LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

SD1: Electronic and Magnetic Materials

Mark Jarrell

Extend local approximations [Density Functional Theory (DFT) and Dynamical Mean Field Approximation (DMFA)] to multi-scale approaches.

FOCUS 1

Multiscale Methods for Strongly Correlated Materials

FOCUS 2

Correlated Organic & Ferroelectric Materials

FOCUS 3

Superconducting Materials

SD1 Research Themes

Electronic & Magnetic Materials

Development Multiscale Methods

Tulane, LSU

- Non-local Approximations for DFT
- Multiscale Many-Body approach
- Inverse LEED method for structural investigations

Organic & Ferroelectric Materials

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

- Metalloporphyrins
- Oxide clusters
- Multiferroic composites

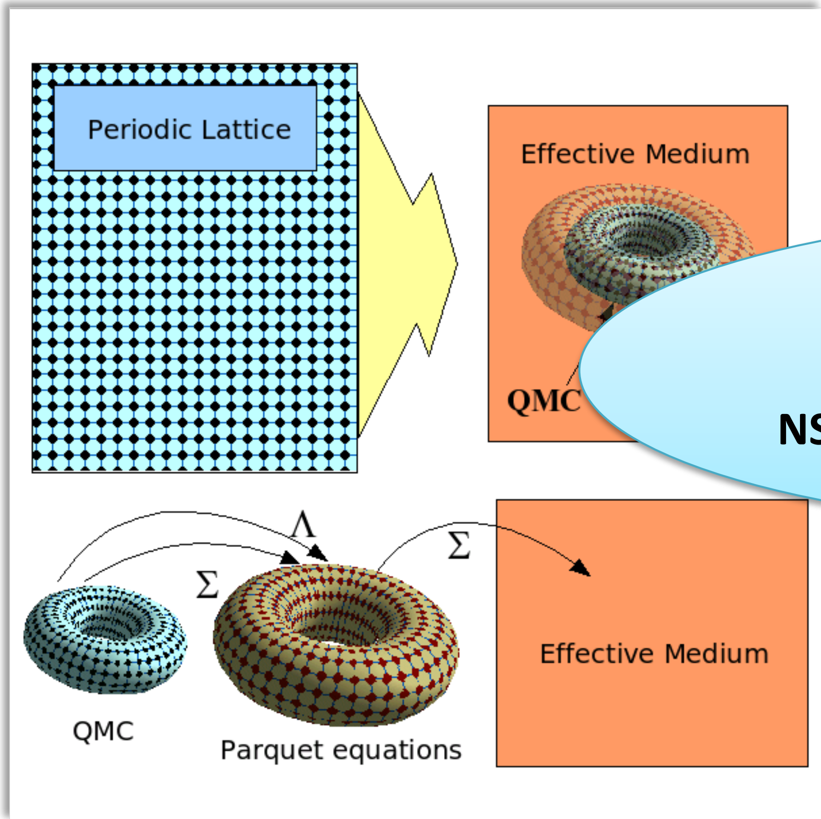
Superconducting Materials

Southern, LSU, UNO, Tulane

- Iron-based superconductors
- Cuprate superconductors

Focus 1: Multiscale Methods for Correlated systems
Computing at the Petascale: Multiscale Many Body

SD1 & CTCI



- QMC for short length scales
- Dual-Fermion diagrammatics for intermediate length scales
- … long
- … gebraically.

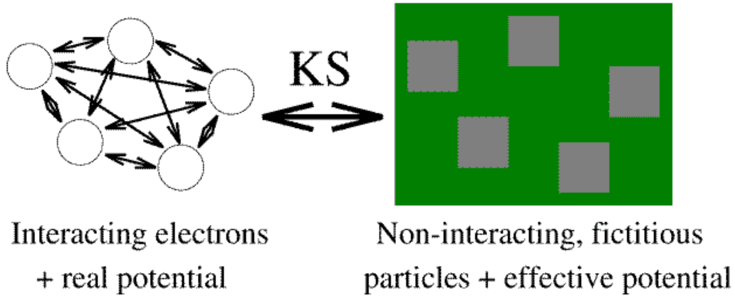
DOE Center and SciDAC Requests
NSF SAVI Request
NSF CRI Award (avail to all LA-SiGMA)

MSMB could lead to simulations of electronic and magnetic materials with predicted capabilities.

- *Dual Fermion Dynamical Cluster Approach for Strongly Correlated Systems*, S.-X. Yang, H. Fotso, H. Hafermann, K.-M. Tam, J. Moreno, T. Pruschke, M. Jarrell, PRB, 84, 155106
- *Solving the Parquet Equations for the Hubbard Model beyond Weak Coupling*, K.M. Tang, S.-X. Yang, H. Fotso, J. Moreno, J. Ramanujam, M. Jarrell. , arXiv:1108.4926.

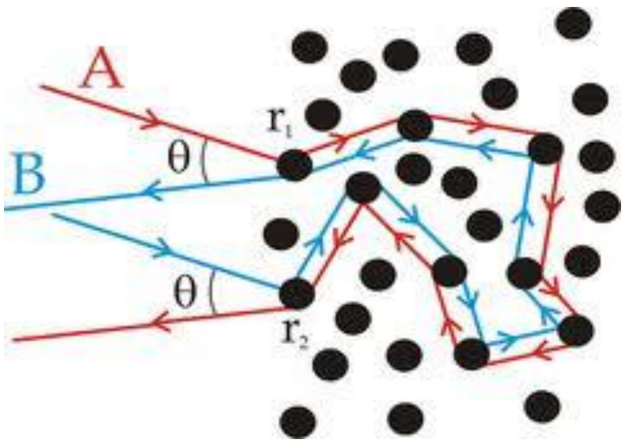
Focus 1

Development of First-Pinciples Multiscale Methods for Strongly Correlated Materials



