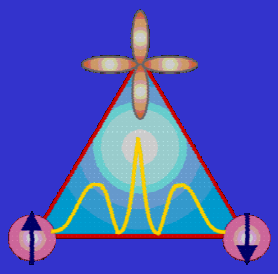
WORKSHOP OVERVIEW PERSPECTIVES, FRONTIERS…



''Realistic Theories of Correlated Electron Materials''

KITP,Dec. 2002

GOALS OF THE WORKSHOP :

* **Bring together** two communities:
many-body and electronic structure

(Over the last few years, ''technology transfer'' between the two fields has progressed tremendously).

* **Advance theoretical methods** in both fields, and especially at the interface

* **Address a wide range of correlated materials.**
  - Get the latest experimental information (the field is experimentally-driven !)
  - Advance qualitative and quantitative understanding of some materials

* **Tutorial aspect**

-Give an idea of the variety of methods discussed here, which were the subject of extended tutorials.

-Highlight some of the experimental results presented at the workshop, often very recent and yet unpublished.

(a personal selection)

-Highlight some of the achievements from collaborative work during the workshop (also: ongoing projects).

⇒ …

- Key open problems, directions, frontiers…

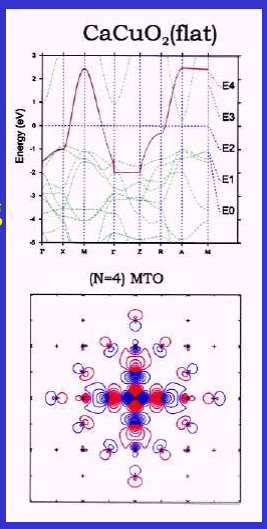
⇒ …

Tutorials on methods

•ELECTRONIC STRUCTURE METHODS:

-"Downfolding" (NMTO)
(O.K. Andersen, T. Saha-Sagupta S.Satpathy)
= A method to construct effective one-electron hamiltonians from DFT/LDA, involving few localised orbitals, valid in a certain energy range

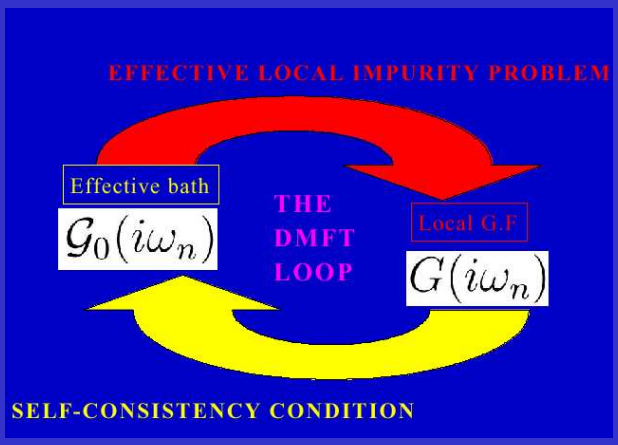
- "Projector augmented wave" (PAW: P. Bloechl
All electron/Combining localised basis functions w/ plane waves



* **MANY-BODY APPROACHES**
& TECHNIQUES TO HANDLE STRONG CORRELATIONS

- DYNAMICAL MEAN-FIELD THEORY

(A.G, G. Kotliar, A. Lichtenstein, M. Rozenberg)



*** QUANTUM MONTE CARLO METHODS**

-Diffusion Quantum Monte Carlo (fixed node approx.)
(M. Foulkes, L. Mitas)

Random walk in Slater determinants space (S. Zhang)

- Monte Carlo cluster algorithms (M. Troyer)

- Other numerical algorithms (M. Imada)

* Renormalization Group methods for fermions

(M. Salmhofer, W. Metzner, K. Schoenhammer, T. Costi, F. Wegner,…)

•Tutorials on several other topics, e.g:

- Fundamental aspects of DFT (E. Gross)

-Frustrated quantum spin systems (F. Mila)

-Ferromagnetic semiconductors (S. Das Sarma)

- Electron interaction effects in mesoscopics (Y. Meir)

-…

SOME EXPERIMENTAL HIGHLIGHTS

* The quasiparticle peak revealed !

