompson "Pseudocapacitive storage via micropores in high-surface area molybdenum nitrides" Nano Energy 51, 122-127.
- Nicolas Jouault, Sanat K Kumar, Robert J Smalley, Changzai Chi, Robert Moneta, Barbara Wood, Holly Salerno, Yuri B Melnichenko, Lilin He, William E Guise, Boualem Hammouda, Michael K Crawford, Do Very Small POSS Nanoparticles Perturb s-PMMA Chain Conformations? Macromolecules, 51, 14, 5278–5293 (2018).
- 16. Djire, A., Siegel J.B., Ajenifujah O., **He L.**, Thompson L.T. Pseudocapacitive storage via micropores in high-surface area molybdenum nitrides Nano Energy 51, 122-127 (2018).
- 17. Heuser B.J., Lin J.L., Do C., **He L**. Small-angle neutron scattering measurements of δ-phase deuteride (hydride) precipitates in Zircaloy 4 Journal of Applied Crystallography, 51, 3, (2018).
- Heller W.T., Cuneo M.J., Debeer-Schmitt L.M., Do C., He L., Heroux L., Littrell K.C., Pingali S.V., Qian S., Stanley C.B., Urban V.S., Wu B., Bras W., The suite of small-angle neutron scattering instruments at Oak Ridge National Laboratory Journal of Applied Crystallography, 51, 2, 1-7 (2018).
- 19. Emilian Popov, Lilin He, Elvis Dominguez-Ontiveros, and Yuri Melnichenko "Detection of vapor nanobubbles by small angle neutron scattering (SANS)" Applied Physics Letters (2018).
- 20. Chen K., Wu B., **He L.**, Smith G.S., Do C., Huang G.R., Zhang G., Wang Y., Strain heterogeneity in sheared colloids revealed by neutron scattering Physical Chemistry Chemical Physics, 20, 9, 6050-6054 (2018).
- 21. Aaron Alford, Veronika Kozlovskaya, Bing Xue, Nirzari Gupta, William Higgins, Dana Pham-Hua, Lilin He, Volker S. Urban, Hubert M. Tse, and Eugenia Kharlampieva, Manganoporphyrin-Polyphenol Multilayer Capsules as Radical and Reactive Oxygen Species (ROS) Scavengers Chem. Mater. (2018)
- 22. Yuan X., **He L.**, Singh S., Simmons B., Cheng G., Effect of ionic liquid pretreatment on the porosity of pine wood: insights from small angle neutron scattering, nitrogen adsorption analysis and x-ray diffraction Energy & Fuels, 31, 10, 10874–10879 (2017).
- 23. Palit S., **He L.**, Hamilton W.A., Yethiraj A., Yethiraj A., The effect of crowder charge in a model polymer–colloid system for macromolecular crowding: Polymer structure and dynamics Journal of Chemical Physics, 147, 11, 114902 (2017).
- 24. Chen X., Wignall G.D., **He L.**, Lopez-Barron C., Alamo R.G., SANS Evidence of Liquid–Liquid Phase Separation Leading to Inversion of Crystallization Rate of Broadly Distributed Random Ethylene Copolymers Macromolecules, 50, 11, 4406–4414 (2017).
- 25. Bridges C.A., Sun X.G., Guo B., Heller W.T., He L., Paranthaman M.P., Dai S., Observing

Framework Expansion of Ordered Mesoporous Hard Carbon Anodes with Ionic Liquid Electrolytes via In-Situ Small-Angle Neutron Scattering ACS Energy Letters, 2, 7, 1698–1704 (2017).

