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

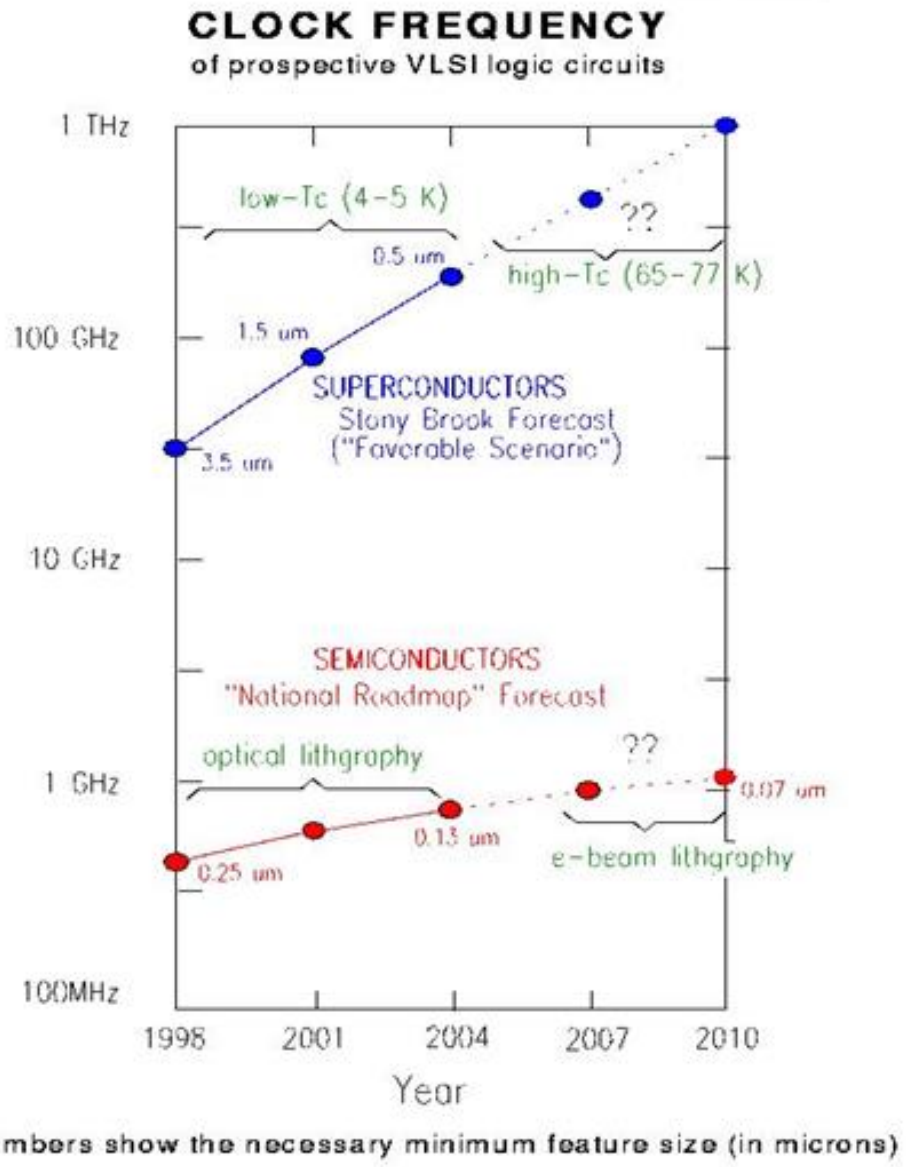
Correlated Organic & Ferroelectric Materials

FOCUS 3

Superconducting Materials

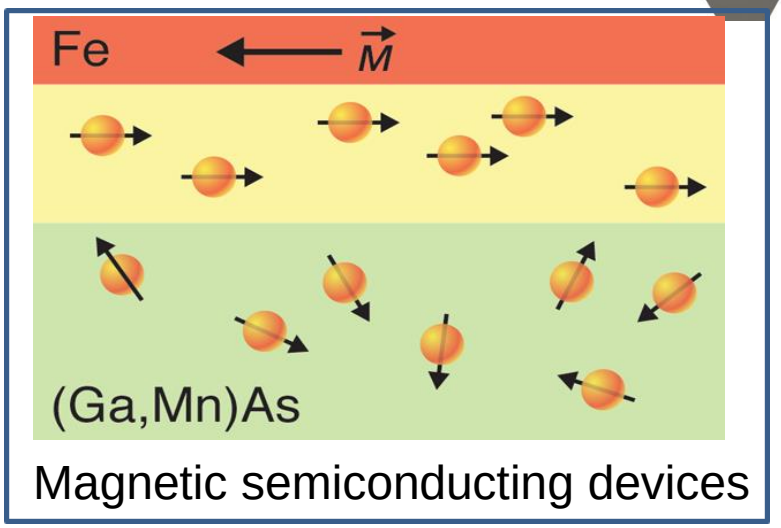
We need faster, smaller, more efficient devices

