

**Sunday, March 13, 2011**

**16:00 Registration**

**19:00 Banquet**

# Monday, March 14, 2011

**8:30 Schlueter, John**

Welcome

## Monday AM: Conductors I

**8:40 Blundell, Stephen**

Muon-spin Rotation as a Probe of Molecule-based Materials

**9:30 Drichko, Natalia**

Interplay of Charge Order and Superconductivity in BEDT-TTF-based Materials with  $\frac{1}{4}$ -filled Conductance Band

**9:50 Streiffer, Stephen**

Physical Sciences and Engineering

**10:00 Break**

**10:30 Brown, Stuart**

Superconductivity in Quasi-one Dimensional and Quasi-two Dimensional Molecular Conductors

**10:50 Kurmoo, Mohamedally**

Magnetism and Porosity in Metal-Organic Frameworks

**11:10 Prassides, Kosmas**

Fullerene Superconductivity 20 Years on

**11:30 Krstovska, Danica**

Magnetothermopower Quantum Oscillations in a Q2D Organic Conductor – a Theoretical Approach

**11:50 Mori, Takehiko**

Requirements for Zero-gap States in Organic Charge-transfer Salts

**12:10 Lunch**

**13:30 Stephens, Peter**

Role of Powder Diffraction in Molecule-based Materials

**14:20 Stephenson, Brian**

Advanced Photon Source

**14:30 Mike Papka**

Advance Leadership Computing

**14:40 Break**

**15:00 Tours**

APS

CNM

ALCF – Jeff Hammond

**17:00 Dinner**

**Monday PM: Extreme Conditions**

**19:00 Musfeldt, Janice**

Spectroscopic Investigations of Materials under Extreme Conditions

**19:20 Halder, Greg**

Pressure-induced Switching in Magnetic Framework Materials

**19:40 Uji, Shinya**

Novel Phenomena in Molecular Conductors under High Magnetic Fields

**20:00 Zvyagin, Sergei**

High-Field ESR in Spin Systems with Reduced Dimensionality

**20:20 Goddard, Paul**

Molecular Magnets and Metals in High Magnetic Fields

**20:40 Wang, Xiaoping**

3D Reciprocal Space Mapping by Neutron Diffraction – Visualization of Molecular and Magnetic Interactions in Real Space for Energy Storage Materials

## Tuesday, March 15, 2011

**8:30 Mori, Take**

Welcome

### Tuesday AM: Molecule-based Magnets I

**8:40 Miller, Joel**

Molecule-based Magnets – A Tutorial Overview

**9:30 Manson, Jamie**

Quantum Magnets Comprised of Strong Hydrogen Bonds

**9:50 Mitchell, John**

Materials for Energy

**10:00 Break**

**10:30 Lahti, Paul**

Development Strategies Taking Paramagnetic Organic Molecules to Molecular Materials

**10:50 Costuas, Karine**

Multifunctional Carbon-rich Organometallic Compounds: Theoretical Aspects

**11:10 Batista, Cristian**

*Title*

**11:30 Jena, Peru**

A New Class of Magnetic Clusters and Their Potential as Building Blocks of Novel Materials

**11:50 McDonald, Ross**

The Role of Charge Degrees of Freedom in Mott Insulators: Coupling of Dielectric and Magnetic Properties via Frustration in Cr-trimer Complexes

**12:10 Lunch**

### Tuesday PM: Multifunctionality

**13:30 Yamashita, Masahiro**

Perspectives on Multi-Functional Single-Molecule Quantum Magnets and Single-Chain Quantum Magnets----Toward Molecular Spintronics

**14:20 Zapf, Vivien**

Multiferroic Behavior in Metal-organics

**14:40 Henne, Tina**

Educational Programs

**14:50 Break**

**15:20 Haddon, Robert**

Magnetic Phase Transitions in Phenalenyl-Based Neutral Radical Conductors

**15:40 Nakhmanson, Serge**

Electroactive Properties of Ferroelectric Polyvinylidene Fluoride and Related Copolymer and Oligomer Compounds

**16:00 Shatruk, Michael**

*Title*

**16:20 Dalal, Naresh**

Multifunctional Metal Organic Framework (MOF) Materials

**16:40 Almeida, Manuel**

Conducting and Magnetic Two Chain Compounds; from 1D systems to Spin-ladders

**17:00 Epstein, Art**

*Title*

**17:20 Dinner**

**19:00 Poster session**

## Wednesday, March 16, 2011

**8:30 Ouahab, Lahcene**

Welcome

### Wednesday AM: Nano and Bio

**8:40 Enoki, Toshiaki**

Graphene Edge is an Important Building Block for Molecule-based Magnetism

**9:00 Firestone, Millie**

Hierarchically Structured Electronic Conducting Polymerized Ionic Liquids

**9:20 Guionneau, Philippe**

Structurally Driven Properties of Molecular Switches

**9:40 Lefort, Ronan**

Toward Functional Hybrid Nanomaterials Based on Confined Calamitic and Discotic Liquid Crystals

**10:00 Petford-Long, Amanda**

Center for Nanostructured Materials

**10:10 Break**

**10:40 Meisel, Mark**

Heterostructural Films and Nanoparticles of Prussian Blue Analogs: Interface Strain Yields New Opportunities