- Abney C.W., Do C., Luo H., Wright J., He L., Dai S., Controlling the Intermediate Structure of an Ionic Liquid for f-Block Element Separations Journal of Physical Chemistry Letters, 8, 9, 2049– 2054 (2017).
- Cooksey T.J., Singh A., Le K.M., Wang S., Kelley E.G., He L., Vajjala Kesava S., Gomez E.D., Kidd B.E., Madsen L.A., Robertson M.L., Tuning Biocompatible Block Copolymer Micelles by Varying Solvent Composition: Core/Corona Structure and Solvent Uptake Macromolecules, 50, 11, 4322–4334 (2017).
- Du P., Li A., Li X., Zhang Y., Do C., He L., Rick S.W., John V.T., Kumar R., Zhang D.H., Aggregation of Cyclic Polypeptoids bearing Zwitterionic End-groups with Attractive Dipole-Dipole and Solvophobic Interactions: A Study by Small-Angle Neutron Scattering and Molecular Dynamics Simulation Physical Chemistry Chemical Physics, 19, 22, 14388-14400 (2017).
- 29. Palit S., **He L.**, Hamilton W.A., Yethiraj A., Yethiraj A., Combining Diffusion NMR and Small-Angle Neutron Scattering Enables Precise Measurements of Polymer Chain Compression in a Crowded Environment Physical Review Letters, 118, 9, 097801 (2017).
- 30. Yuan X., Duan Y., **He L.**, Singh S., Simmons B., Cheng G., Characterization of white poplar and eucalyptus after ionic liquid pretreatment as a function of biomass loading using x-ray diffraction and small angle neutron scattering Bioresource Technology, 232, 113-118 (2017).
- 31. Zhao W., Xiao L.P., Song G., Sun R.C., **He L.**, Singh S., Simmons B., Cheng G., From lignin subunits to aggregates: insights into lignin solubilization Green Chemistry, 19, 3272-3281 (2017).
- 32. Thusitha Etampawala, Dipak Aryal, Naresh Osti, **Lilin He**, William Heller, Carl Willis, Gary Grest, and Dvora Perahia "Association of a Multifunctional Ionic Block Copolymer in a Selective Solvent " *Journal of Chemical Physics*, 145, 184903, 18 (2016)
- 33. Jitendra Bahadur, Cristian Medina, **Lilin He**, Yuri Melnichenko, John Rupp, Tomasz Blach and David Mildner "Determination of closed porosity by (ultra) small-angle neutronscattering: a new approach" *Journal of Applied Crystallography*, 2016, 49, Part 6.
- Lilin He, Bin Hu, Danie M. Henn, and Bin Zhao "Influence of Cleavage of Photosensitive Group on Micellization and Gelation of a Doubly Responsive Diblock Copolymer in Aqueous Solutions: A SANS Study" *Polymer*, 2016, 105, 25-34.
- 35. Jouault N., Crawford M.K., Chi C., Smalley R.J., Wood B., Jestin J., Melnichenko Y.B., **He L**., Guise W.E., Kumar S.K., "Polymer Chain Behavior in Polymer Nanocomposites with Attractive Interactions", *ACS Macro Letters*, 2016, 5, 523-527.
- Li A., Lu L., Li X., He L., Do C., Garno J.C., Zhang D.H., "Amidine-Mediated Zwitterionic Ring-Opening Polymerization of N-Alkyl N-Carboxyanhydride: Mechanism, Kinetics, and Architecture Elucidation", *Macromolecules*, 2016, 49, 1163-1171.
- 37. Zhang G., Yang H., **He L.**, Hu L., Lan S., Li F., Chen H., Guo T., "Importance of domain purity in semi-conducting polymer/insulating polymer blends transistors", Journal of Polymer Science Part B: Polymer Physics, 2016, 54, 1760-1766.

