US Department of Energy
Planning meeting to form the CMSN Team:
Building a unified computational model for the resonant X-ray
scattering of strongly correlated materials
Grant: FG02-07ER46385

Applicant/Institution: Northern Illinois University

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The planning meeting was held May 21-23 2008 at Argonne National Laboratory (ANL). The purpose of the meeting was to establish a network on building computational model for resonant elastic and inelastic x-ray scattering. This course of action was recommended by program officer Dale Koelling after the initial submission of a proposal for a Computational Materials Science Network to Basic Energy Sciences. The meeting consisted of talks and discussion. At the end of the meeting three subgroups were formed. After the successful formation of the team, a new proposal was written which was funded by BES. Since this was a planning meeting there were no proceedings. The program and titles of talks are given below.

Participants:

U. S. participants

Ken Ahn	New Jersey Institute of Technology
Arun Bansil	Northeastern University
Jim Freericks	Georgetown University
Mark Jarrell	University of Cincinnati
Bob Markiewicz	Northeastern University
John Rehr	University of Washington
Eric Shirley	National Institute for Standards and Technology
Michel van Veenendaal	Northern Illinois University/Argonne National Laboratory

International participants

Tom Devereaux	University of Waterloo, Canada
Sadamichi Maekawa	Tohoku University, Japan
George Sawatzky	University of British Columbia, Canada
Andrij Shvaika	Institute of Condensed Matter Physics, Ukraine
Jeroen van den Brink	University of Leiden, the Netherlands

Experimental Participants

Peter Abbamonte	University of Illinois, Urbana Champaign
Zahid Hasan	Princeton University
John Hill	Brookhaven National Laboratory
Ben Larson	Oak Ridge National Laboratory

Time and location.

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PLANNING MEETING PROGRAM

Each talk will had 40 minute time slot of 25 minutes plus 15 minutes for discussion.

DAY 1:

8:00-8:30 Welcome, Goals of the planning meeting

8:30-10:30 Scientific talks 1,2,3

10:30-11:00 Integrative Discussion

11:00-12:20 Talks 4,5

12:20-1:30 Lunch with Working Groups

1:30-3:30 Talks 6,7,8

3:30-4:00 Integrative Discussion

4:00-6:00 Talks 9,10,11

6:00-6:30 Integrative Discussion

6:30-8:30 Dinner and Working Groups

8:30-10:00 Working Groups

DAY 2:

8:00-8:30 Reports of the Working Groups

8:30-10:30 Talks 12,13,14

10:30-11:00 Integrative Discussion

11:00-1:00 Talks 15,16,17,18

1:00-2:30 Lunch and Working Groups

2:30-4:00 Plenary Discussion on the organization of the teams. Tasks are defined and final teams are formed.

4:00-6:00 Team members got together to set up an action plan for the network, to establish the subjects each Collaborative Research Team (CRT) will focus on and to find a workable plan to optimize the collaborative aspect of the CRT.

6:00-8:00 Dinner and working CRT groups

8:00-9:30 CRT teams finalize their plans and timelines

DAY 3:

8:30-10:00 Reports of the detailed working plans of the CRTs

10:00-10:30 Integrative Discussion for final plans

10:30-12:00 Wrap up planning for new proposal for the CMSN

Afternoon: Meeting Adjournment

Titles of talks

1. **Jeroen van den Brink**, New light on magnetic excitations: indirect resonant inelastic X-ray scattering on magnons
2. **Bob Markiewicz**, Mott gap collapse in electron-doped cuprates probed by RIXS
3. **Ken Ahn**, X-ray spectroscopy on transition metal oxides-- Probe for band structures and inhomogeneities
4. **Mark Jarrell**, Dynamical Cluster Quantum Monte Carlo simulations of the cuprates and how to relate these many body problems to resonant x-ray scattering
5. **Michel van Veenendaal**, Resonant Inelastic X-ray Scattering in early transition-metal compounds
6. **Arun Bansil**, Realistic Modeling of Resonant X-Ray Scattering Spectra of the Cuprates: Opportunities and Challenges
7. **Jim Freericks**, Many-body physics issues associated with the core-hole propagator and resonant inelastic x-ray scattering
8. **Eric Shirley**, Density functional theory approaches to the Bethe-Salpeter equation and resonant x-ray scattering
9. **Tom Devereaux**, K-edge RIXS in edge and corner sharing cuprates
10. **Andrij Shvaika**, Kadanoff-Baym-Keldysh techniques for determining the core-hole propagator and associated charge vertices
11. **Zahid Hasan**, Charge excitations, collective modes and order in Low-D and doped Mott insulators probed by Elastic & Inelastic Resonant X-ray Scattering
12. **John Rehr**, Multiple Scattering Approach to Inelastic X-ray Scattering
13. **George Sawatzky**, Resonant Elastic Soft-X-ray Scattering
14. **Young-June Kim/John Hill**, Recent experimental progress in Resonant Elastic and Inelastic X-ray Scattering
15. **Ben Larson**, Inelastic X-ray Scattering as a probe of the dynamic structure factor
16. **Peter Abbamonte**, Orbital and charge order studied by Resonant soft X-ray Scattering
17. **Sadamichi Maekawa**, Resonant Inelastic X-ray Scattering on undoped and doped Hubbard systems.
18. **Aleksi Soininen**, Recent Developments in Calculations and Analysis of Inelastic X-ray Scattering