DMFT: Correlated metals have coexisting Hubbard bands and low-energy quasiparticle peak

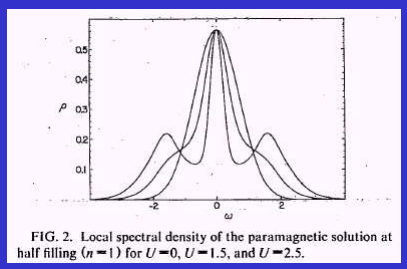
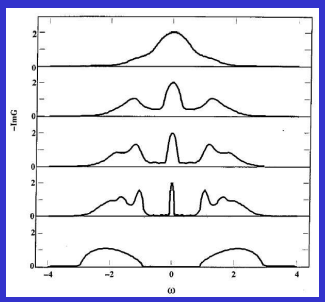
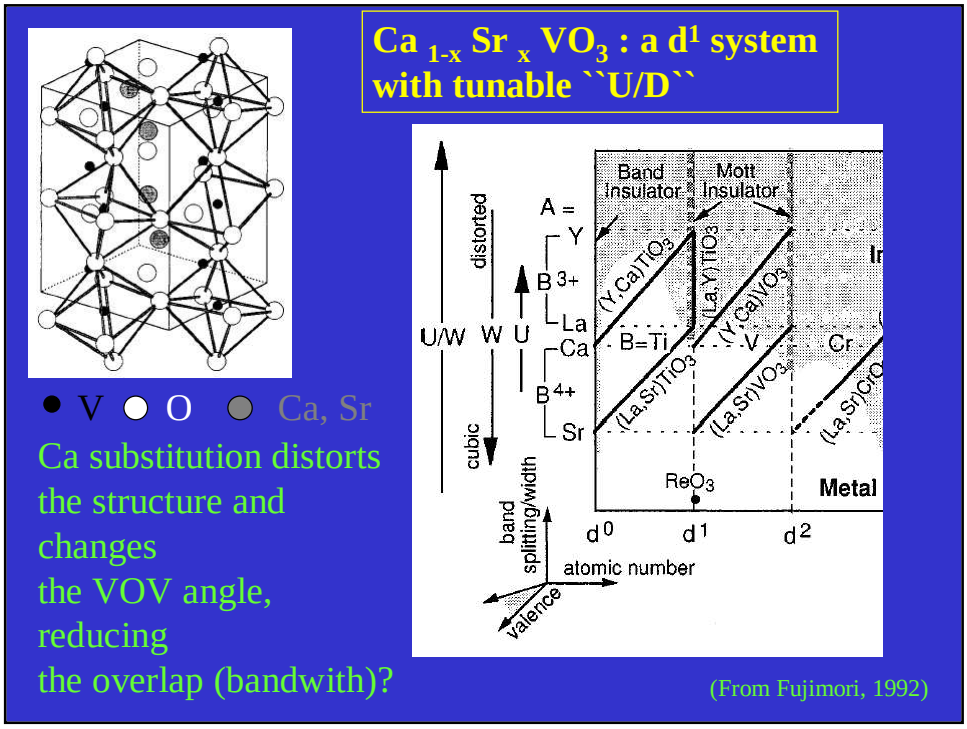