- Non-local Approximations for Density Functional Theory
- Long-range van der Waals attractions between two distant objects,
  - $-C_6/R^6 - C_8/R^8 - C_{10}/R^{10} - ...$
- Combine LDA + Many Body
  - Poster by Ryky Nelson
- First-principles study of localization
  - Poster By Chinedu Ekuma

- J. Tao, J.P. Perdew, and A. Ruzsinszky, Proc. Nat. Acad. Sci. (USA) **109**, 18 (2012)
- J.P. Perdew, J. Tao, P. Hao, A. Ruzsinszky, G.I. Csonka, and J.M. Pitarke, submitted to J. Phys.: Condens. Matter
- J. Tao and J.P. Perdew, in preparation
- Ekuma Chinedu E.; Singh David J.; Moreno J.; et al. PRB, 85, 085205
- Chinedu E. Ekuma, M Jarrell, J. Moreno, and D. Bagayoko, AIP Advances 2, 012189 (2012).



Anderson localization

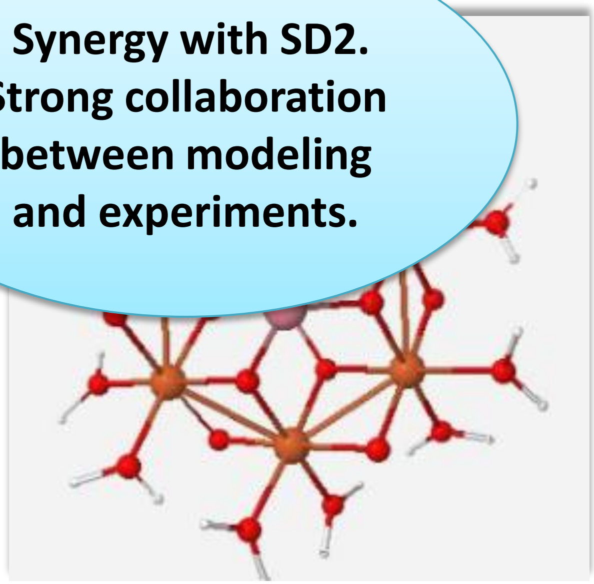
SD1 Focus 1 Milestones

Milestones	Y1	Y2	Y3	Y4	Y5	
Develop QMC solver for GPU supercomputers .	X	X				*On Track*
Incorporate Hyper-GGA functionals into common DFT codes including VASP.		X	X			*Ahead*
Develop MSMB solver able to treat multiple correlated orbitals.		X	X	X		*Ahead*
Port hyperparallel codes to NSF national leadership class machines (Blue Waters).			X	X	X	*Ahead*

Focus 2: Magnetic and Ferroelectric Materials
Iron Oxide Molecular Clusters as Building Blocks of Non-Volatile Memory (Xavier, Tulane, UNO)

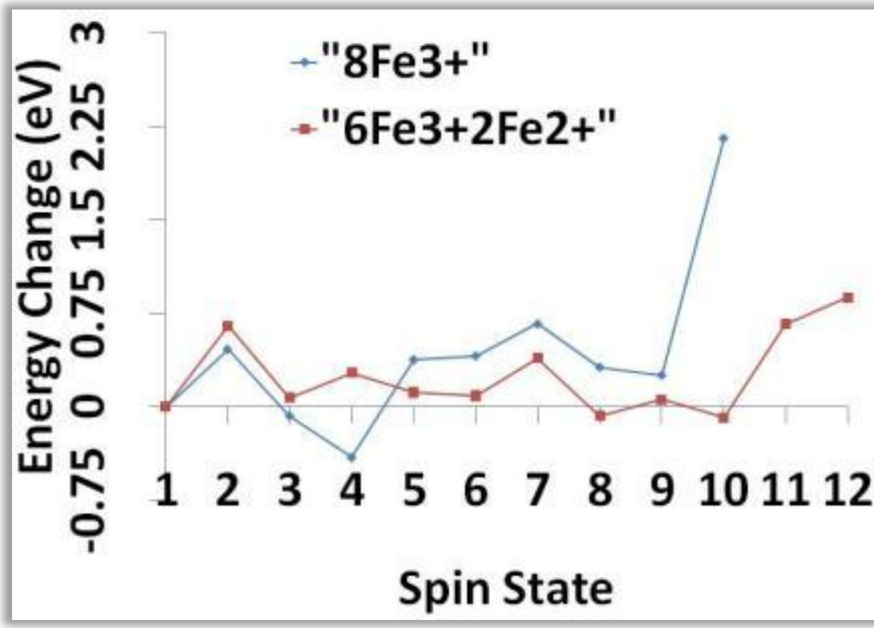
SD1 & CTCI, SD2

Synergy with SD2. Strong collaboration between modeling and experiments.



$Co_2Fe_6H_{24}O_{24}$ cluster. Spinel-type structure with water ligands.