- 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

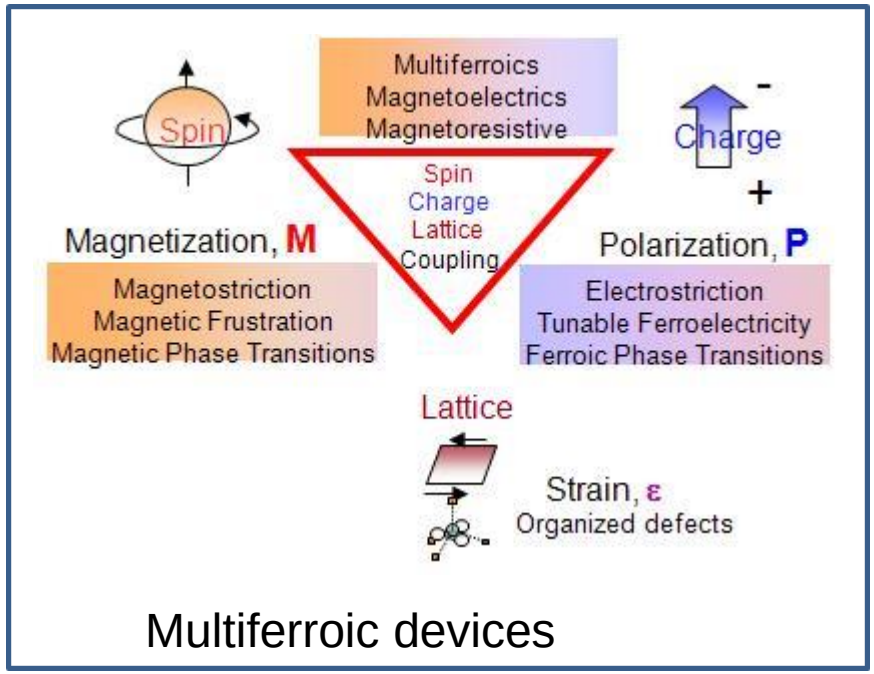


We need faster, smaller, more efficient devices

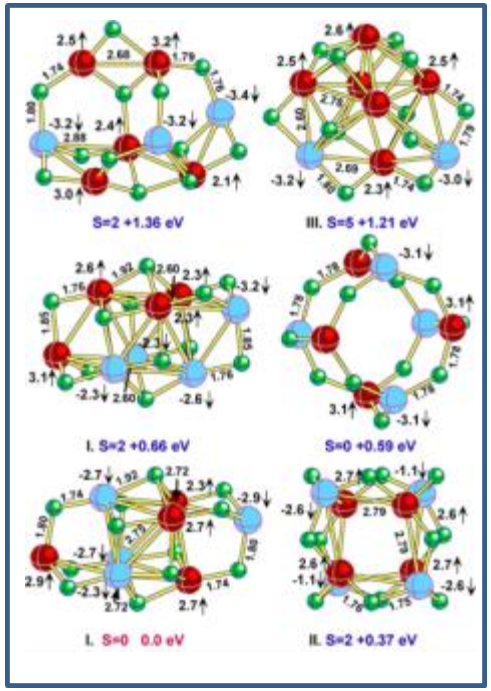
- Materials studied by LA-SiGMA promise devices employing other degrees of freedom
  - Magnetic semiconductors use both spin and charge
  - Magnetic nanoparticles instead of domains
  - Multiferroics use both spin and polarization