- Sudheer K. Molugu, Zacariah L. Hildenbrand, David Gene Morgan, Michael B. Sherman, Lilin He, Costa Georgopoulos, Natalia V. Sernova, Lidia P. Kurochkina, Vadim V. Mesyanzhinov, Konstantin A. Miroshnikov, and Ricardo A. "Ring separation highlights the protein folding mechanism used by the phage EL encoded chaperonin" *Structure*, 24, 2016, 537-546.
- 39. Zhicai He, Feng Liu, Cheng Wang, Jihua Chen, **Lilin He**, Dennis Nordlund,Hongbin Wu, Thomas P. Russell, Yong Cao "Simultaneous Spin-Coating and Solvent Annealing: Manipulating the Active Layer Morphology to a Power Conversion Efficiency of 9.6% in Polymer Solar Cells" *Mater. Horiz.* 2015,2, 592-597.
- 40. Rui Zhang, Shimin Liu, Jitendra Bahadur, Derek Elsworth, Yuri Melnichenko, Lilin He, Yi Wang "Estimation and modeling of coal pore accessibility using small angle neutron scattering" *Fuel*, 2015, 161, 323-332.
- 41. J. Bahadur, Y. B. Melnichenko1, L. He, C. Contescu, N.C. Gallego, J. R. Carmichael "SANS Investigations of CO2 Adsorption in Microporous Carbon" Carbon, 2015, 95, 535-544.
- 42. Lilin He, Do C., Qian S., Wignall G. D., Heller W. T., Littrell K. C., Smith G. S., "Corrections for the Geometric Distortion of the Tube Detector at HFIR Small Angle Neutron Scattering Beamlines" Nuclear Instruments and Methods in Physics Research A, 2015, 775, 63-70.
- Scott A. Jamieson, Katie W. K. Tong, William A. Hamilton, Lilin He, Michael James and Pall Thordarson "Small Angle Neutron Scattering (SANS) Studies on the Structural Evolution of Pyromellitamide Self-assembled Gels" *Langmiur* 2014, 30, 13987-13993.
- 44. Lilin He, Yuri B. Melnichenko, Nidia C. Gallego, Cristian I. Contescu, Junjie Guo, Jitendra Bahadur, "Investigation of morphology and hydrogen adsorption capacity of disordered carbons" *Carbon*, 2014, 80, 82-90.
- 45. Yuri B. Melnichenko, N. V. Lavrik, E. Popov, J. Bahadur, **Lilin. He**, I. I. Kravchenko, G. Smith, V. Pipich, and N. K. Szekely, "Cavitation on deterministically nanostructured surfaces in contact with an aqueous phase: A small-angle neutron scattering study" *Langmiur* 2014, 30, 9985-9990.
- 46. Lilin He, Chris J. Cornelius, Dvora Perahia "Water dynamics within a highly rigid sulfonated polyphenylene" *European Polymer Journal* 56, 2014, 168-173.
- Sofiane Boukhalfa, Daniel Gordon, Lilin He, Yuri B. Melnichenko, Naoki Nitta, Alexandre Magasinski, and Gleb Yushin, "In Situ Small Angle Neutron Scattering Revealing Ion Sorption in Microporous Carbon Electrical Double Layer Capacitors" ACS Nano 2014, 8(3), 2495-2503.
- 48. Sai Venkatesh Pingali,\* Hugh M. O'Neill, Yoshiharu Nishiyama, **Lilin He**, Yuri B. Melnichenko, Volker Urban, Loukas Petridis, Brian Davison, Paul Langan. "Morphological changes in the cellulose and lignin components of biomass occur at different stages during steam pretreatment" *Cellulose*, 2014, 21, 873-878.
- 49. Brent J. Heuser, Dallas R. Trinkle, Tai-Ni Yang, and <u>Lilin He</u>, "Hydrogen Trapping at Dislocation Cores at Room Temperature in Deformed Pd" *J. of Alloys and Compound*, 2013, 577, 189-191.
- 50. J. R. Morris, C. I. Contescu, M. F. Chisholm, V. R. Cooper, J. Guo, <u>L. He</u>, Y. Ihm, E. Mamontov, Y. B. Melnichenko, R. Olsen, S. J. Pennycook, M. Stone, H. Zhang, N. C. Gallego, "Modern

approaches to studying gas adsorption in nanoporous carbons", *Journal of Materials Chemistry A*, 2013, 1, 9341-9350.