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

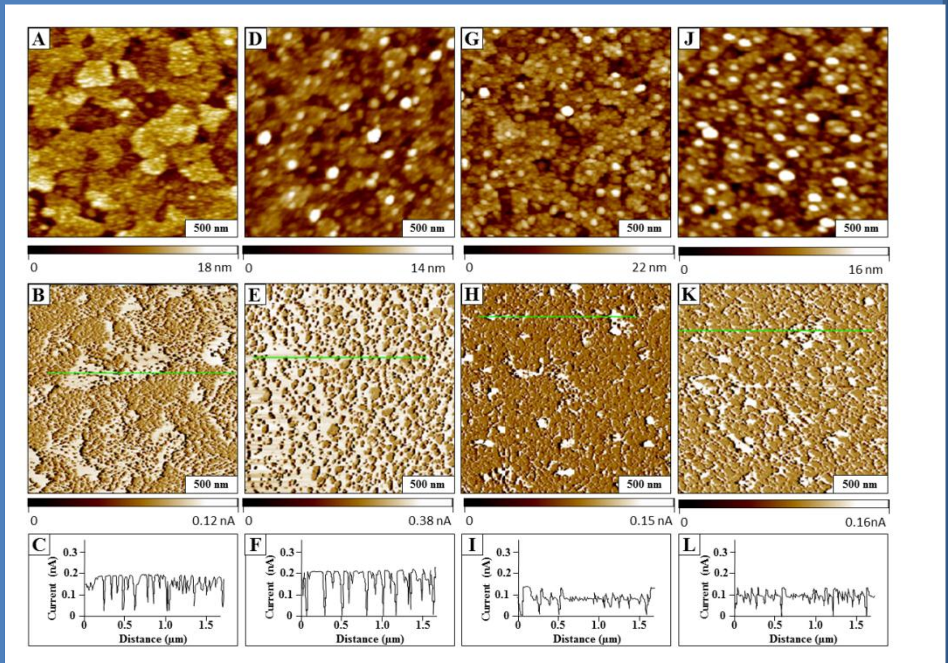


Elementary clusters derived from spinel-type structures are candidates for molecular magnets which can be used for high capacity memory devices.

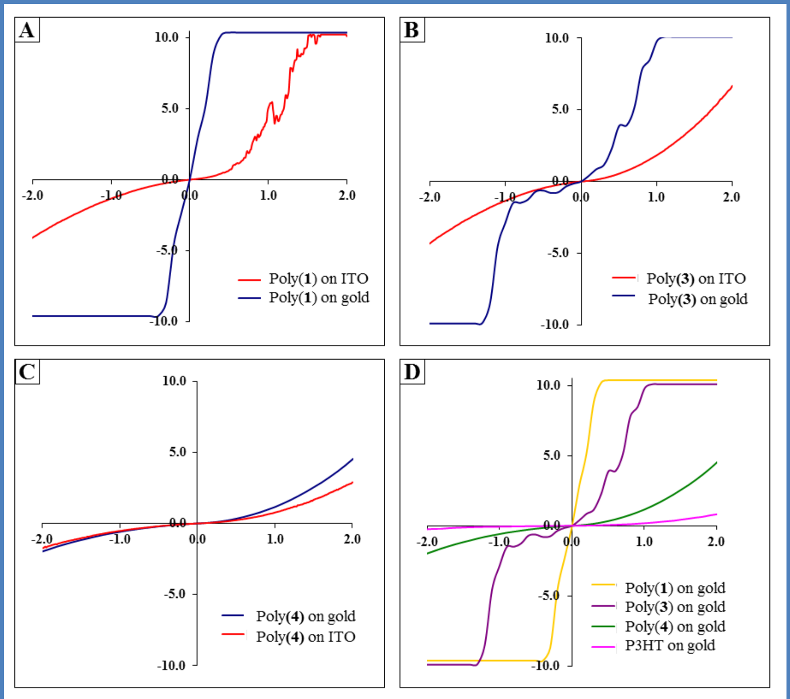
Predict charge transport in metalloporphyrins and compare with experiments (Garno)

AFM Current Imaging (fixed bias)

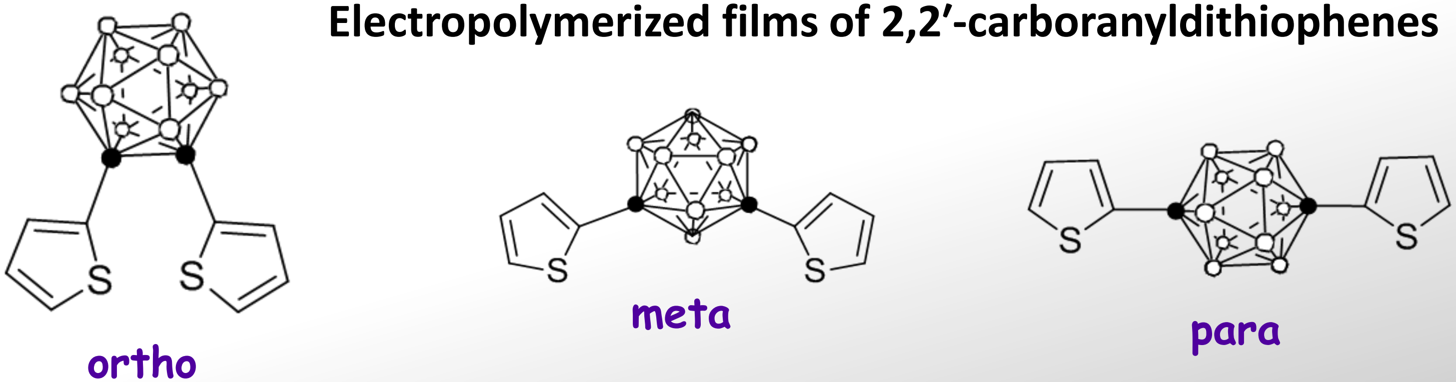
bare ITO ortho meta para



AFM I-V Spectra ITO vs Au substrates



Electropolymerized films of 2,2′-carboranyldithiophenes



SD1 & CTCI

Exploring the interplay between magnetism and electrical conduction in iron-based semiconductors and related materi...

LSU

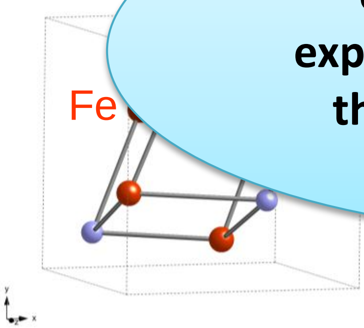
Small band gap insulators that can be doped into fe... create materials where disorder, magnetism, and crys... ...rise to novel phenomen...