Magnetic semiconducting devices



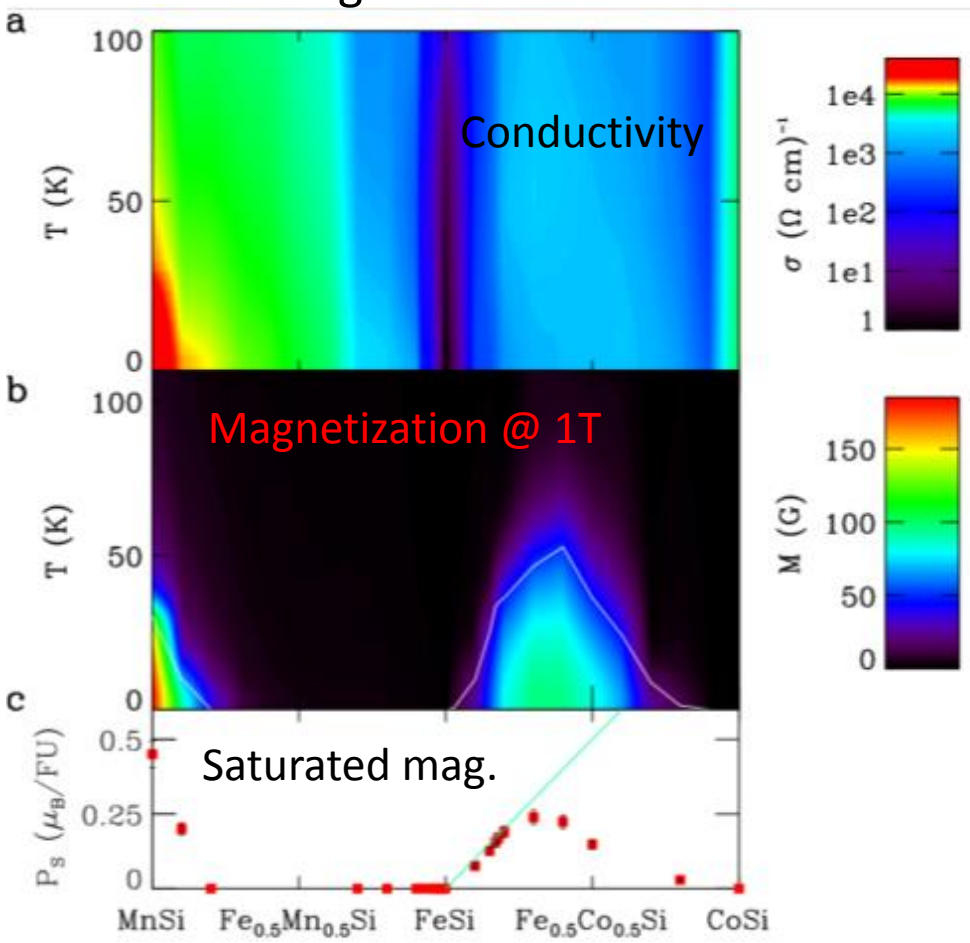
Multiferroic devices



Iron-oxide nanoclusters for memory devices

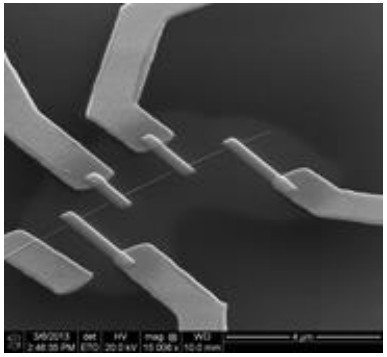
Strongly Correlated Systems: Complexity and Competing Orders

Phase diagram of MnFeCoSi



- 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.

$Fe_{1-x}Co_xSi$ nanowire, Rebar & DiTusa



Manyala et al, Nature 2000; Nature 2008

SD1: Electronic and Magnetic Materials

Development Multiscale Methods

Tulane, LSU

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

Correlated Organic & Ferroelectric Materials

Tulane, LA Tech, Grambling, UNO, Xavier, LSU

- Metallo-organics
- Oxide clusters
- Multiferroic composites

Electronic & Magnetic Materials

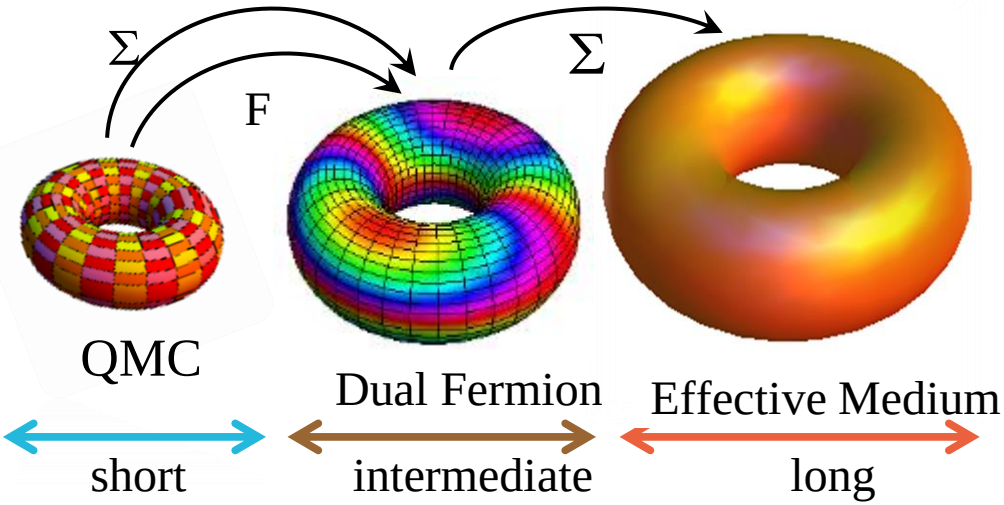
Superconducting Materials

Southern, LSU, UNO, Tulane

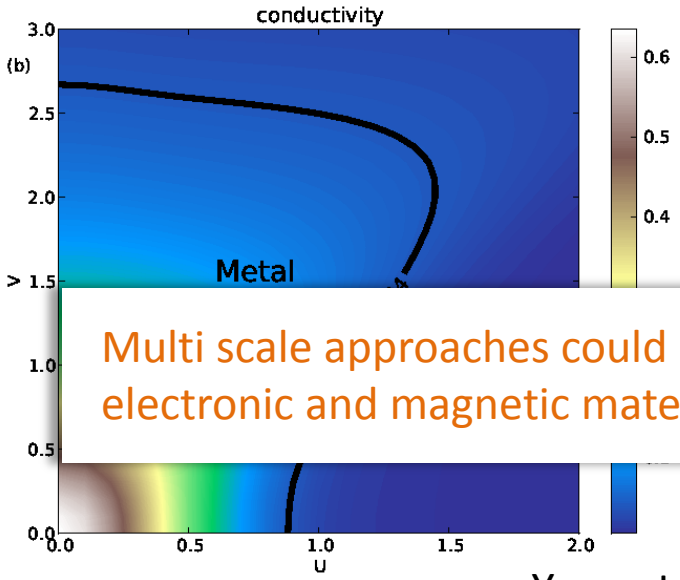
- Iron-based superconductors
- Cuprate superconductors