- 51. M. K. Crawford, R. J. Smalley, G. Cohen, B. Hogan, S. K. Kumar, Y. B. Melnichenko, L. He, W. Guise, B. Hammouda, "Chain conformation in polymer nanocomposites with uniformly dispersed nanoparticles," *Physical Review Letters* 2013, 110, 196001.
- 52. Stan Martin, <u>Lilin He</u>, William Heller, Flora Meilleur, "New Insight into the Structure of RNA in *Red Clover Necrotic Mosaic Virus* and the role of divalent cations revealed by Small Angle Neutron Scattering".*Archives of Virology* 2013, 158, 1661-1669.
- Sofiane Boukhalfa, <u>Lilin He</u>, Yuri B. Melnichenko, Gleb Yushin "Small-Angle Neuron Scattering for In-Situ Probing the Ion Adsorption Inside Micropores" *Angewandte Chemie International Edition* 2013, 52, 4618-4622.
- 54. Leslie F. Ruppert, Richard Sakurovs, Tomasz P. Blach, <u>Lilin He</u>, Yuri B. Melnichenko, David F.R. Mildner and Leo Alcantar-Lopez "A USANS/SANS Study of the Accessibility of Pores in the Barnett Shale to Methane and Water" *Energy & Fuels* 2013, 27, 772-779.
- 55. Richard Sakurovs, <u>Lilin He</u>, Yuri B. Melnichenko, Andrzej P. Radlinski, Tomas Blach, Hartmut Lemmel, David F.R. Mildner "Pore size distribution and accessible pore size distribution in bituminous coals" *International Journal of Coal Geology*, 2012, 100,51-64.
  - This paper was awarded the best paper in geochemistry and/or mineralogy of coal for 2013. (the 2013 Dal Swaine Award)
- 56. <u>Lilin He</u>, Gang Cheng, Yuri B. Melnichenko "Partial collapse and reswelling of a polymer in the critical demixing region of good solvents" *Physical Review Letters*, 2012, 109, 067801
  Highlighted by ORNL website
- Gang Cheng, Michael Kent, <u>Lilin He</u> et al. "Effect of Ionic Liquid Treatment on the Structures of Lignins in Solutions: Molecular Subunits Released from Lignin" *Langmuir*, 2012, 28, 11850-7
- Jayant J. Jayasundar, Jeong Ho Ju; <u>Lilin He</u>, Dazhi Liu, Flora Meilleur, Jinkui Zhao, David J.E. Callaway, and Zimei Bu "Open Conformation of ezrin bound to PIP2 and to F-actin by neutron scattering" *Journal of Biological Chemistry*, 2012, 287, 37119-37133.
- C.R.Clarkson, N.Solano, R.M.Bustin, A.M.M. Bustin, G.R.L.Chalmers, <u>L.He</u>, Y.B. Melnichenko, A.P. Radlinski, T.P. Blach. "Pore Structure Characterization of North American Shale Gas Reservoirs using USANS/SANS, gas adsorption, and Mercury Instrusion" *Fuel*, 2012, 103, 606-616.
- 60. Maria Mastalerz, <u>Lilin He</u>, Yuri B Melnichenko, John A Rupp "Porosity of coal and shale: Insights from gas adsorption and SANS/USANS techniques" *Energy & Fuels* 2012, 26, 5109-5120.
- 61. <u>Lilin He</u>, Amanda Piper, Flora Meilleur, Raquel Hernandez, William T. Heller, Dennis T. Brown, "Conformational changes in Sindbis virus induced by decreased pH revealed by Small-Angle Neutron Scattering"*J. Virol.*2012, 86,1982-1987.
- 62. <u>Lilin He</u>, Melnichenko et al. "Pore Accessibility by Methane and Carbon Dioxide in Coal as Determined by Neutron Scattering" *Energy&Fuels* 2012, 26, 1975-1983.
  - It has been cited as "Probing Nanopores: Neutrons Shine a light on geological nanostructures" http://www.ornl.gov/info/ornlreview/v45\_1\_12/article05.shtml

