



The Gene and Linda Voiland School of  
**Chemical Engineering and  
Bioengineering**  
2015 Seminar Series  
Monday, April 6, 2015  
12:10 p.m. Wegner G1



Jianzhi Hu  
Senior Research Scientist  
Pacific Northwest National Laboratories

Dr. Hu has more than 18 years of research experience, with more than 70 publications in the field of NMR, and three pending US patents. He joined PNNL in 2000 and has been associated with the Macromolecular Structure and Dynamics group in the EMSL since 2000.

He earned his PhD in Applied Physics at the Wuhan Institute of Physics, the Chinese Academy of Sciences. His thesis work was granted permission by the University of Utah (1991-1994). In 1986, he obtained an MS in Applied Physics at Wuhan Institute of Physics, the Chinese Academy of Sciences and in 1983 his BS in Semiconductor Physics, Lanzhou University, China.

Dr. Hu specializes in nuclear magnetic resonance (NMR) spectroscopy. Recent interest includes: Development and application of novel Magnetic Resonance techniques, such as the magic angle turning experiments, applied at very slow sample spinning rate from 1 to 100 Hz, to enhance NMR spectral resolution in intact cells, excised organs, excised tissues and live animals. Developing spectral resolution enhanced localized NMR spectroscopy/imaging to study biological samples. Application of solid state NMR techniques to investigate molecular structure and dynamics of catalyst materials, polycrystalline and amorphous solids, fossil fuels, polymers and biological solids. Developing a novel in-situ NMR method to characterize real time catalytic reaction. Ab-initio calculations using quantum chemistry theory to predict molecular geometry and NMR parameters. NMR Pulse sequence development and data processing. NMR probe design and construction.

**In Situ and Ex Situ NMR: Development and Applications**

Basic NMR principles will be briefly introduced first. I'll then talk about a few unique in situ and ex situ NMR capabilities that have been developed in my group. These capabilities include but not limited to the followings.

- (1) In situ high resolution magic angle spinning (MAS) NMR with constant flow of reactants into the catalyst bed for studying catalytic reactions using heterogeneous catalysts;
- (2) The combined high temperature and high pressure high resolution MAS NMR capability using sealed MAS rotors for in situ investigation of the reaction mechanisms associated with (a) zeolite synthesis, (b) biogenic molecules to fuels in the presence of zeolites and aqueous water and (c) geological carbon sequestration where supercritical fluid CO<sub>2</sub> is reacting with minerals to form stable metal carbonates;
- (3) Ex situ ultra-high field natural abundance <sup>25</sup>Mg and <sup>17</sup>O NMR capability for studying the solvation mechanisms of the ions in electrolytes associated with Li-ion and Mg-batteries; and
- (4) In situ NMR capabilities for investigating the detailed electrochemistry and reaction mechanisms associated with energy storage systems such as Li-ion and Li-sulfur batteries under real world working conditions, i.e., electric wires are attached to the batteries for discharge-charge while the NMR data are acquired.