Focus 1: Computing at the Petascale: dual-fermion mean-field embedding

SD1 & CTCI



- 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

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

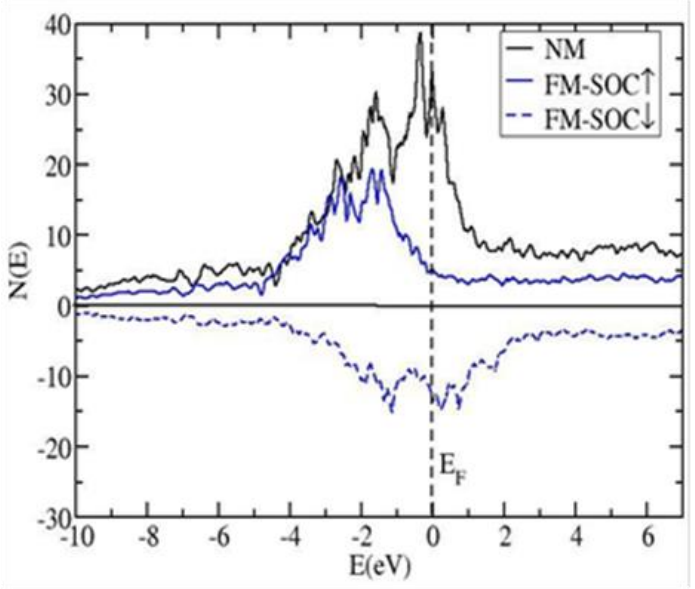
Errors in lattice constants of ionic insulators and semiconductors from diferent functionals..

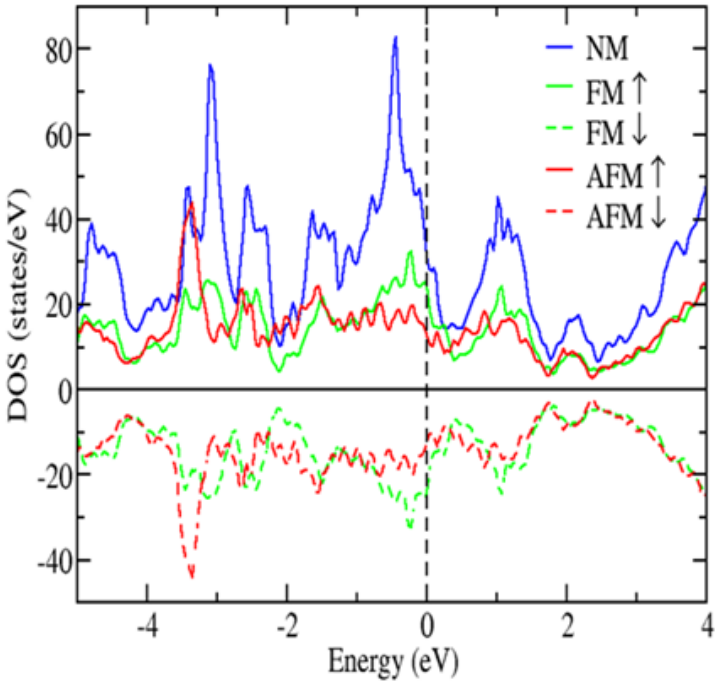
solids	LDA	PBE	M06L	revTPSS	MGGA_MS2	Expt.
C	-0.022	0.014	-0.010	0.003	-0.007	3.555
Si	-0.017	0.046	-0.010	0.017	0.005	5.422
Ge	-0.013	0.124	0.137	0.038	0.005	5.644
GaAs	-0.026	0.111	0.143	0.039	0.002	5.641
NaCl	-0.098	0.130	0.117	0.102	0.029	5.565
MgO	-0.018	0.073	0.012	0.052	0.019	4.188
ME	-0.032	0.083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

J. Sun et al., unpublished (2013);
J. Sun et al., J. Chem. Phys. (2013)

Focus 1: Non-local Approximations for Density Functional Theory

Electronic properties of Fe_3Ga_4: An Ab-initio Study, **C. Ekuma et al., Proceedings p. 53.** Ferromagnetic ground state corroborated by experimental results of **Mendez et al., Proceedings p. 93**

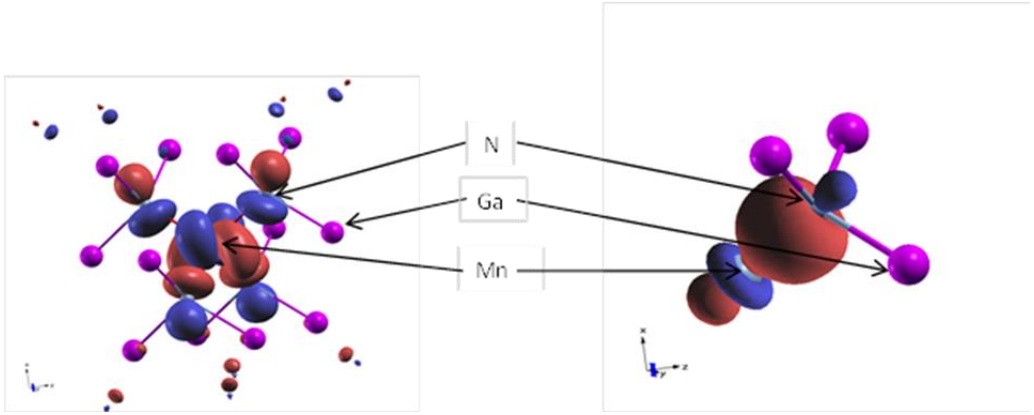




First Principles Study of Electronic Properties of $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$, **E. Hilliard et al, Proceedings p. 61.**

Ca-Fe-Pt-As family with T_c =11 – 35 K.