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- 64. Salvino Ciccariello, Yuri B. Melnichenko and <u>Lilin He</u>, "Phase Behavior of Carbon Dioxide Confined in Silica Aerogel in the Vicinity of the Bulk Critical Point" *J.Phys.Chem. C*, 2011, 115, 22336-22346.
  - It was reported by 2010 ORNL neutron science review, cited as "A new home for greenhouse gases"
- Nidia C. Gallego, <u>Lilin He</u>, Dipendu Saha, CristianI. Contescu, Yuri B. Melnichenko"Hydrogen Confined in Carbon Nanopores: Extreme Densification at Ambient Temperature" *J. Am. Chem. Soc.*,2011, 133 (35),13794–13797.
  - It was selected as highlight submitted to Basic Energy Sciences, Office of Science, U.S. Department of Energy
  - It was reported by *NOTIZIARIO Neutroni e Luce di Sincrotrone*, (a publication that addresses the needs of neutron and synchrotron users worldwide). The article entitled "Neutrons measure phase behavior in pores at Angstrom size"
- 66. Yuri B. Melnichenko, <u>Lilin He</u> et al., "Accessibility of Pores in Coal to Methane and Carbon Dioxide" *Fuel*, 2012, 91, 200-208.
  - It was highlighted by *Science* as Editor's Choice [*Science*, Vol. 334, Oct. 7, P.19, (2011)] <u>http://www.sciencemag.org/content/334/6052/twil.full.pdf</u>
  - It was reported by DOE Pulse website. The article entitled "Energy and Environmental Solutions Under our Feet" <u>http://neutrons.ornl.gov/research/highlights/GPSANS/accessibility-coal-pores.shtml</u> <u>http://www.ornl.gov/info/news/pulse/no345/story5.shtml</u>
- 67. <u>Lilin He</u>, Suresh. M. Chathoth et al. "Small-Angle Neutron Scattering Characterization of the Structure of Nanoporous Carbons for Energy-related Applications" *Microporous and Mesoporous Materials*, 2012, 149, 46-54.
- Suresh M. Chathoth, <u>Lilin He</u>, E. Mamontov and Yuri. B. Melnichenko, "Effect of Carbon Dioxide and Nitrogen on the Diffusivity of Methane Confined in Nano-porous Carbon Aerogel" *Microporous and Mesoporous Materials*, 2012, 148, 101-106.
- 69. Xin Li, Chwen-Yang Shew, <u>Lilin He</u> et al., "Scattering Functions of Platonic Solids" J. Appl. Cryst. 2011. 44, 545-557.
  Selected from all crystallography Hoursels for highlight
  - Selected from all crystallography Hournals for highlight
- Salvino Ciccariello, Yuri B. Melnichenko and <u>Lilin He</u>, "Supercritical Carbon Dioxide Behavior in Porous Silica Aerogel" J. Appl. Cryst. 2011. 44, 43-51.
- <u>Lilin He</u>, Amanda Piper, Flora Meilleur, Dean A. A. Myles, Raquel Hernandez, Dennis T. Brown, William T. Heller "The structure of sindbis virus produced from vertebrate and invertebrate hosts determined by small angle neutron scattering" *J. Virol.*, 2010, 84(10), 5270-5276.
  - It was reported by ORNL News, cited as "Neutrons 'go viral' at ORNL: ORNL neutron scattering study yields new insights into virus life cycle"
  - It was reported by 2010 ORNL neutron science review, cited as "Neutron scattering studies promise better antiviral drugs"

- 72. <u>Lilin He</u>, C. J. Cornelius and Perahia Dvora, "From Solution to Membranes: Structure Studies of Sulfonated Polyphenylene" *Macromolecules*, 2009, 42(18), 7084-7090.
- 73. <u>Lilin He</u>. Hillary Smith, J. Majewski, Christopher J. Cornelius, Perahia Dvora. "Interfacial Effects on Water Penetration into Ultrathin Ionomer Films: An in-situ Study Using Neutron Reflectometry" *Macromolecules*, 2009, 42(15), 5745-5751.
- 74. Changqing Wu, Feng Chen, Xi Wang, Yonnie Wu, Meidui Dong, Guoqing He, Ronald D. Galyean, <u>Lilin He</u>, Guohui Huang "Identification of antioxidant phenolic compounds in feverfew (*Tanacetumparthenium*) by HPLC-ESI-MS/MS and NMR" *Phytochemical Analysis* 2007 Vol 18, 401.

#### **CONFERENCE PROCEEDINGS**

- Dipendu Saha, <u>Lilin He</u>, Cristian I. Contescu, Nidia C. Gallego, Yuri B. Melnichenko "Experimental Evidence of Super Densification of Adsorbed Hydrogen by in-situ Small Angle Neutron Scattering (SANS)" *Materials Research Society Proceedings* 2011,1334
- 2. Hongxin Zhang, <u>Lilin He</u>, Yuri B. Melnichenko, Cristian I. Contescu, Nidia C. Gallego "Monitoring phase behavior of hydrogen confined in carbon nanopores by *in-situ* Small Angle Neutron Scattering technique" *Materials Research Society Proceedings* 2012,1440
- 3. Yuri B. Melnichenko, <u>Lilin He</u>, Maria Mastalerz "Pore Size Specific Characterization of the Adsorption of CO2 and Methane in Coals using SANS" *Geochimica ET Cosmochimica Acta*, 2012, 74, A697-A697

