Computational Materials Science Network:

Predictive Capability for Strongly Correlated Electron Materials

[1] Density Functionals: Correlated Bands and Charge/Spin Respons
Eguiluz, Pickett

[2] Dynamical Mean Field Theory and Cluster Extensions
Savrasov, Jarrell, Scalettar

[3] Emerging Downfolding Approaches
Ku, White, Eguiluz

Global Collaborative Activities

Fall 2003 Coordination Meeting– University of Tennessee

- 41 participants
- External Speakers: Ole. K. Anderson, Jörg Fink

Fall 2004 Coordination Meeting– Oak Ridge National Laboratory

- 44 participants
- External Speakers: K. Held, S. Nagler, G. Sawatzky, A. Moreo

Fall 2005 Coordination Meeting– Chicago

- 31 participants from PCSCS CRT.
- In coordination with 'Excited States' CRT.

Satellites of March APS meetings

- Montreal 2004: 19 CMSN talks
- Los Angeles 2005: 45 CMSN talks (5 invited)
- Baltimore 2006: Planned

Team A Collaborative Activities

Postdoctoral Exchange:

Jan Kunes (Davis) visits Eguiluz group (Tenn./ORNL), 3 weeks, Jan. 2005.

Linear response in LDA+U

Jan Kunes (UCD) visits to Savrasov group (NJIT), 3 weeks, Jan. 2005.

Development of Impurity Solvers

Student Exchange:

Kwan-Woo Lee (UCD) visits Eguiluz group (Tenn./ORNL), 2 weeks, Nov. 2003

Investigate Na_xCoO_2 by linear response methods.

Oscar Restrepo (Tenn./ORNL) visits Pickett group (UCD), 2 weeks, July, 2005

Development of Many-Body Kernel in LAPW code.

Exciton effects in Mott insulators.

Team A Collaborative Activities

Publications acknowledging CMSN

"Magnetic Coupling Between Non-Magnetic Ions: Eu3+ in EuN and EuP", M. I Johannes and W. E. Pickett, Phys. Rev. B, to appear.

"NaxCoO2 in the $x \rightarrow 0$ Regime: Coupling of Structure and Correlation Effects K.-W. Lee and W. E. Pickett, Phys. Rev. B 72, 115110 (2005).

"Disproportionation, Metal-Insulator Transition, and Critical Interaction Strengt in Na1/2CoO2", K.-W. Lee, J. Kunes, P. Novak, and W. E. Pickett, Phys. Re Lett. 94, 026403 (2005).

"Pressure Driven Nonmagnetic to Ferromagnetic Transition in CoN" D. Kas nathan and W. E. Pickett, submitted (2005).

Team B Collaborative Activities

Postdoctoral Exchange:

Nick Zein (Kurchatov) visits Savrasov/Kotliar groups (NJIT/Rutgers),
6 months, 2004-5.
Development of GW+DMFT.

Ping Sun (Rutgers) visits Pickett/Scalettar groups (Davis).
Development of GW+DMFT.

Alexandru Macridin (Cincinnati) visits Pickett/Scalettar groups (Davis),
3 weeks, June, 2005.
Study of 2D extended Hubbard model with DCA.
Phonon softening due to electron-phonon interaction in the Holstein model.
and visits Kent/Schulthess groups (ORNL), 2 weeks, Jan. 2005.
Realistic simulations of the cuprates.

Student Exchange:

Luke Shulenberger (Illinois) works with S. Zhang (W&M).
Auxiliary Field Quantum Monte Carlo.

Team B Collaborative Activities

Publications acknowledging CMSN

Kristjan Haule, Viktor Oudovenko, Sergej Y. Savrasov, Gabriel Kotliar "The alph to gamma transition in Ce: a theoretical view from optical spectroscopy," K. Haul V. Oudovenko, S.Y. Savrasov, and G. Kotliar, Phys. Rev. Lett. 94, 036401 (2005

"Program LMTART for Electronic Structure Calculations", S. Y. Savrasov, Zeitsc fuer Kristallography 220, 555 (2005).

"Interpolative Approach for Solving Quantum Impurity Model," S. Y. Savraso V. Oudovenko, K. Haule, D. Villani, and G. Kotliar Phys. Rev. B71, 1151 (2005).

"Spectral Density Functional for Electronic Structure Calculations," S. Y. Savrasc and G. Kotliar, Phys. Rev. B 69, 245101 (2004).

"Combined local-density and dynamical mean field theory calculations for the com pressed lanthanides Ce, Pr, and Nd", A. K. McMahan, Phys. Rev. B 72, 11512 (2005).

"Physics of cuprates with the two-band Hubbard model: The validity of the on band Hubbard model," A. Macridin, M. Jarrell, Th. Maier, and G. A. Sawatzk Phys. Rev. B 71, 134527 (2005).

"Phase separation in the Hubbard model," A. Macridin, M. Jarrell, Th. Mai
preprint, cond-mat/0506148.

"Pseudogap and antiferromagnetic correlations in the Hubbard model," A. Macric
M. Jarrell, T. Maier, P.R.C. Kent, preprint, cond-mat/0509166.

Team C Collaborative Activities

PI Exchange:

Wei Ku (BNL) visits B.C. Larson (ORNL), 1 week, Sept. (2004).

Wannier function analysis of non-resonant IXS of NiO and CoO.

Cyrus Umrigar (Cornell) visits Wilkins group (Ohio State), 1 week, October 200

Also involved: Scuseria, Hennig, Martin.

QMC calculations for defects and phase transitions in silicon.

Postdoctoral Exchange:

Weiguo Yin (BNL) visits Steven White (UCI), 4 weeks, Jan. 2005.

Development of numerical canonical transformations for infinite lattices.

Student Exchange:

Travis Sjostrom (Utah) visits Ku group (BNL), 4 weeks, July 2005.

First-principles modeling of strongly correlated nano-wire arrays.

Dmitri Volja (BNL) attends Cornell Summer School, 1 week, July 2005.

Wavelet Bases for DFT.

Team C Collaborative Activities

Publications acknowledging CMSN

"Electron-hole and plasmon excitations in 3d transition metals: Ab initio calcul
tions and inelastic x-ray scattering measurements", I.G. Gurtubay, Wei Ku, J.M
Pitarke, A.G. Eguiluz, B.C. Larson, J. Tischler, and P. Zschack, Phys. Rev. B7
125117 (2005).

"Strong correlation effects in trapped atomic bose gases", W. Purwanto and
Zhang, Phys. Rev. A, to appear.

"Orbital ordering in $LaMnO_3$: Electron-electron versus electron-lattice intera
tions," Wei-Guo Yin, D. Volja, and Wei Ku, submitted to Phys. Rev. Lett.

"Coexistence of gapless excitations and commensurate charge-density wave in th
2H-transition metal dichalcogenides", R.L. Barnett, A. Polkovnikov, E. Demle
Wei-Guo Yin, and Wei Ku, submitted to Phys. Rev. Lett.

"Electronic Mechanism for the Coexistence of Ferroelectricity and Ferromagnetism
C. Batista, J.E. Gubernatis, and Wei-Guo Yin, cond-mat/0508113.