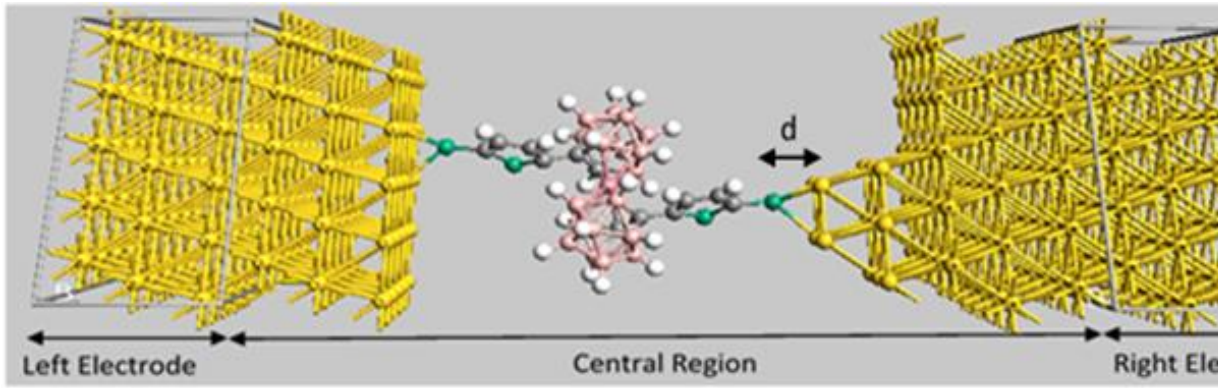
First reported computed ground state of this parent material showing an AFM state.

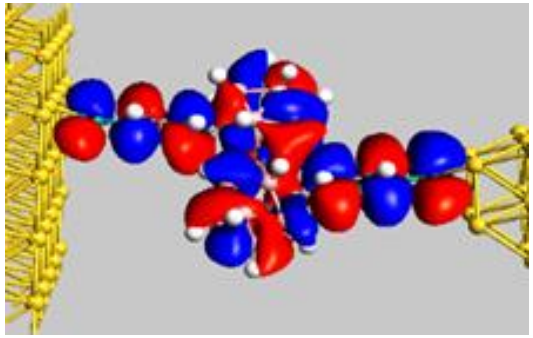


Mn-d_{yz} and (b) N-sp^3 Wannier orbitals.

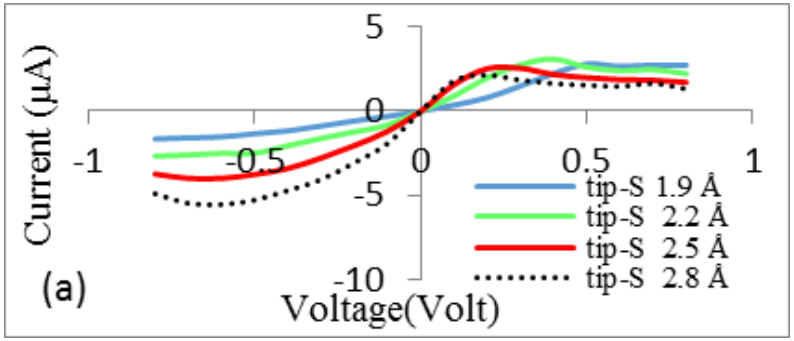
Ryky Nelson et al, Proceedings p. 37
Using a Wannier function-based first-principles method study the Mn valence state in GaMnN.

Effect of molecule-contact distance and coordination geometry of clip atom in I-V characteristics of thiophenes containing cobalt bisdicarbollide.
Anjana Paudyal et al, Proc. p. 41.

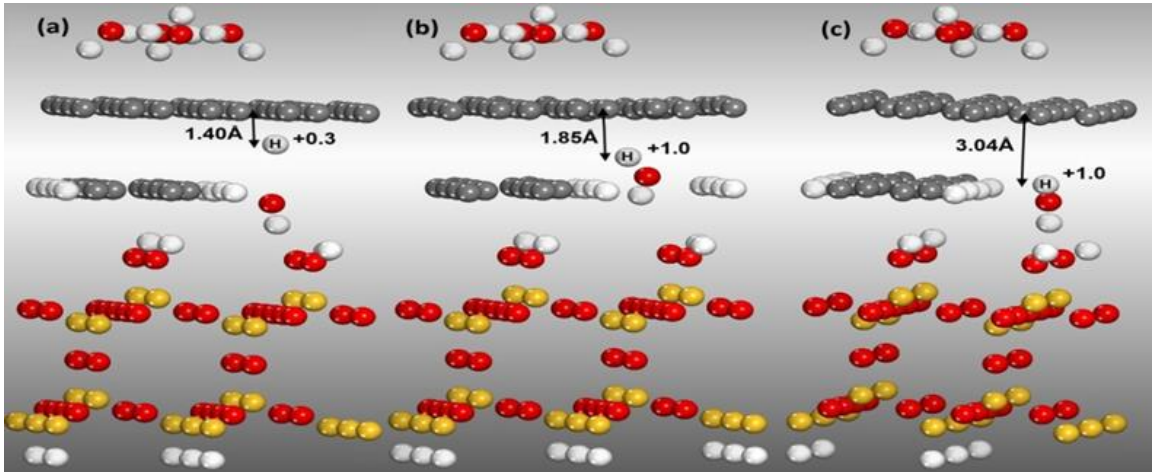




HOMO-2 (-0.326 eV)