### **ARITICLES UNDER REVIEW** (*The following manuscript is available upon request*)

- 1. Etampawala, Thusitha; Tehrani, Mehran; Nematollahi, Ali; He, Lilin; Dadmun, Mark "The Impact of Solvent Doping on the Morphology and Performance of Spray-coated PEDOT:dPSS: A USANS and SANS Study" (submitted to Macromolecules)
- 2. Nidia C Gallego, Timothy D Burchell, Lilin He, Melanie J. Kirkham, Cristian I Contescu "Neutron irradiation effects on the structure of highly oriented pyrolytic graphite: A XRD and SANS Study" (Submitted to Conference Proceeding of Carbon 2016, the world conference on Carbon)
- 3. Tyler J. Cooksey, Avantika Singh, Kim Mai Le, Shu Wang, Elizabeth G. Kelley, Lilin He, Sameer Vajjala Kesava, Enrique D. Gomez, Bryce E. Kidd,f Louis A. Madsen,f and Megan L. Robertson "Tuning Biocompatible Block Copolymer Micelles by Varying Solvent Composition: Core/Corona Structure and Solvent Uptake" (submitted to Macromolecules)

### **CONFERENCE ORAL PRESENTATIONS**

- 1. Lilin He, Xiaoliang Wang, Shuo Qian, and Shengqian Ma "Small-angle Neutron Scattering Study of Enzyme Encapsulation in Nanoporous Metal-Organic Frameworks" (American Crystallographic Association, 2019, Covington, KY)
- 2. Lilin He, Xiaoliang Wang, Shuo Qian, Shengqian Ma "Enzyme Immobilization in Mesoporous Metal-Organic Frameworks by SANS" (American Physical Society, 2019, Boston, MA)

- Lilin He, Luming Yang, Rui Zhang, Jianlin Li, Mircea Dinca "Operando SANS Study on Ion Adsorption in Conductive Porous MOF Electrodes" (American Physical Society, 2018, Los Angeles, CA)
- 4. Lilin He, William Hamilton, Tao Hong, X. Tong, Lowell Crow, Katherine Bailey, Nidia Gallego "Observation of Anomalous Neutron Scattering Ring in Highly Oriented Pyrolytic Graphite" (American Physical Society, 2017, New Orleans, LA)
- <u>Lilin He</u>, Bin Hu, Bin Zhao "Micellizationa and Gelation of Water Soluable Thermo-and Lightsensitive Block Copolymer Investigated by SANS" (American Physical Society, 2016, Baltimore, MD)
- 6. <u>Lilin He</u>, Bin Hu, Bin Zhao "Micellizationa and Gelation of Water Soluable Thermo-and Lightsensitive Block Copolymer Investigated by SANS" (2015 APS meeting, San Antonio, TX)
- 7. <u>Lilin He</u>, Bin Hu, Bin Zhao "Thermo- and Light-Sensitive Hydrophilic Block Copolymer in Water Investigated by SANS" ACA 2014, Albuquerque, NM, TN
- Lilin He, Cristian Contescu, Yuri Melnichenko, Nidia Gallego, Junjie Guo, Jitendra Bahadur "Morphology and Hydrogen Adsorption Capacity of Nanoporous Carbons" ACNS 2014, Knoxville, TN (Oral presentation).
- 9. <u>Lilin He</u>, Yuri Melnichenko et al. "Microstructural Characterization of Nanoporous Carbon Fibre as Determined by Neutron Scattering" (American Physical Society, 2013, Baltimore, MD)
- 10. <u>Lilin He</u>, Gang Cheng, Yuri B. Melnichenko "Conformation Transition of Polyethylene Glycerol near the Critical Demixing Point of a Binary Mixture" (American Neutron Scattering Society, June 25-28, 2012, Washington D.C., USA)
- 11. Nidia C. Gallego, Cristian Contescu, **Lilin He**, Yuri Melnichenko and Hongxin Zhang "Characterization of the Phase Behavior of Hydrogen Confined in the Pores of Nanostructured Carbons" (New Diamond and Nano Carbons Conference, May 20-24, 2012, San Juan, Puerto Rico)
- 12. <u>Lilin He</u>, Amanda Hafer et al. "The Structure of Sindbis Virus Produced from Vertebrate and Invertebrate Hosts Determined by Small Angle Neutron Scattering" (American Neutron Scattering Society, 2010, Ottawa, Canada)
- 13. <u>Lilin He</u>, Rakchart Traiphol, Dennis W. Smith, Dvora Perahia "Confinement induced crystallinity in semiflurinated polymer thin film" (2003 APS Meeting, Austin,TX)
- 14. <u>Lilin He</u>, Dvora Perahia, Christopher Cornelius "The correlation between molecular and phase structure in highly ionic polymer" (2004 APS meeting, Montreal, Canada)
- 15. <u>Lilin He</u>, Christopher Cornelius "Structure of highly rigid ionic polymers from single molecules to membranes" (2005 APS meeting, Los Angeles, CA)
- 16. <u>Lilin He</u>, Cy Fujimoto, Christopher Cornelius, Dvora Perahia "Confined water in ionic membranes: studied by NMR"(2006 APS meeting, Baltimore, MD)

