LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

SD1: Electronic and Magnetic Materials
Juana Moreno
Louisiana State University

FOCUS 1
Multiscale Methods for Strongly Correlated Materials

FOCUS 2
Correlated Organic & Ferroelectric Materials

FOCUS 3
Superconducting Materials
We need faster, smaller, more efficient devices

• By 2020 a transistor in a chip may reach the size of a few atoms
• To continue Moore’s law we need to use other degrees of freedom
  • E.g., a single flux quantum transistor
We need faster, smaller, more efficient devices

- Materials studied by LA-SiGMA promise devices employing other degrees of freedom
  - Magnetic semiconductors use both spin and charge
  - Magnetic nanoparticles instead of domains
  - Multiferroics use both spin and polarization

Magnetic semiconducting devices

Iron-oxide nanoclusters for memory devices
Strongly Correlated Systems: Complexity and Competing Orders

- Competing phases emerge as a function of control parameter.
- Electron correlations at different length scales.
- Correlations lead to complex spin, charge, and orbital phases.
- Tunability allows device applications.

Phase diagram of MnFeCoSi

Fe_{1-x} Co_{x} Si nanowire, Rebar & DiTusa

SD1: Electronic and Magnetic Materials

**Development Multiscale Methods**
Tulane, LSU

- Non-local Approximations for DFT
- Multiscale Many-Body approach

**Electronic & Magnetic Materials**

**Superconducting Materials**
Southern, LSU, UNO, Tulane

- Iron-based superconductors
- Cuprate superconductors

**Correlated Organic & Ferroelectric Materials**
Tulane, LA Tech, Grambling, UNO, Xavier, LSU

- Metallo-organics
- Oxide clusters
- Multiferroic composites
Focus 1: Computing at the Petascale: dual-fermion mean-field embedding

- QMC for short length scales
- Dual-Fermion diagrammatics for intermediate length scales
- Mean-field approximation for long length scales
- QMC scales exponentially with problem size, while multi scale approaches scale algebraically.

Metal-insulator transition as a function of disorder and interaction strength.

Multi scale approaches could lead to simulations of electronic and magnetic materials with predicted capabilities.

Yang et al., unpublished
Focus 1: Non-local Approximations for Density Functional Theory

Perdew’s group developed a new computationally-efficient semilocal meta-GGA (MGGA) accurate for strong and weak bonds. This will allow an efficient modeling of molecules, surfaces, and solids with same DFT functional

Errors in lattice constants of ionic insulators and semiconductors from different functionals..

<table>
<thead>
<tr>
<th>solids</th>
<th>LDA</th>
<th>PBE</th>
<th>M06L</th>
<th>revTPSS</th>
<th>MGGA_MS2</th>
<th>Expt</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.022</td>
<td>0.014</td>
<td>-0.010</td>
<td>0.003</td>
<td>-0.007</td>
<td>3.555</td>
</tr>
<tr>
<td>Si</td>
<td>-0.017</td>
<td>0.046</td>
<td>-0.010</td>
<td>0.017</td>
<td>0.005</td>
<td>5.422</td>
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<tr>
<td>Ge</td>
<td>-0.013</td>
<td>0.124</td>
<td>0.137</td>
<td>0.038</td>
<td>0.005</td>
<td>5.644</td>
</tr>
<tr>
<td>GaAs</td>
<td>-0.026</td>
<td>0.111</td>
<td>0.143</td>
<td>0.039</td>
<td>0.002</td>
<td>5.641</td>
</tr>
<tr>
<td>NaCl</td>
<td>-0.098</td>
<td>0.130</td>
<td>0.117</td>
<td>0.102</td>
<td>0.029</td>
<td>5.565</td>
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<tr>
<td>MgO</td>
<td>-0.018</td>
<td>0.073</td>
<td>0.012</td>
<td>0.052</td>
<td>0.019</td>
<td>4.188</td>
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<tr>
<td>ME</td>
<td>-0.032</td>
<td>0.083</td>
<td>0.065</td>
<td>0.042</td>
<td>0.009</td>
<td></td>
</tr>
<tr>
<td>MAE</td>
<td>0.032</td>
<td>0.083</td>
<td>0.072</td>
<td>0.042</td>
<td>0.011</td>
<td></td>
</tr>
</tbody>
</table>