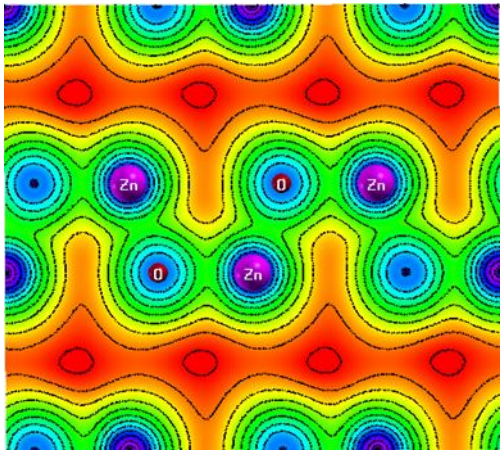


First Principles Simulation on the Graphene Defect and H_2O Molecule Interaction.
S. Yang et al., Proc. P. 57



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

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.



C. Ekuma and Fanklin

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)

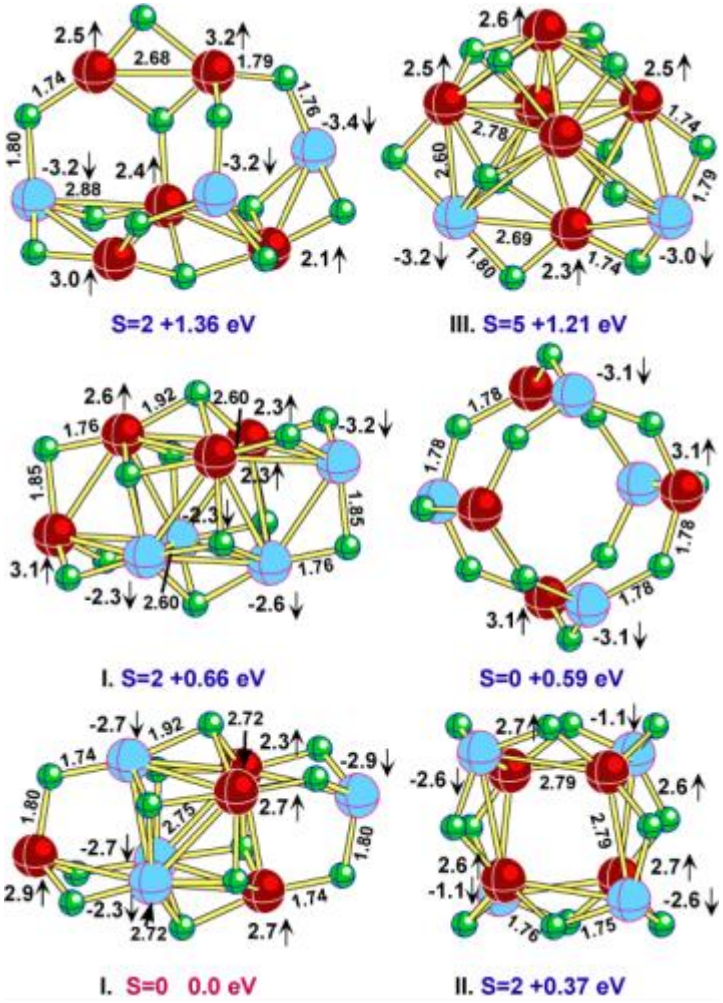
SD1 Focus 1 Milestones

Milestones	Y1	Y2	Y3	Y4	Y5	
Develop continuous time QMC solver for 16-way multicore supercomputers.	X	X				*Completed*
Incorporate long-range van der Waals corrections to semi-local DFT potentials into widely used codes by Y3.		X	X			*In progress**
Develop MSMB solver able to treat multiple correlated orbitals.		X	X	X		*On target*
Port hyperparallel codes to NSF national leadership class machines (Blue Waters).			X	X	X	*On target*

* Unforeseen difficulties in finding a 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)