- 17. <u>Lilin He</u>, Erik Watkins, Jaroslaw Majewski, Cy Fujimoto, Christopher Cornelius, Dvora Perahia "Water diffusion in ultrathin ionomer thin films: neutron reflectivity study" (2007 APS meeting, Denver, CO)
- 18. Christopher Cornelius, Cy H. Fujimoto, <u>Lilin He</u>, Dvora Perahia "Interfacial Characteristics of a Potentially Antifouling Highly Rigid Ionomer" (2007 APS meeting, Denver, CO)
- 19. <u>Lilin He</u> "Methanol Diffusion into Thin Ionomer Films: An in situ Study Using Neutron Reflectometry" (2008 APS March meeting, New Orleans, LA)
- 20. Thusitha Etampawala, Dvora Perahia, <u>Lilin He,</u> Christopher Cornelius "*In situ* neutron reflectivity study of alcohols into ultra-thin ionomer films" (2009 APS March meeting, Pittsburg, PA)

#### **CONFERENCE POSTERS**

- 1. Lilin He et al, "From Chain Conformation to Morphology: Fundamental Understanding of Polymeric Materials by Neutron Scattering" SHUG meeting, 2018, ORNL.
- 2. Lilin He et al. "PARADYSE: A Highly Efficient, Multiscale Modeling Framework for Hierarchical Materials" SAS, 2018, Traverse City, MI.
- 3. Lilin He et al. "Study of Ring Scattering by Highly Oriented Pyrolytic Graphite" at the American Conference on Neutron Scattering" 2016, Long Beach, CA
- 4. Cristian I. Contescu, Nidia C. Gallego, Eugene Mamontov, Yuri B. Melnichenko, <u>Lilin He</u>, Alexander I. Kolesnikov, Raina J. Olsen, James R. Morris "Hydrogen confined and restrained in overcrowded carbon" (6th International Conference on Carbon for Energy Storage/Conversion and Environment Protection, 2015, Poznan, Poland)
- <u>Lilin H</u>., Do C., Qian S., Wignall G. D., Heller W. T., Littrell K. C., Smith G. S., "Geometric Corrections of the Tube Detectors on SANS Instruments" (16th International Conference on Small-Angle Scattering, 13 - 18 September, 2015, Berlin, Germany)
- Abdoulaye Djire, Olabode T Ajenifujah, Alice Sleightholme, Paul Rasmussen, <u>Lilin He</u>, Jason Siegel, Levi T Thompson "Charge Storage Mechanisms of Carbides and Nitrides" (227th The Electrochemical Society meeting, May 2-28, 2015, Chicago, IL, USA)
- 7. <u>Lilin He</u> Yuri B. Melnichenko et al. "Correlating Morphology and Hydrogen Adsorption Capacity of Disordered Carbons" ACA 2014, Albuquerque, NM, TN
- 8. <u>L. He</u>, C. Do, S. Qian, G. D. Wignall, W. T. Heller, K. C. Littrell, and G.S. Smith "Understanding Geometric Distortion of the Tube Detectors on SANS Instruments at ORNL" ACNS 2014, Knoxville, TN(Poster presentation).
- 9. <u>Lilin He</u>, Yuri B. Melnichenko et al. "Structure and Adsorption Characteristics of Porous Materials as Determined by Small-angle Neutron Scattering" (American Neutron Scattering Society, June 25-28, 2012, Washington D.C., USA)