**11:00 Iwasa, Yoshi**

Physics of Electrochemical Interfaces

**11:20 Bendeif, Eleulmi**

Structural Properties of the Thermal and Photo induced Spin Transition in Iron(II) Complexes: from the Macroscopic to the Nanoscopic Scale

**11:40 Anthony, John**

Molecular Design for Organic Electronic Devices: Transistors and Photovoltaics

**12:00 Darling, Seth**

Toward Idealized Bulk Heterojunctions in Organic Photovoltaics

**12:20 Lunch**

**2:00 Depart for Chicago**

# Thursday, March 17, 2011

**8:30 Prassides, Kosmas**

Welcome

## Thursday AM: Surfaces, Films and Interfaces

**8:40 Boukheddaden, Kamel**

Photoswitchable Spin-Crossover Solids: From Equilibrium to Non-equilibrium Properties

**9:30 Nicolazzi, William**

New model for Simulation of Domain Spatio-temporal Propagation in Spin Crossover Solids: A Defect-mediated Phase Transition?

**9:50 Brooks, James**

National High Magnetic Field Laboratories

**10:00 Break**

**10:20 Awaga, Kunio**

Organic Electronics based on Paramagnetic Species

**10:40 Kaneto, Keiichi**

Development of Extremely Air Stable n-type Organic Semiconductor for Thin Film Flexible Complementary-Field Effect Transistors

**11:00 Makiura, Rie**

Surface Molecular Architecture of Coordination Materials

**11:20 Van Ruitenbeek, Jan**

Highly Conductive Single Molecule Junctions without Anchoring Groups

**11:40 Rabiller, Philippe**

Original Aspects of Phase Transitions in Aperiodic Alkane-urea Inclusions Compounds

**12:00 Lunch**

## Thursday PM: Photoproperties

**13:30 Buron-Le Cointe, Marylise**

Structure and Dynamics of Photo-induced Transformations: From Photostationary to Ultrafast

**14:20 Pointillart, Fabrice**

The Tetrathiafulvalene-amido-2-Pyridine-N-oxide Ligand as Efficient Organic Chromophore for the Sensitization of Yb(III) Luminescence: Experimental and Theoretical Studies

**14:40 Vinokur, Valerii**

Materials Theory Institute

**14:50 Break**

**15:20 Neville, Suzanne**

Spin Crossover Nano-materials: Thermal and Light-Induced Properties

**15:40 Boillot, Marie-Laure**

Photoreactive Materials Based on Spin-Crossover Fe<sup>II</sup> Complexes: Properties of Nanocomposite Silica Thin Films

**16:00 Koshihara, Shinya**

Search for the Photo-induced Hidden Phase in Strongly Correlated Systems

**16:20 Malfant, Isabelle**

Molecular Switching in Photochromic Materials based on Ruthenium Nitrosyl Complexes

**16:40 Yonemitsu, Kenji**

Photoinduced Phase Transition Dynamics: Interplay between Correlated Electrons and Molecular Vibrations during Insulator-metal and Neutral-ionic Transitions

**19:00 Banquet**

# Friday, March 18, 2011

## Friday AM: Molecule-based Magnets II

**8:30 Cador, Olivier**

Some Theoretical Aspects in Molecular Magnetism

**9:20 Booth, Corwin**

Correlated Electron Effects in Lanthanide Organometallic Molecules

**8:40 Flash presentation poster prize winner (Theory)**

**8:45 Flash presentation poster prize winner (Chemistry)**

**8:50 Flash presentation poster prize winner (Physics)**

**8:55 Flash presentation poster prize winner (Nano)**

**10:00 Break**

**10:20 Clerac, Rodolphe**

Single Chain Magnets – New Developments

**10:40 Fishman, Randy**

Molecule-based Diruthenium Magnet with Interpenetrating Sublattices

**11:00 Holmes, Steve**

Tuning Magnetic and Optical Bistability via Building Block Synthetic Approaches

**11:20 Novoa, Juan**

The First-Principles Bottom-Up Methodology: A General, Systematic, and Unbiased Form of Analyzing the Magnetic Interactions in Molecule-based Magnets

**11:40 Hill, Steve**

Single-Molecule Magnets

**12:00 Lunch**

## Friday PM: Spin Liquids/Conductors

**13:30 Kanoda, Kazushi**

Mott Physics of Correlated Electrons in Molecular Conductors

**14:20 Kato, Reizo**

Molecular Quantum Spin Liquid and Related Electronic States

**14:40 Chakoumakos, Bryan**

Neutrons at Oak Ridge National Laboratory

**14:50 Break**

**15:20 Kuroki, Kazuhiko**

Origin of Magnetism and Large Thermopower in Tau-type Organic Conductors

**15:40 Wallis, John**

The Synthesis and Properties of Functionalized Organosulfur Donors

**16:00 Suzumura, Yoshikazu**

Dirac Electron and Berry Curvature in Organic Conductors

**16:20 Tanatar, Makariy**

Non-magnetic Insulating Ground State of  $\kappa$ -(ET)<sub>2</sub>Cu[N(CN)<sub>2</sub>]I and Mott Transition Scheme for Two-dimensional Organic Superconductors

**16:40 De Souza, Mariano**

Lattice Effects in Organic Charge-Transfer Salts Close to the Mott Transition

**17:00 Schlueter, John**

Closing comments