SD1 & CTCI, SD2



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

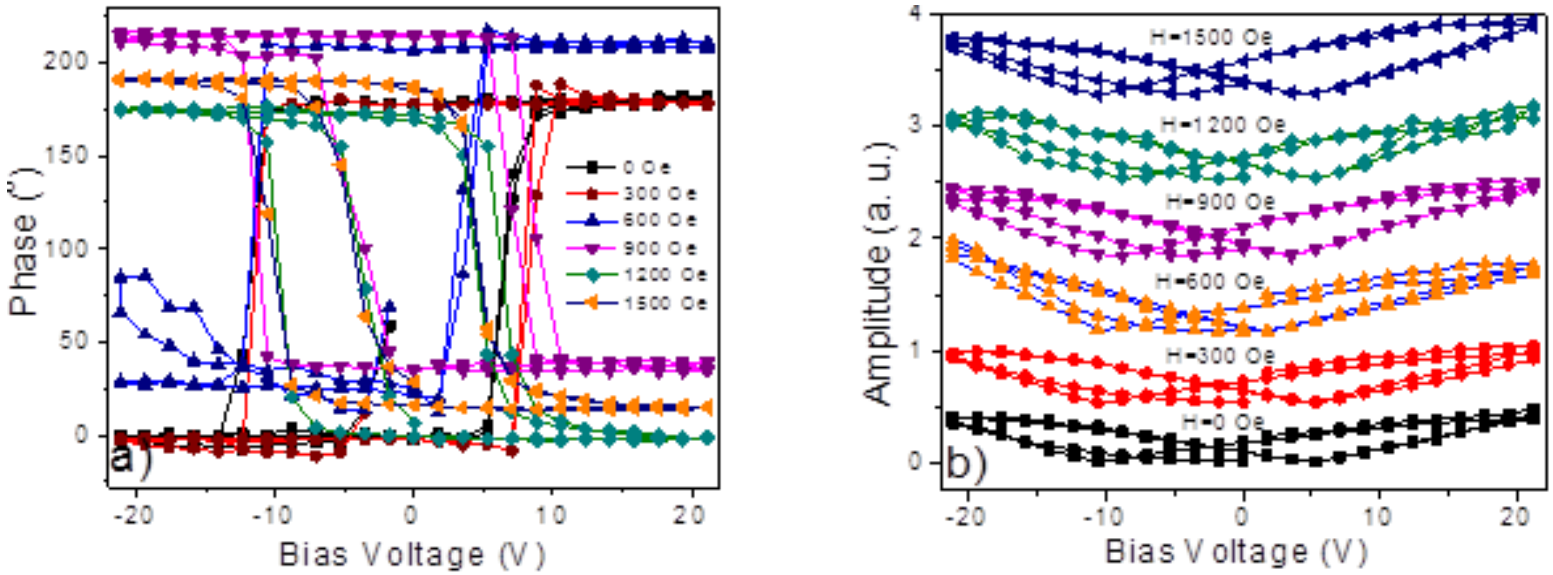
Synergy with SD2. Strong collaboration between modeling and experiments.

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 Fe_2O_3 Based Single Molecular Magnets
J. M. Leveritt et al, Proc. p. 161; also **P. Kucheryavy et al., Proc. p. 165**

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 $PbTiO_3$-$NiFe_2O_4$ bilayered structure under different magnetic fields.

Caruntu et al., *Probing the local strain-mediated magnetoelectric coupling in multiferroic nanocomposites by magnetic field*, Nanoscale (2012)

SD1 Focus 2 Milestones

Milestones	Y1	Y2	Y3	Y4	Y5	
Test array of DFT functionals for prediction of metalloporphyrin and ferroelectric properties.	X	X				*Completed*
Prepare and measure electrical/magnetic properties of metalloporphyrin.	X	X				*Completed*
Develop experimentally validated computational models for organic magnets, organometallics and ferroelectric systems using measurements as guide.		X	X	X	X	*On Track*
Develop multiscale models of organometallics, organic magnets systems using DFT parameters.			X	X	X	*On Track*
Predict properties of organometallics and ferroelectrics and compare with experiments. .			X	X	X	*On Track*
Prepare organic magnets, organometallics and ferroelectrics.	x	x	X	X	X	*On Track*
Predict properties of ferroelectrics using new nonlocal meta-GGA DFT functionals.			X	X	X	*On Track*

Focus 3

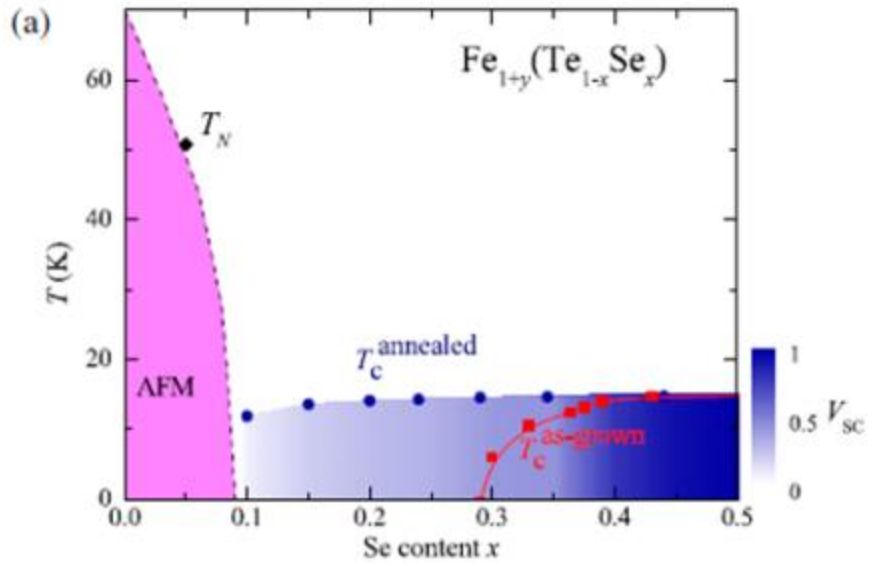
Superconducting Materials

What is the pairing mechanism in pnictides?

