Computational Materials Science Network:

Predictive Capability for
Strongly Correlated Electron Materials

[1] Density Functionals: Correlated Bands and Charge/Spin Responses
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$_x$CoO$_2$ 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


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:


Auxiliary Field Quantum Monte Carlo.
Team B Collaborative Activities

Publications acknowledging CMSN


“Pseudogap and antiferromagnetic correlations in the Hubbard model,” A. Macridin, M. Jarrell, T. Maier, P.R.C. Kent, preprint, cond-mat/0509166.
Team C Collaborative Activities

PI Exchange:
   Wannier function analysis of non-resonant IXS of NiO and CoO.
Cyrus Umrigar (Cornell) visits Wilkins group (Ohio State), 1 week, October 2005.
   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