Collaboration with researchers in Switzerland, Japan, Canada, and England.

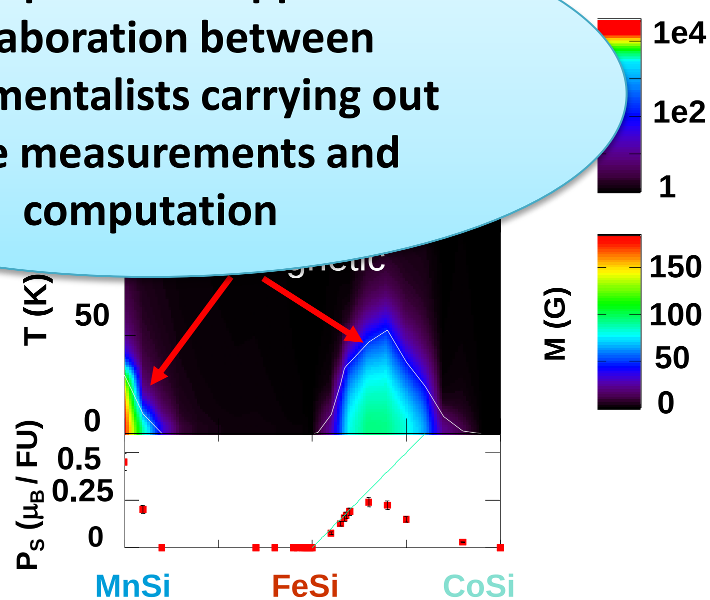
LaSigma provides support for a collaboration between experimentalists carrying out these measurements and computation

FeSi

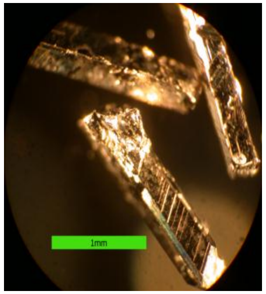
Fe



N. Manyala *et al*, Nature (2008)
N. Manyala et *al*, Nature (2000)

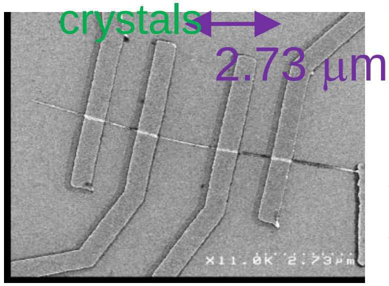


Magnetic semiconductor with high degree of carrier polarization that is compatible with silicon technology

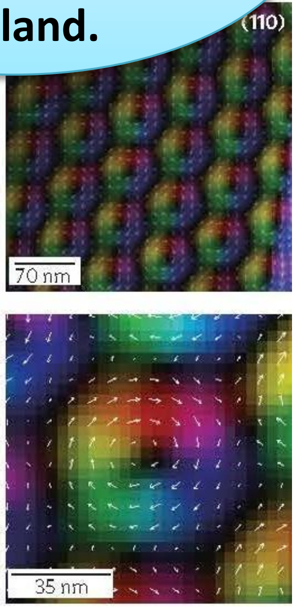


$Fe_{0.98}Co_{0.02}Si$

Single crystals



Nanowires



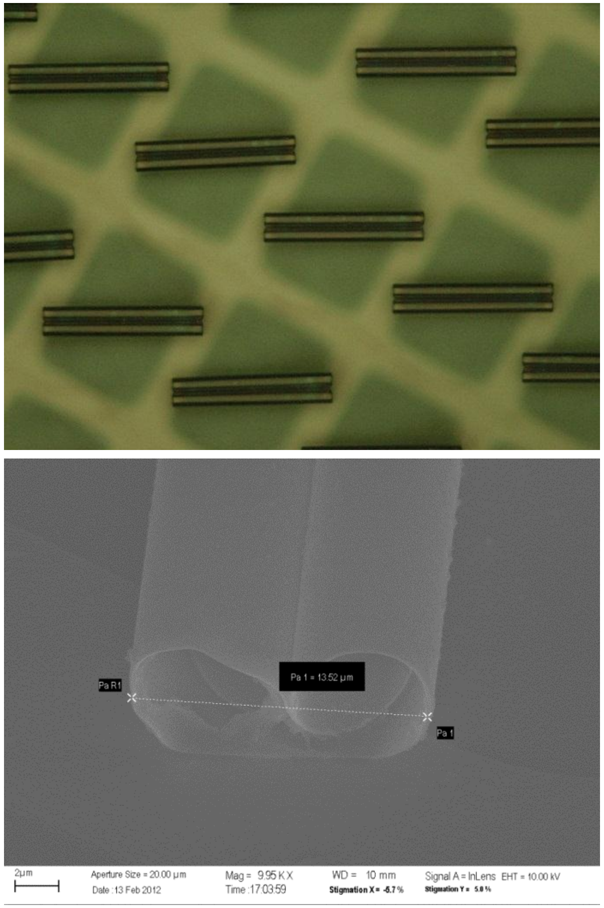
Novel Magnetic States: Skyrmions

X. Z. Yu *et al*. Nature Materials (2011)

UNO: L. Malkinski

SD1

Fabrication and properties of magnetic and multiferroic multi-wall tubes using stress engineering in bilayered film patterns