- 10. <u>Lilin He</u>, Gang Cheng, Yuri B. Melnichenko "Polymer Conformation near the Critical Demixing Point of a Binary Mixture of Solvents" (2012 APS Meeting, Boston, MA)
- 11. <u>Lilin He</u>, Yuri B. Melnichenko et al. "Structure and Adsorption Properties of Carbonaceous Adsorbents Characterized using Small-angle Neutron Scattering" (2012 Symposium/Workshop "Carbons for Energy Applications" Organized by the American Carbon Society, Stone Mountain, GA)
- Lilin He, Yuri B. Melnichenko et al. "Neutron Scattering Studies of the structure and Adsorption of Carbon Dioxide and Methane in Coals" (International Pittsburgh Coal Conference, 2011, Pittsburgh, PA)
- Lisa Debeer-Schmitt, Kathy Bailey, <u>Lilin He</u>, George Wignall, Yuri Melnichenko, Ken Littrell "Have some large structures? Try small-angle neutron scattering (SANS)" (2011 APS Meeting, Dallas, TX)
- Lilin He, Yuri B. Melnichenko, Maria Mastalerz "The Porosity Characterization and Phase Behavior of Greenhouse Gases Confined in Coals" (American Neutron Scattering Society, 2010, Ottawa, Canada)
- 15. <u>Lilin He</u>, Amanda Hafer et al. "Solution Structure of Sindbis Virus: A Small Angle Neutron Scattering (SANS) Study" (International Conference on *Neutron Scattering 2009*, Knoxville, TN)
- 16. Yiming Mo, <u>Lilin He</u> et al. "SANS Investigations on E1 (1-129) Protein from Sindbis Virus" (International Conference on *Neutron Scattering 2009*, Knoxville, TN)
- Etampawala, T.N., <u>Lilin He</u> et al. "Long chain alcohol penetration into ultrathin ionomer films: An in-situ kinetic study using Neutron reflectivity" (International Conference on *Neutron Scattering* 2009, Knoxville, TN)
- Leslie F. Ruppert, Richard Sakurovs, Tomasz P. Blach, David F.R. Mildner, <u>Lilin He</u>, Yuri B. Melnichenko "A USANS/GP-SANS Study of the Accessibility of Pores in Gas Shale to Methane, Water, and Brine" American Association of Petroleum Geologists, Sep 25-27, 2011, Arlington, Virginia

### **INVITED TALKS**

- "Small Angle Neutron Scattering (SANS) and Its Applications in Structural Characterization of Nanostructured Materials" (ORNL CNMS Seminar Series, Oak Ridge National laboratory, Oak Ridge, TN, September 2020)
- "Capabilities for Soft Matter Studies on the Neutron Scattering Beamlines at ORNL" (SHUG meeting, 2019)
- "Exploring Nanoporous Materials with Small-angle Neutron Scattering (SANS)" (ORNL CSD Seminar Series, Oak Ridge, TN, September 2019)
- "Investigate Energy Materials with Small-angle Neutron Scattering (SANS)" (ORNL ETSD Seminar, Oak Ridge, TN, September 2019)
- "Insights into Ion adsorption in Conductive Porous MOF Electrodes using SANS" (SERACS, 2018, Augusta, GA)
- "Time-Resolved SANS Experiments on GP-SANS" (Time-Resolved Neutron Scattering Workshop, ORNL, 2018)

- "Investigating Hierarchical Materials with Small angle Neutron Scattering (SANS)" (Early Carrer Scientist Forum, ORNL, 2018)
- "Hierarchical Structures of Disordered Materials" (Chemistry Department, The University of Nottingham, May, 2018)
- "Applications of Small Angle Neutron Scatterings for Polymer Studies" (Eastman Chemical Company, TN, Oct, 2017)
- "Exploring Hierarchical Structures of Soft Materials with Small Angle Neutron Scattering" (Physical Sciences Directorate Seminar Series, Oak Ridge National laboratory, Oak Ridge, TN, September 2016)
- "Investigation of Hierarchically Structured Soft Materials using Small Angle Neutron Scattering" (Shanghai Jiaotong Univ., May of 2016, Shanghai, China)
- "SANS Capabilities at Oak Ridge National Laboratory" (Neutron and Nano User Meeting, Oak Ridge, August, 2013)
- "Small Angle Neutron Scattering Study of Sindbis Virus Produced from Vertebrate&Invertebrate Hosts" (The University of Tennessee, Knoxville, April, 2013)
- "The characterization of porous materials using small angle neutron scattering" (Porous Materials Inc, Ithaca, NY. May, 2010)
- "Carbon sequestration in porous coals" (Workshop "SANS for geology", ORNL June, 2010)
- "Structure and Transport Characteristics of Highly Rigid Ionomers" (Henkel, Irvine, CA, October, 2007)