SD1 & CTCI

Tulane/UNO/LSU collaboration:
Unusual interplay between magnetism and superconductivity in iron chalcogenide $Fe_{1.02}$ (Te_{1-x} Se_x)

Collaboration with NIST , SLAC & researchers in China, Germany and France.



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

Liu et al., Nature Materials 9, 716 (2010) , Liu et at. Phys. Rev. Lett.. 110 037003 (2013).

J. Hu et al, Proc. p. 13

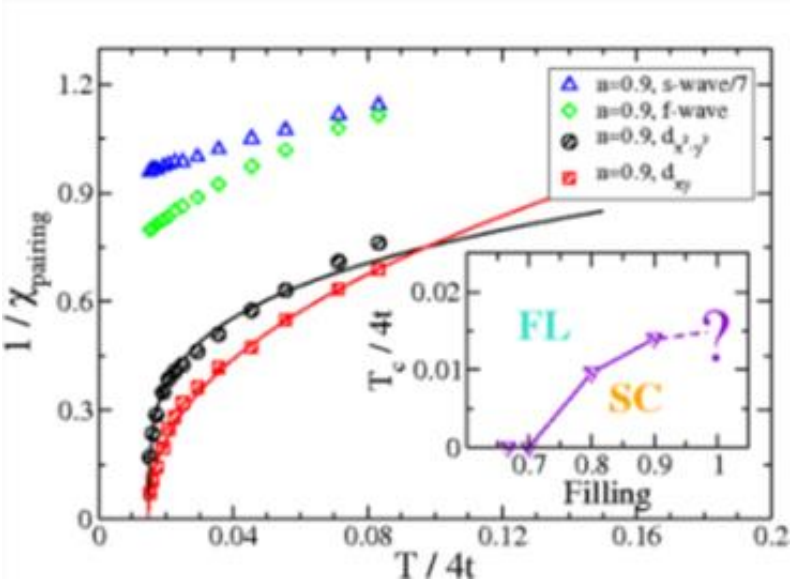
Focus 3

Superconducting Materials

What is the pairing mechanism in cobaltates? Organic salts?

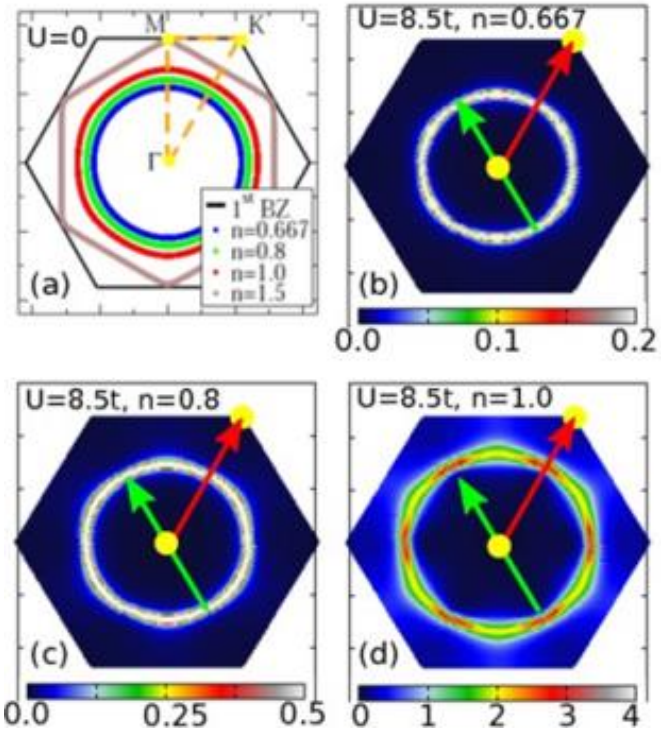
SD1 & CTCI

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.

K.S Chen et al., Phys. Rev. B (2013)



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

SD1 Focus 3 Milestones

Milestones	Y1	Y2	Y3	Y4	Y5	
Address the bottlenecks and numerical instabilities in the parquet equations by employing better parallel linear systems solvers and develop multiband parquet codes.	X	X	X	X	X	*On Track*
Incorporate Ramanujam's advanced tensor rotation and contraction methods (Tensor Contraction Engine) into parquet codes.	X	X				*Completed*
Use hybrid QMC to address the origin of the QCP and competing order in cuprate models.	X	X				*Completed*
Study overscreening in pnictide models using new Hyper-GGA functionals.	X	X	X			*On Track*
Use methods that combine LDA models obtained from downfolding and DCA/MSMB to study correlation and phonon effects in the pnictides.	X	X	X	X	X	*On Track*

Workfoce development & External Engagement

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

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

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
- Janet B. Ruscher
  Professor of Psychology and the Associate Dean for Graduate Programs in Science and Engineering
  Tulane
- 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.

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

She received her B.S., cum laude, from Jackson State University and her Ph.D. in Inorganic Chemistry, from LSU. Within the Office of Strategic Initiatives, she works collaboratively with the Vice Chancellor and program managers to increase and improve the educational experiences of students.

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LA-SiGMA