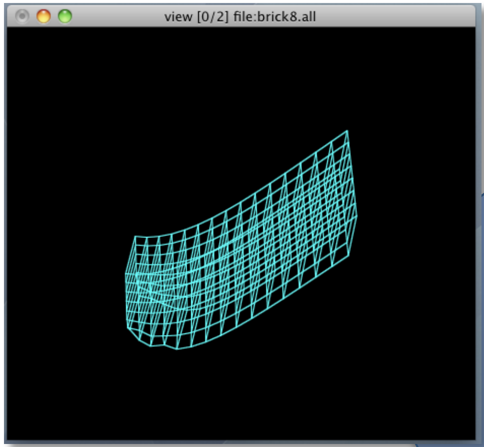
"Double barrelled shotgun" structures of /Au(5 nm)/AlN(20 nm)/CoFe(40 nm)/Au(5 nm)

Interfacial stresses between two layers of dissimialr materials can be used to form tubular or helical shapes of thin film patterns which roll when released from the sacrificial layer. Tubular shape of the structures alters their magnetic properties. We have also used this method to fabricate arrays of magnetoelectric composites of AlN/CoFe with protective Au coating in the form of double tubes.

S. Min, J.H, Lim, J. Gaffney, K. Kinttle, J. B. Wiley, L. Malkinski, J. Appl. Phys.,**111**, 07A320 (2012)

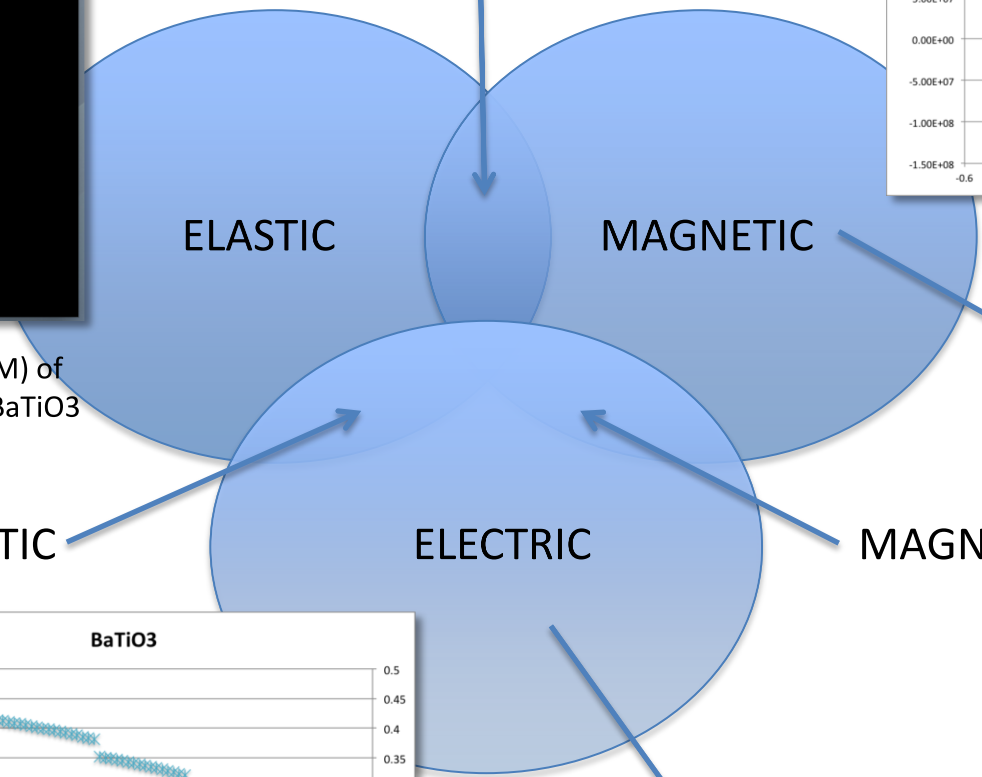
Combined Elastic Micromagnetic Ferroelectric Simulations of Multiferroic Materials

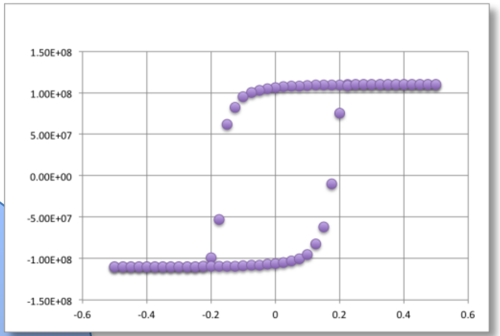
Scott L. Whittenburg, AMRI



Finite Element Modeling (FEM) of nano-origami in $CoFe_2O_4$ – $BaTiO_3$ bilayer due to misfit strain

MAGNETOELASTIC



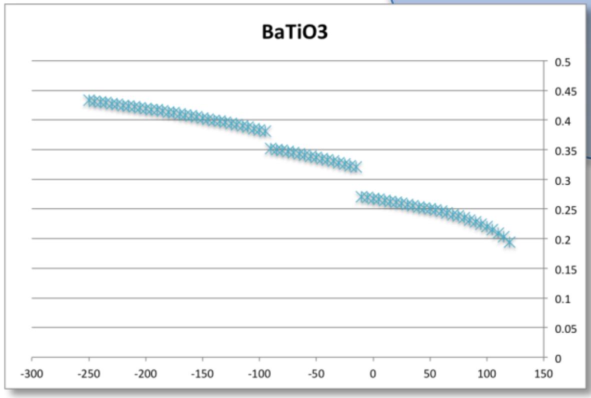


Hysteresis in $CoFe_2O_4$

Micromagnetic Simulations

FERROELASTIC

MAGNETOELECTRIC



Ferroelectric Simulations

Landau Devonshire simulation of ferroelectric phase transitions (spontaneous polarization vs temperature) in Barium Titanate.