First Principles Study of Electronic Properties of Ca$_{10}$(Pt$_3$As$_8$)(Fe$_2$As$_2$)$_5$, E. Hilliard et al, Proceedings p. 61. Ca-Fe-Pt-As family with $T_c = 11 – 35$ K. First reported computed ground state of this parent material showing an AFM state.
Using a Wannier function-based first-principles method study the Mn valence state in GaMnN.

Mn-$d_{yz}$ and (b) N-$sp^3$ Wannier orbitals.

Effect of molecule-contact distance and coordination geometry of clip atom in I-V characteristics of thiophenes containing cobalt bisdicarbollide.

HOMO-2 (-0.326 eV)
Density Functional Theory Revisited: The Mathematical and Physical Conditions for the Physical Content of the Eigenvalues, Bagayoko et al., Proc. p. 21

The Bagayoko-Zhao-Williams method as enhanced by Ekuma-Franklin using optimal basis sets.

First Principles Simulation on the Graphene Defect and H$_2$O Molecule Interaction. S. Yang et al., Proc. P. 57

Silicon atoms (yellow), oxygen (red), carbon (black), hydrogen (white)

A 2-D contour plot of the electron charge density in w-ZnO. Note well that in the vicinity of atomic sites, one finds spherical symmetry. For the valence electrons, polarization (i.e., p, d and f) prime spherical symmetry as found in the work of Ekuma and Franklin (EF)

C. Ekuma and Fanklin
## SD1 Focus 1 Milestones

<table>
<thead>
<tr>
<th>Milestones</th>
<th>Y1</th>
<th>Y2</th>
<th>Y3</th>
<th>Y4</th>
<th>Y5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop continuous time QMC solver for 16-way multicore supercomputers.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Incorporate long-range van der Waals corrections to semi-local DFT potentials into widely used codes by Y3.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Develop MSMB solver able to treat multiple correlated orbitals.</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Port hyperparallel codes to NSF national leadership class machines (Blue Waters).</td>
<td>X</td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
</tbody>
</table>

* Unforeseen difficulties in finding an effective cut off strategy for the short range correlations delayed the porting to widely used codes.
Focus 2
Iron Oxide Molecular Clusters as Building Blocks of Non-Volatile Memory (Xavier, Tulane, UNO)

Computational/Experimental effort to synthesize spinel-type iron oxide clusters, and investigate their ground state using QM/MM approach.

Synergy with SD2.
Strong collaboration between modeling and experiments.

Elementary clusters derived from spinel-type structures are candidates for molecular magnets which can be used for high capacity memory devices.

Structure and Properties of Fe₂O₃ Based Single Molecular Magnets
Focus 2: Synthesis and Processing of Nanoscale Multiferroic Structures (UNO)

It is not known whether the magnetoelectric coupling properties are retained in nanostructured multiferroics. Maximize the coupling between the ferroelectric and magnetostrictive phases and enhance the ME response at room temperature.

Phase and amplitude curves of the piezoresponse of the PbTiO$_3$-NiFe$_2$O$_4$ bilayered structure under different magnetic fields.

Caruntu et al., Probing the local strain-mediated magnetoelectric coupling in multiferroic nanocomposites by magnetic field, Nanoscale (2012)
## SDI Focus 2 Milestones

<table>
<thead>
<tr>
<th>Milestones</th>
<th>Y1</th>
<th>Y2</th>
<th>Y3</th>
<th>Y4</th>
<th>Y5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test array of DFT functionals for prediction of metalloporphyrin and ferroelectric properties.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Prepare and measure electrical/magnetic properties of metalloporphyrin.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Develop experimentally validated computational models for organic magnets, organometallics and ferroelectric systems using measurements as guide.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Develop multiscale models of organometallics, organic magnets systems using DFT parameters.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Predict properties of organometallics and ferroelectrics and compare with experiments.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Prepare organic magnets, organometallics and ferroelectrics.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Predict properties of ferroelectrics using new nonlocal meta-GGA DFT functionals.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>
What is the pairing mechanism in pnictides?

