Zero-field Spin Effects in Chemical Systems

Organizers
James K. McCusker, Michigan State University
David A. Shultz, North Carolina State University
Martin Kirk, University of New Mexico
Remi Beaulac, Michigan State University

(TRSC Host: Mark Kozak 970-708-4426)

June 23 – June 27, 2015
Telluride Elementary School, 447 West Columbia Avenue, Telluride, CO

Tuesday, June 23
- 6:00pm: Town Talk (Telluride Elementary School)
- 8:30pm: Conference meet-and-greet (Cosmopolitan, 301 West San Juan Avenue)

Wednesday, June 24
- 8:15 – 8:45am: Continental breakfast at the Telluride Elementary School
- Morning Session (Chair: Jim McCusker)
  - 8:45 – 9:00am: Opening remarks
  - 9:00 – 9:40am: Josef Michl (Univ. of Colorado at Boulder/IOCB ASCR, Prague)
    “T1-S0 Spin-orbit Coupling in Biradicals and Biradicaloids”
  - 9:40 – 10:20am: Mike Wasielewski (Northwestern University)
    “Spin Coherence Transfer within Photogenerated Three-spin Systems”
  - 10:20 – 10:40am: Coffee break
  - 10:40 – 11:20am: Yoshio Teki (Osaka City University)
    “Excited-state Spin Alignment and Spin Dynamics of Acene Derivatives having Radical Components”
  - 11:20 – 12:00pm: Marty Kirk (University of New Mexico)
    “Spin Effects on Donor-Acceptor Charge-transfer Excited States”
  - 12:00 – 2:00pm: Lunch
- Afternoon Session (Chair: Jeff Long)
  - 2:00 – 2:40pm: Danna Freedman (Northwestern University)
    “Rational Design of Magnetic Molecules for Quantum Information Processing”
  - 2:40 – 3:20pm: Trisha Andrew (University of Wisconsin)
    “Spin-Spin Interactions in Open-Shell Organic Semiconductors”
  - 3:20 – 3:40pm: Coffee break
• 3:40 – 4:20pm: **Dave Harris** (Northwestern University)
  “Synthesis of Iminobenzoquinone-bridged Dinuclear Complexes with Strong Magnetic Coupling”

• 4:20 – 5:00pm: **Carmen Herrmann** (University of Hamburg)
  “Chemical Control of Spin Coupling in Molecules – A Theoretical Analysis”

• 5:00 – 5:30pm: Discussion

• 6:00pm: TSRC Picnic and Poster Session (Telluride Elementary School)

**Thursday, June 25**

• *Morning free*

• *Afternoon Session (Chair: Marty Kirk)*

  • 1:30 – 2:10pm: **Jeff Long** (University of California at Berkeley)
    “New Single-Molecule Magnets with High Blocking Temperatures”

  • 2:10 – 2:50pm: **Jorge Rodriguez** (Purdue University)
    “Accurate Computation of Magnetic Properties in Metal-containing (bio)Molecular Complexes: Development and Application of Post-SDFT Methodologies”

  • 2:50 – 3:10pm: Coffee break

  • 3:10 – 3:50pm: **Rodolphe Clerac** (University of Bordeaux)
    “Rational Design of Magnetic Materials Based on “Single-Molecule Magnet” Building-Blocks”

  • 3:50 – 4:30pm: **Corine Mathoniere** (University of Bordeaux)
    “Rational Design of Switchable Electron Transfer Compounds”

  • 4:30 – 5:10pm: **Tony Rappe** (Colorado State University)
    “Multi-Determinant Density Functional Theory for Spin Multiplet Structure”

  • 5:10 – 5:30pm: Discussion

• *Dinner on your own*

**Friday, June 26**

• 8:30 – 9:00am: Continental breakfast at the Telluride Elementary School

• *Morning Session (Chair: Dave Shultz)*

  • 9:00 – 9:40am: **Caroline Saouma** (University of Utah)
    “Novel Approaches for CO₂ Reduction Catalysis”

  • 9:40 – 10:20am: **Ted Betley** (Harvard University)
    “Engineering high-spin electronic states via direct and double exchange.”

  • 10:20 – 10:40am: Coffee break

  • 10:40 – 11:20am: **Jeremy Smith** (Indiana University)
    “Magnetic Properties of 3d Nitride Complexes in Three-fold Symmetry”
• 11:20 – 12:00pm: Jeff Rinehart (University of California at San Diego)  
“Law and (magnetic) order in colloidal metal nanoparticles - Molecular magnetism as a guide to better defining the properties of nanoscale systems.”

• Lunch and afternoon free

• 7:30pm: Conference Banquet at Rustico Ristorante (http://www.rusticoristorante.com)

Saturday, June 27
• 8:30 – 9:00am: Continental breakfast at the Telluride Elementary School

• Morning Session (Chair: Jim McCusker)
  • 9:00 – 9:40am: Dave Shultz (North Carolina State University)  
  • 9:40 – 10:20am: Matt Shores (Colorado State University)  
  “Switching Magnetic Behaviors in Complexes with Atomic Number Containing a ”2””
  • 10:20 – 10:40am: Coffee break
  • 10:40 – 11:20am: Phil Duxbury (Michigan State University)  
  “Ultrafast Photo-induced Phase Transitions in the Solid State”
  • 11:20 – 12:00pm: Jim McCusker (Michigan State University)  
  “The Thermodynamic Effects of Zero-field Spin Exchange”
  • 12:00 – 12:30pm: Discussion/Summary

End of Conference