Louisiana Alliance for Simulation-Guided Materials Applications
LA-SiGMA (NSF LA-BoR #EPS1003897)

SD1 Focus 2 Milestones

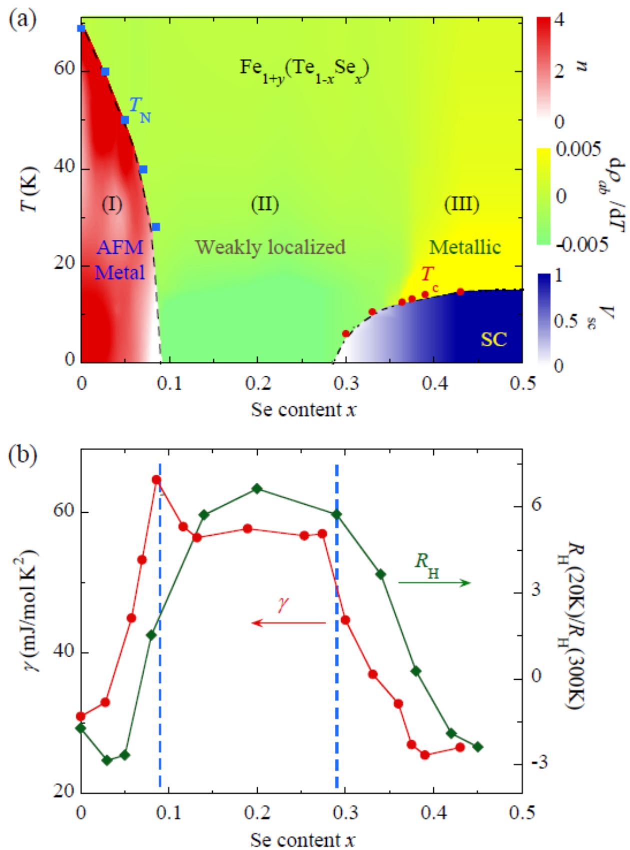
Milestones	Y1	Y2	Y3	Y4	Y5	
Test array of DFT functionals for prediction of metalloporphyrin and ferroelectric properties.	X	X				*On Track*
Prepare and measure electrical/magnetic properties of metalloporphyrin nanostructures.	X	X				*On Track*
Prepare organic magnets and ferroelectrics.	X	X	X			*On Track*
Develop experimentally validated computational models for porphyrin systems using magnetoresistance and electrical conductance measurements as guides		X	X	X	X	*??*
Develop multiscale models of metalloporphyrin systems using DFT parameters			X	X	X	
Predict charge transport in metalloporphyrins and compare with experiments			X	X	X	
Predict properties of ferroelectrics using new nonlocal meta-GGA DFT functionals			X	X	X	
Develop experimentally validated models of organic magnets and ferroelectrics			X	X	X	

Focus 3
Superconducting Materials

SD1 & CTCI

What is the pairing mechanism in pnictides?

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



- The remarkable increase of the superconducting volume fraction V_{SC} and the normal state metallicity occurs when the normal state Sommerfeld coefficient γ and Hall coefficient R_H drop drastically.
- Superconductivity is surprisingly enhanced by magnetic field for x-0.3-0.4.
- The $(\pi,0)$ magnetic fluctuations in the underdoped region gives rise to incoherent magnetic scattering, resulting in electronic disorders and low charge mobility.
- The Short-range ordered glassy magnetism at $(\pi,0)$ in superconducting samples arises from magnetic Friedel-like oscillations surrounding interstitial Fe forming magnetic polarons

Hu et al., arXiv 1111.0699, submitted to PRL.
Thampy et al., PRL 108, 107002 (2012), in collaboration with John Hopkins

Enabling International collaborations

CNRS, Grenoble and Paris, France

Quantum critical phenomena and spin fluctuations from ferromagnetic superconductors to iron pnictides

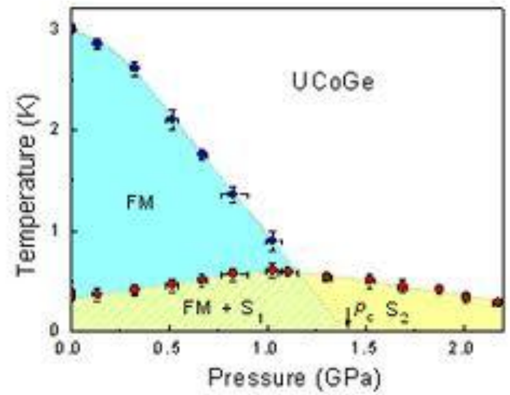
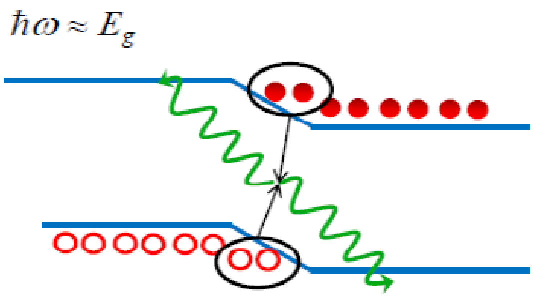


Fig. from E. Slooten et al.: Phys. Rev. Lett. 103 (2009) 097003.

Indranil Paul, visitor, April 2012

Karlsruhe Institute of Technology, Germany

Super-luminescence in superconductor-semiconductors junctions: underlying physics and pathways to phase detection



pn-junction

Paul Baireuther, student visitor, March-April 2012

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				*On Track*
Use hybrid QMC to address the origin of the QCP and competing order in cuprate models.	X	X				*On Track*
Study overscreening in pnictide models using new Hyper-GGA functionals.	X	X	X			*Behind*
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*

Challenge/Barrier: Additional time was required to test the Hyper-GGA functional before porting it to Solid State codes.

Mitigation Plan: Testing is almost complete & porting will take place in the 2nd year of the award.