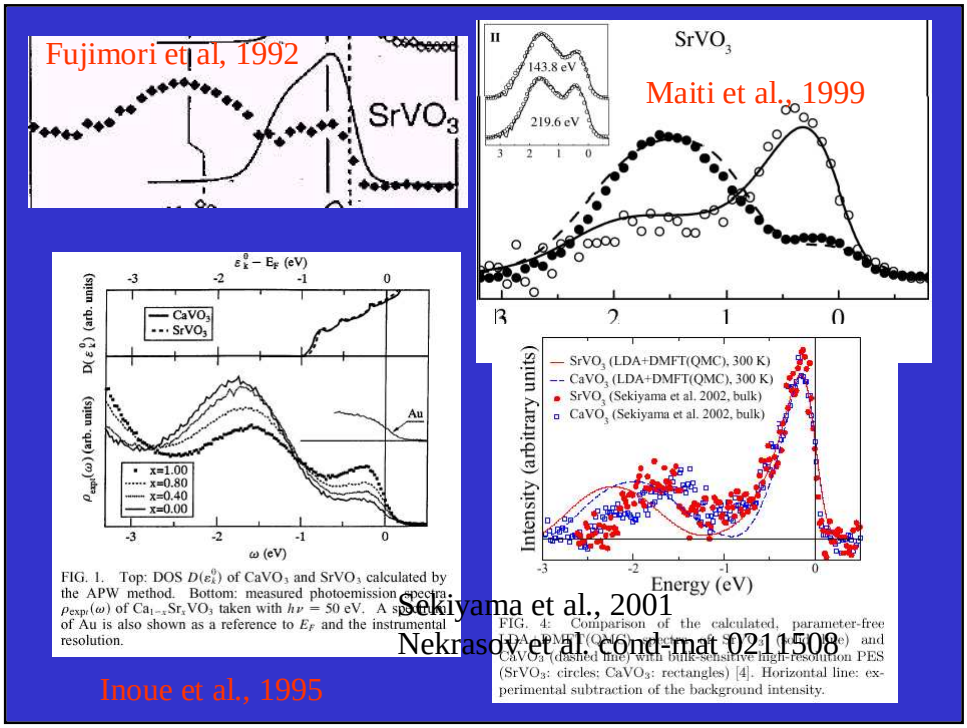
FIG. 2. Local spectral density of the paramagnetic solution at half filling ($n=1$) for $U=0$, $U=1.5$, and $U=2.5$.

A.G & G. Kotliar, 1991



Rev. Mod. Phys. 1996


Ca 1-x Sr x VO3 : a d1 system with tunable ``U/D``
● V ○ O ● Ca, Sr
Ca substitution distorts the structure and changes the VOV angle, reducing the overlap (bandwith)?
Band Insulator
Mott Insulator
distorted
cubic
U/W
W
U
A =
Y
B 3+
La
Ca
B 4+
Sr
B=Ti
V
Cr
(Y,Ca)TiO3
(La,Y)TiO3
(Y,Ca)VO3
(La,Sr)TiO3
(La,Sr)VO3
(La,Sr)CrO
ReO3
Metal
band splitting/width
d 0
d 1
d 2
atomic number
valence
(From Fujimori, 1992)


Fujimori et al, 1992
SrVO3
Maiti et al., 1999
143.8 eV
219.6 eV
SrVO3 (LDA+DMFT(QMC), 300 K)
CaVO3 (LDA+DMFT(QMC), 300 K)
SrVO3 (Sekiyama et al. 2002, bulk)
CaVO3 (Sekiyama et al. 2002, bulk)
Intensity (arbitrary units)
Energy (eV)
CaVO3
SrVO3
Au
x=1.00
x=0.80
x=0.40
x=0.00
ω (eV)
Inoue et al., 1995
Sekiyama et al., 2001
Nekrasov et al. cond-mat 0211508

Genuine Electronic States Insensitive to the Distortion in Perovskite Vanadium Oxides Revealed by High-Energy Photoemission

A. Sekiyama,[1,*] H. Fujiwara,[1] S. Imada,[1] H. Eisaki,[2,†] S. I. Uchida,[2] K. Takegahara,[3] H. Harima,[4] Y. Saitoh,[5] and S. Suga[1]

Bulk-sensitive high-resolution photoemission was carried out $Sr_{1-x}Ca_xVO_3$. In a strong contrast to so far reported results, t revealed to be insensitive to x. The conservation of the density of s ppression tance of l tronic st

