

Zero-field Spin Effects in Chemical Systems

Organizers

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(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)
“Donor-Acceptor Biradicals in Ground- and Excited States. Photophysics of Planar, Pt(II) Complexes with Donor-Acceptor Chromophores having Covalently-attached Stable Radicals”
 - 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