New Focus

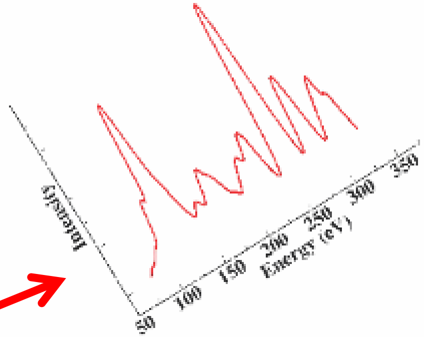
Low Energy Electron Diffraction: An Inverse Problem for Structural Determination

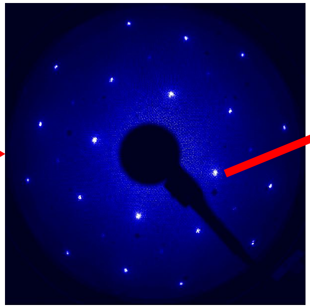
(LI/LA-SiGMA seed funded)

SD1 & CTCI, SD2

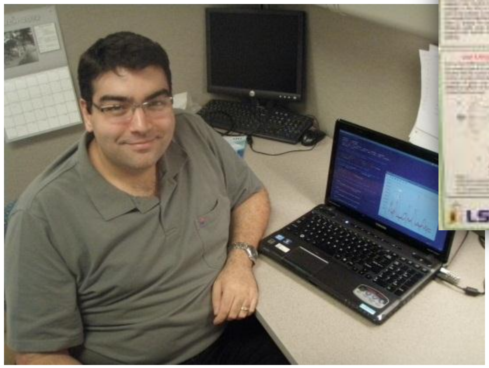
Surface Probe: I vs. V curves contain structural information.

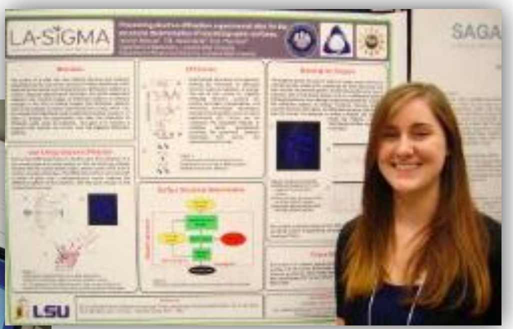
Since new complex materials have **many** atoms in the unit cell, extracting the structure is computationally challenging.



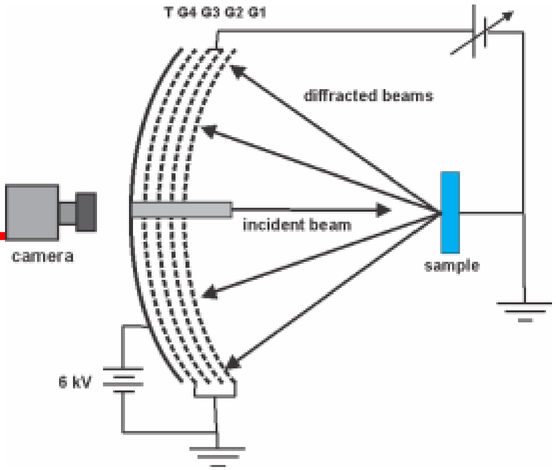


D.D. dos Reis





H. Manuel

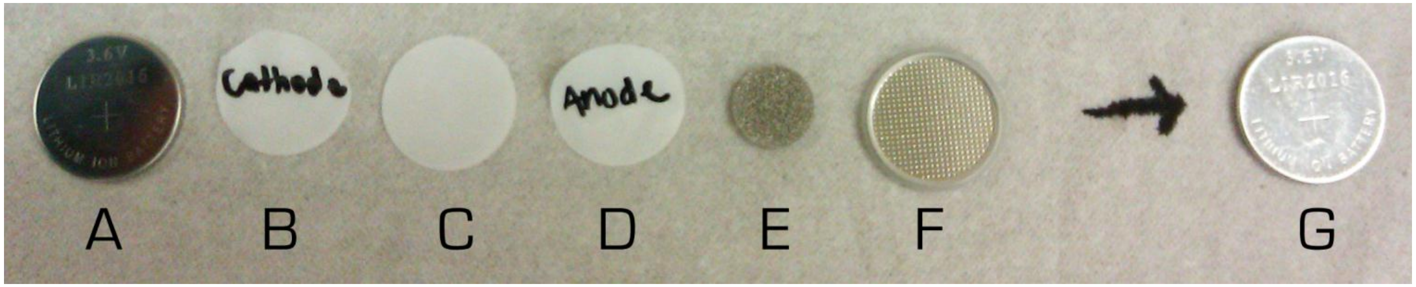


Better inverse problem techniques will improve material characterization

Outreach Activities (Tulane)

- Provided summer research opportunities for the undergraduates supported by the LA-SiGMA REU program. Two students from this program worked with Prof. Mao last summer and they were involved in the research searching for novel superconductor in iron chalcogenides using chemical intercalation.
- Outreach activity

Offered research opportunities to students from Benjamin Franklin High School (BFHS) in New Orleans. Prof. Mao has directed two students from BFHS to complete their independent research project. This project aimed at searching for alternative cathode materials for developing high energy density lithium-ion battery. This project was successful; some promising materials have been found.



