DOE/BES Computational Materials Science Network

Predictive Capabilities for Strongly-Correlated Systems

Fall 2008 Coordination Meeting

Oak Ridge National Laboratory

November 14-16, 2008

All talks are held at:

Joint Institute for Computational Sciences

http://www.jics.utk.edu/

5100 Building, Lecture Hall 128

Bethel Valley Road

Oak Ridge, Tennessee 37830

Sponsored by the US Department of Energy
Supported in part by the BES/ORNL FWP ERKCS93: *"Theory of Complex Collective Phenomena"*

Friday, November 14

7:50 AM — Pick up at hotel

8:10 AM — Getting Badges at the Visitors Center

8:50 – 9:00 **Richard Scalettar,** University of California, Davis; **Adolfo Eguiluz,** University of Tennessee and ORNL
Welcome to Fall 2008 PCSCS coordination meeting

Chair: Malcolm Stocks, Oak Ridge National Laboratory

9:00 – 9:40 **Helmut Eschrig,** Leibniz IFW, Dresden, Germany
The Electronic Structure of Layered Iron Chalcogenides/Pnictides

9:40 – 10:20 **George Sawatzky,** University of British Columbia, Canada
Interplay between Atomic and Molecular Physics, and Translational Symmetry in the high-Tc Cuprates

10:20 – 10:50 **Coffee Break**

Chair: Elbio Dagotto, University of Tennessee and ORNL

10:50 – 11:30 **Jim Allen,** University of Michigan
The correlation problem in the heavy fermions: An overview

11:30 – 12:10 **Steve Nagler,** Oak Ridge National Laboratory
Neutron scattering and quantum materials: some existing results and future prospects

12:10 – 13:50 **Lunch**

Chair: Thomas Schulthess, Oak Ridge National Laboratory

13:50 – 14:30 **Mikhail Katsnelson,** University of Nijmegen, The Netherlands
Graphene: Electronic structure, chemistry, and magnetism

14:30 – 15:10 **Werner Hanke,** University of Würzburg, Germany
From the microscopic cluster to the infinite lattice: Does the Hubbard model describe high-Tc superconductivity?

15:10 – 15:50 **Adriana Moreo,** University of Tennessee and ORNL
Modeling of $LaO_{1-x}FeAs$: The Magnetic Order and Pairing Channels

16:00 – 17:30 **Tour of the Spallation Neutron Source**

18:00 – 21:00; **Buffet Dinner** + Networking

Saturday, November 15

8:15 AM — Pick up at hotel

Chair: George Sawatzky, University of British Columbia

9:00 – 9:40 **Pengcheng Dai,** University of Tennessee and ORNL
Magnetic order close to superconductivity in the iron-based layered $RFeAsO_{1-x}F_x$ (R = La, Ce) systems

9:40 – 10:20 **Adam Kaminski,** Ames National Laboratory
Photoemission investigation of the LaOFeAs superconductors

10:20 – 11:00 **Sergey Savrasov,** University of California, Davis
Electronic structure of the LaOFeAs superconductors

11:00 – 11:30 **Coffee Break**

Chair: Shiwei Zhang, College of William and Mary

11:30 – 12:10 **David Ceperley,** University of Illinois
Coupled Electron Ion Simulations of Dense Hydrogen

12:10 – 12:50 **Lubos Mitas,** North Carolina State University
QMC calculations for transition-metal oxides

12:50 – 14:20 **Lunch**

Chair: Wei Ku, Brookhaven National Laboratory

14:20 – 15:00 **Takeshi Egami,** University of Tennessee and ORNL
Phonons in $BaFe_{1.8}Co_{0.2}As_2$ single crystal observed by pulsed neutron inelastic scattering

15:00 – 15:40 **John Hill,** Brookhaven National Laboratory
Inelastic X-ray Scattering Studies of Strongly Correlated Electron Systems: Recent Results and Outlook

15:40 – 16:20 **Chris Marianetti,** Columbia University
Electronic Coherence in plutonium: A DMFT study

16:20 – 16:50 **Coffee Break**

Chair: Werner Hanke, University of Würzburg

16:50 – 17:30 **Thomas Maier,** Oak Ridge National Laboratory
Pairing in the Hubbard model of the high-Tc cuprates: Insights from dynamic cluster simulations

17:30 – 18:10	**Jan Kunes,** University of Augsburg, Germany *Correlation vs. hybridization in transition-metal compounds: a DMFT picture*
18:10 – 18:50	**Satoshi Okamoto,** Oak Ridge National Laboratory *Enhanced superconductivity in superlattices of high-Tc cuprates*

19:15 Dinner / Discussions **— American Science and Energy Museum**

Sunday, November 16

8:30 AM — Pick up at hotel

CMSN Nano-Woodstock

Chair: Richard Hennig, Ohio State University

9:00 – 9:20	**Wirawan Purwanto,** College of William and Mary *Quantum Monte Carlo Study of Bulk MnO*
9:20 – 9:40	**Chia-Chen Chang**, College of William and Mary *Spatially inhomogeneous phase in the 2D repulsive Hubbard model*
9:40 – 10:00	**Tom Berlijn**, BNL and Stony Brook University *Influence of disorder on the Fermi-surface of* Na_xCoO_2
10:00 – 10:20	**Simone Chiesa**, University of California, Davis *A robust pseudogap anomaly in the heavily-disordered 2D Hubbard model*
10:20 – 10:40	**Anton Kozhevnikov**, ORNL and University of Tennessee *TBA*

10:40 – 11:10 Coffee Break; networking

Chair: Jan Kunes, University of Augsburg, Germany

11:10 – 11:30	**Erik R. Ylvisaker**, University of California, Davis *LDA+DMFT: Yb valence transition and charge self-consistency*
11:30 – 11:50	**Yucel Yildrim**, Brookhaven Nacional Laboratory *Strong-coupling limit of superconductivity in anti-ferromagnetic phase: Extended hardcore boson picture of d-wave order and phase fluctuation*
11:50 – 12:10	**Myung Joon Han**, University of California, Davis *Magnetic interaction and superconductivity in Fe-based superconductors*
12:10 – 12:30	**Alexandru Macridin**, University of Cincinatti *TBA*

12:30 **Closing Remarks**

12:45 **Lunch**; networking