Tulane/UNO/LSU collaboration: Unusual interplay between magnetism and superconductivity in iron chalcogenide Fe$_{1.02}$ (Te$_{1-x}$ Se$_x$)

Bulk superconductivity occurs only when the ($\pi$, 0) magnetic correlations are strongly suppressed and spin fluctuations near ($\pi$, $\pi$) become dominant.


J. Hu et al, Proc. p. 13
Superconductivity on triangle lattices in organic materials & cobaltates: interplay between strong electron correlations and spin frustration

Large-scale cluster QMC simulations predict a chiral $d+id$ singlet superconducting phase in the hole-doped Hubbard model on the triangular lattice.

The pairing is due to antiferromagnetic spin fluctuations at the magnetic order wavevector nesting the deformed Fermi surface.

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<th>Milestones</th>
<th>Y1</th>
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<th>Y3</th>
<th>Y4</th>
<th>Y5</th>
<th>On Track</th>
</tr>
</thead>
<tbody>
<tr>
<td>Address the bottlenecks and numerical instabilities in the parquet equations by employing better parallel linear systems solvers and develop multiband parquet codes.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>Completed</td>
</tr>
<tr>
<td>Incorporate Ramanujam’s advanced tensor rotation and contraction methods (Tensor Contraction Engine) into parquet codes.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td>Completed</td>
</tr>
<tr>
<td>Use hybrid QMC to address the origin of the QCP and competing order in cuprate models.</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td>On Track</td>
</tr>
<tr>
<td>Study overscreening in pnictide models using new Hyper-GGA functionals.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td>On Track</td>
</tr>
<tr>
<td>Use methods that combine LDA models obtained from downfolding and DCA/MSMB to study correlation and phonon effects in the pnictides.</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td>On Track</td>
</tr>
</tbody>
</table>
**Workforce development & External Engagement**

4 of the 5 graduate level distance-learning courses taught by SD1 faculty and international collaborators

**High-Performance Computing** short course at students & faculty at Baton Rouge Community College

Super Science Saturday, Baton Rouge, October 26, 2012. Over 1,600 people attended

NanoDays in Baton Rouge, March 30 & April 6, 2013. Over 500 visitors

Public talks by DiTusa & Kurtz

Balloon Nanotube at the **2013 NanoDays** hosted at the Louisiana Art & Science Museum, Baton Rouge
LSU’s Center for Computation & Technology (CCT) and Innovation through Institutional Integration (I3) at the LSU Office of Strategic Initiatives invite all summer research programs to attend

Minorities in STEM Panel
Moderated by: Joel Tohline, LSU CCT, Director

Tuesday, July 30, 2 p.m. - 4 p.m.
130 Nicholson Hall

Guest Speakers

John Harkless
Associate Professor of Chemistry
Howard University, DC
He obtained his B.S. from Morehouse College, and his Ph.D. at the University of California at Berkeley. His research interests are Quantum Monte Carlo wavefunction development, Electronic structure of metallic systems, and Electronic excitations.

Janet B. Ruscher
Professor of Psychology and the Associate Dean for Graduate Programs in Science and Engineering
Tulane
She joined the Tulane faculty in 1991 after earning the Ph.D. in experimental social psychology from the University of Massachusetts at Amherst. Prior to assuming her current administrative position, she served for 9 years as Department Chair. Her primary research lies at the interface of social cognition, prejudice, and language. These topics include subtle (as opposed to blatant) prejudiced language, cross-race performance feedback, and the persistence of stereotypes in conversation.

Zakiya Wilson
Assistant Director of Graduate Studies in Chemistry and Executive Assistant of Strategic Initiatives
Louisiana State University

On the agenda

- Why it is important to have a diverse pool of people in research groups
- How to recruit minorities and women to the sciences and how to mentor & retain them
- How to avoid unintentional and implicit biases

Refreshments at 3:30 p.m.