Assembly of a lithium ion coin cell. (A) positive terminal; (B) cathode; (C) insulator; (D) anode (lithium); (E) current collector (nickel foam); (F) negative terminal; (G) completed lithium ion coin cell

Preparation of cathode

Outreach

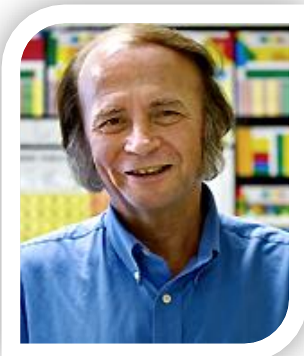
- Nanodays. LA-SiGMA faculty members gave four public lectures and graduate students led demonstrations at the BREC's Highland Road Observatory and the Louisiana Arts and Science Museum: over 300 visitors.
- CCT and LA-SiGMA REU programs

Outreach, education, funding initiatives (Garno)

- ***NanoDays***
- ***Super Science Saturday***
- ***Chem Demos,***
- ***Saturday Science***

Graduate Students and Postdoctoral Education

Density Functional Workshop, Summer 2011
(40 registrants, 5 speakers, LA Tech, LSU, SUBR, Tulane, Xavier)



John Perdew
Tulane

Shobhana Narasimhan
Jawaharlal Nehru Centre

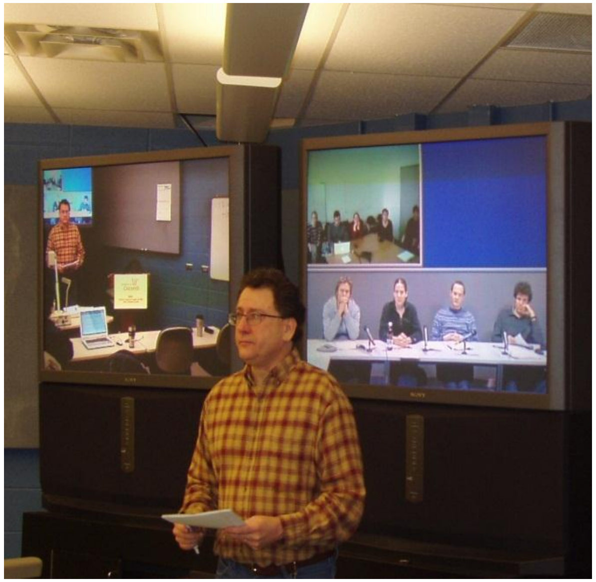
Kieron Burke
UC Irvine

Mel Levy
Tulane & N.C. A&T

Weitao Yang
Duke

Tanusri Saha-Dasgupta
S.N. Bose National Centre

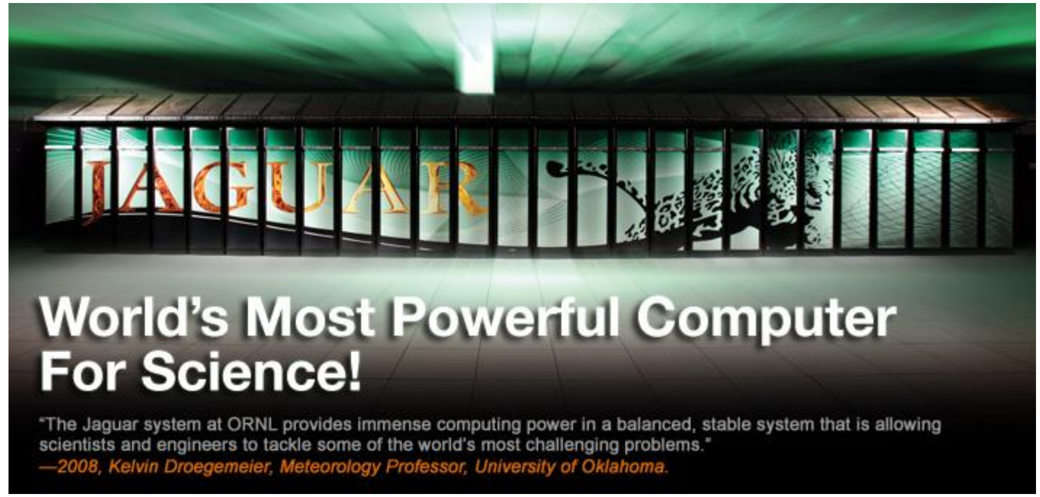
Graduate Student Education



- Distance Learning Courses:
  - Computational Solid State Physics
  - Advanced Solid State Physics with Computation
  - Computational Physics
  - Simulations of Quantum Many-Body Systems
  - …Ten courses total
- SD1 International Computational Materials Science Seminar Series (EVO)
  - Wednesdays at 10:00
  - (http://www.institute.loni.org/lasigma/lasigma-int-seminarseries.php)
  - Kieron Burke, Karol Kowalski, Bayo Lau…
- GPU Team Meetings
  - Monday, 12:30-1:30 (EVO)

Partnership with Pacific Northwest National Lab

- Environmental Molecular Sciences Laboratory (EMSL)
  - Home of NWChem!
- SciDAC3 request
- Invited DOE Center request ($11M)
- Internship program for LA-SiGMA students
  - 3-6 month visits
  - Working with EMSL Open Source Code Developers
  - undergraduate to PhD
- Indo-US SCES Centre



EMSL Associate Lab Director Bill Shelton participating in LA-SiGMA REU panel

Pacific Northwest NATIONAL LABORATORY

Funding

- Two Computational Materials Science and Chemistry Network awards (BNL, Ames, SLAC, Argonne, PNNL)
- NSF CRI Award
  - About $500K
  - Shelob Cluster available to LA-SiGMA investigators
- Indo-US Center preliminary approval (IUSSTF)
- SciDAC request (submitted)
- DOE Center request (invited)
- NSF SAVI request (white paper).
  - Extend LA-SiGMA into an international virtual org.

Summary

- Meeting Goals and Milestones
- Strong Overlap with CTCI
- Outreach and Education
  - Courses
  - DFT Workshop
  - GPU Team
- Partnerships with National Labs (BNL+PNNL)
- Seeking Other Sources of Funding
  - DOE Center of Excellence