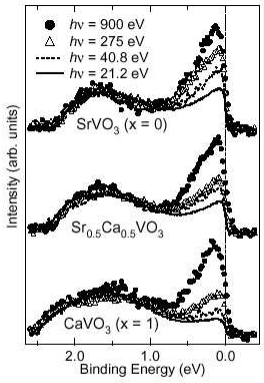


FIG. 2: Photon-energy dependence of the V 3*d* spectral weights for $Sr_{1-x}Ca_xVO_3$. The V 3*d* spectra are normalized by the integrated intensities of the incoherent part ranging from 0.8 to 2.6 eV.

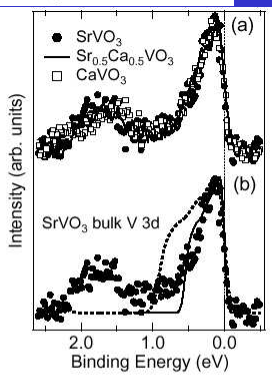


FIG. 3: (a) Bulk V 3*d* spectral functions of $SrVO_3$ (closed circles), $Sr_{0.5}Ca_{0.5}VO_3$ (solid line) and $CaVO_3$ (open squares). (b) Comparison of the experimentally obtained bulk V 3*d* spectral function of $SrVO_3$ (closed circles) to the V 3*d* partial density of states for $SrVO_3$ (dashed curve) obtained from the band-structure calculation, which has been broadened by the experimental resolution of 140 meV. The solid curve shows the same V 3*d* partial density of states but the energy is scaled down by a factor of 0.6.

More to come…

VOLUME 88, NUMBER 23 PHYSICAL REVIEW LETTERS 10 JUNE 2002

Fermi Surface of $3d^1$ Perovskite $CaVO_3$ near the Mott Transition

I. H. Inoue,[1,2] C. Bergemann,[3] I. Hase,[4] and S. R. Julian[3]

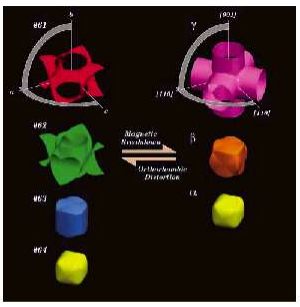


FIG. 3 (color). FS sheets predicted by LDA. The right panels show the FS sheets in a *cubic* TB fit to the LDA data, while on the left side these sheets are folded over into the orthorhombic BZ. The field directions in the rotation study are indicated around the surfaces in the top row.

