

Sunday, March 13, 2011

17:00 Registration – Guest House

19:00 Reception – Guest House

Monday, March 14, 2011

8:30 Schlueter, John

Welcome

Monday AM: Conductors I

Chair: John Schlueter

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 Norman, Mike

Materials Science Division, Materials Theory Institute

10:00 Break

Chair: Tadashi Kawamoto

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

Magneto-thermopower 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 – Guest House

Chair: Gregory Halder

13:30 Stephens, Peter

Role of Powder Diffraction in Molecule-based Materials

14:20 Linda Young

Advanced Photon Source

14:30 Susan Coghlan

Advanced Leadership Computing Facility

14:40 Break

15:00 Tours

APS – Karena Chapman, Gregory Halder, Daniel Haskel

CNM – Kathleen Carrado Gregar

ALCF – Jeff Hammond

17:00 Dinner – Guest House

Monday PM: Extreme Conditions

Chair: Jamie Manson

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, Takehiko

Welcome

Tuesday AM: Molecule-based Magnets I

Chair: Takehiko Mori

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

Chair: Olivier Cador

10:30 Batista, Cristian

Field Induced Thermodynamic and Transport Properties of the Quantum Magnet
 $\text{NiCl}_2[\text{SC}(\text{NH}_2)_2]_4$

10:50 Costuas, Karine

Multifunctional Carbon-rich Organometallic Compounds: Theoretical Aspects

11:10 McDonald, Ross

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

11:30 Jena, Peru

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

11:50 Hill, Steve

Single-Molecule Magnets

12:10 Lunch – Guest House

Tuesday PM: Multifunctionality

Chair: Yasuhiro Tanaka

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 Nakhmanson, Serge
Electroactive Properties of Ferroelectric Polyvinylidene Fluoride and Related Copolymer and Oligomer Compounds

15:00 Henne, Tina
Educational Programs

15:10 Break

Chair: Vivien Zapf

15:40 Haddon, Robert
Magnetic Phase Transitions in Phenalenyl-Based Neutral Radical Conductors

16:00 Shatruk, Michael
Functionalizing Spin-Crossover Complexes for Preparation of Multifunctional Materials

16:20 Dalal, Naresh
Designing New Magnetic Ferroelectrics (Multiferroics)

16:40 Almeida, Manuel
Conducting and Magnetic Two Chain Compounds; from 1D systems to Spin-ladders

17:00 Poster Session – APS Gallery

19:00 Dinner – Guest House

Wednesday, March 16, 2011

8:30 Ouahab, Lahcene

Welcome

Wednesday AM: Nano and Bio

Chair: Danica Krstovska

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 Kathleen Carrado Gregar

Center for Nanostructured Materials

10:10 Break

Chair: Paul Goddard

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

Excursion to Chicago, March 16, 2011

12:30 Pick up box lunches – Guest House

13:30 Excursion to Chicago

13:30 Buses depart Argonne Guest House

14:15 Buses arrive Museum Campus for optional Field Museum or American Sightseeing coach bus tour

14:25 Buses drop off at Millennium Park – on your own (no tour)

14:30 Buses drop off at the Magnificent Mile Shopping/Dining District – on your own (no tour)

14:35 Buses drop off at Navy Pier – on your own (no tour)

20:20 Buses pick up at Water Tower Plaza– Please be on time (Chestnut Street Door in front of the John Hancock Tower)

20:30 Buses pick up at Navy Pier – Please be on time (Entrance #1 on north dock)

21:15 Buses arrive at Argonne Guest House

Thursday, March 17, 2011

8:30 Prassides, Kosmas

Welcome

Thursday AM: Surfaces, Films and Interfaces

Chair: Kosmas Prassides

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

Chair: Sergei Zvyagin

10:30 Awaga, Kunio

Organic Electronics based on Paramagnetic Species

10:50 Kaneto, Keiichi

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

11:10 Makiura, Rie

Surface Molecular Architecture of Coordination Materials

11:30 Van Ruitenbeek, Jan

Highly Conductive Single Molecule Junctions without Anchoring Groups

11:50 Rabiller, Philippe

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

12:10 Lunch – Guest House

Thursday PM: Photoproperties

Chair: Eric Collet

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 Neville, Suzanne

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

15:00 Wang, Xiaoping

Neutrons at Oak Ridge National Laboratory

15:10 Break

Chair: Janice Musfeldt

15:40 Boillot, Marie-Laure

Photoreactive Materials Based on Spin-Crossover Fe^{II} 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

17:00 Collet, Eric

Detection of 1D Precursor of the Photoinduced Transition of TTF-CA

19:00 Banquet – Guest House

Friday, March 18, 2011

Friday AM: Molecule-based Magnets II

Chair: James Brooks

8:30 Cador, Olivier

Some Theoretical Aspects in Molecular Magnetism

9:20 Booth, Corwin

Correlated Electron Effects in Lanthanide Organometallic Molecules

9:40 Flash presentation poster prize winner (Chemistry)

9:45 Flash presentation poster prize winner (Physics)

9:50 Flash presentation poster prize winner (Theory)

9:55 Flash presentation poster prize winner (Nano/Devices)

10:00 Break

Chair: Kamel Boukhedaden

10:20 Lahti, Paul

Development Strategies Taking Paramagnetic Organic Molecules to Molecular Materials

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 Clerac, Rodolphe

Single Chain Magnets – New Developments

12:00 Lunch – Guest House

Friday PM: Spin Liquids/Conductors

Chair: Tadahiko Ishikawa

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 Kuroki, Kazuhiko

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

15:00 Break

Chair: Mitsuhiro Maesato

15:30 Wallis, John

The Synthesis and Properties of Functionalized Organosulfur Donors

15:50 Suzumura, Yoshikazu

Dirac Electron and Berry Curvature in Organic Conductors

16:10 Tanatar, Makariy

Non-magnetic Insulating Ground State of κ -(ET)₂Cu[N(CN)₂]I and Mott Transition Scheme for Two-dimensional Organic Superconductors

16:30 De Souza, Mariano

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

16:50 Schlueter, John

Closing comments