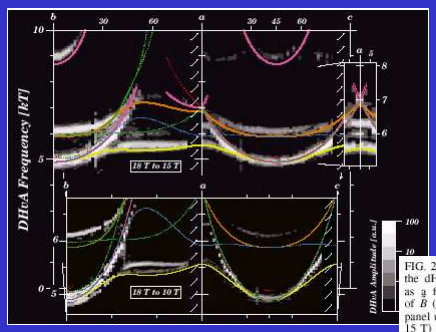
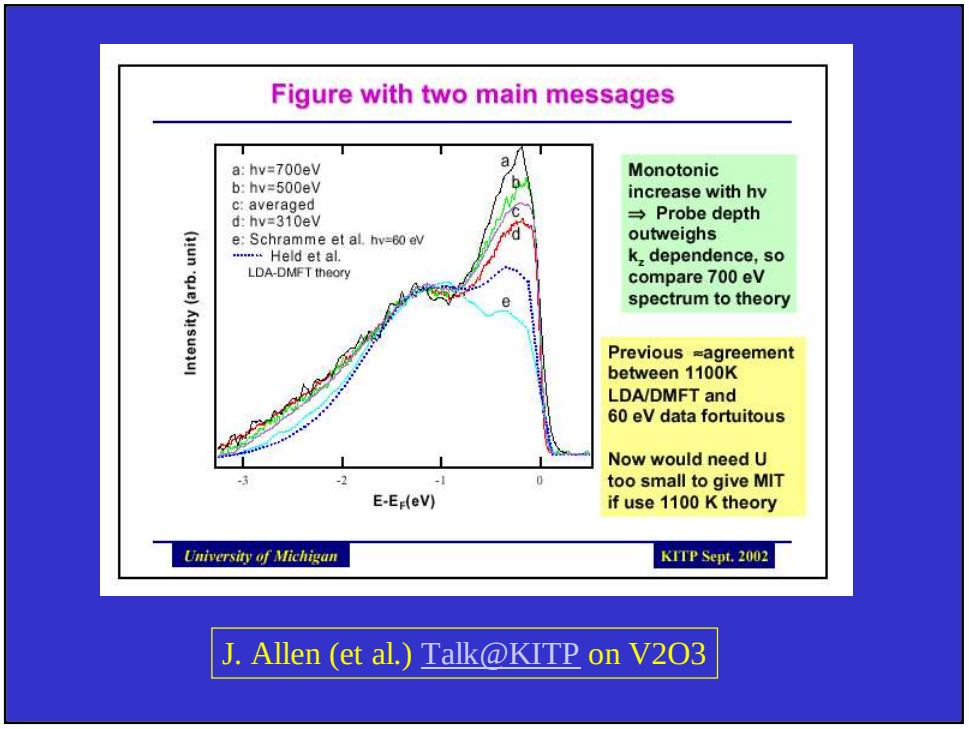
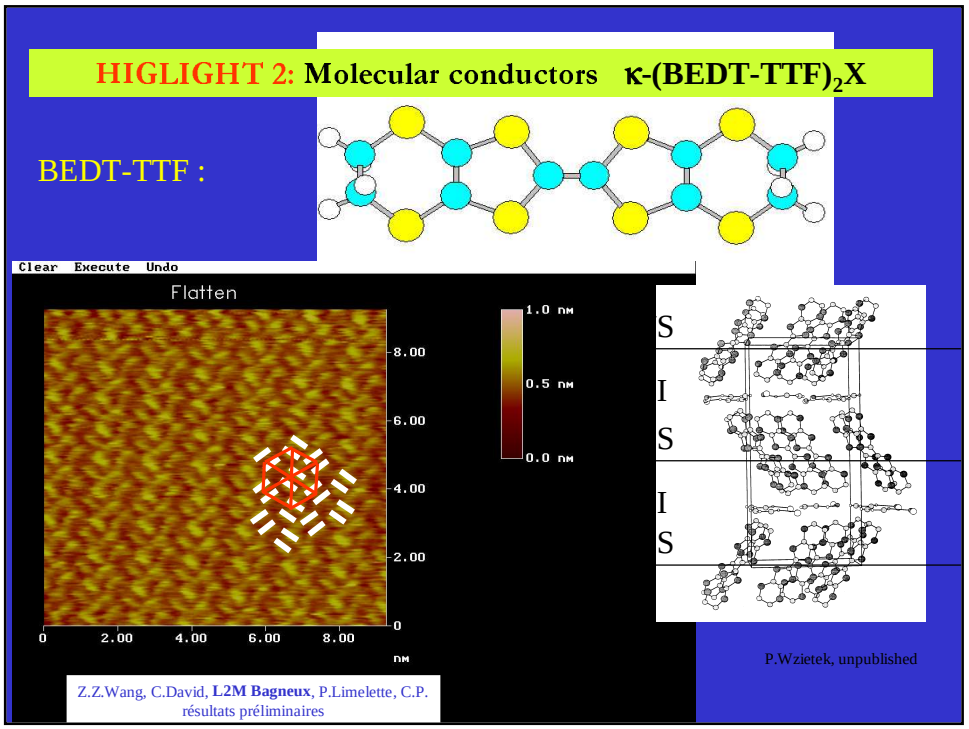


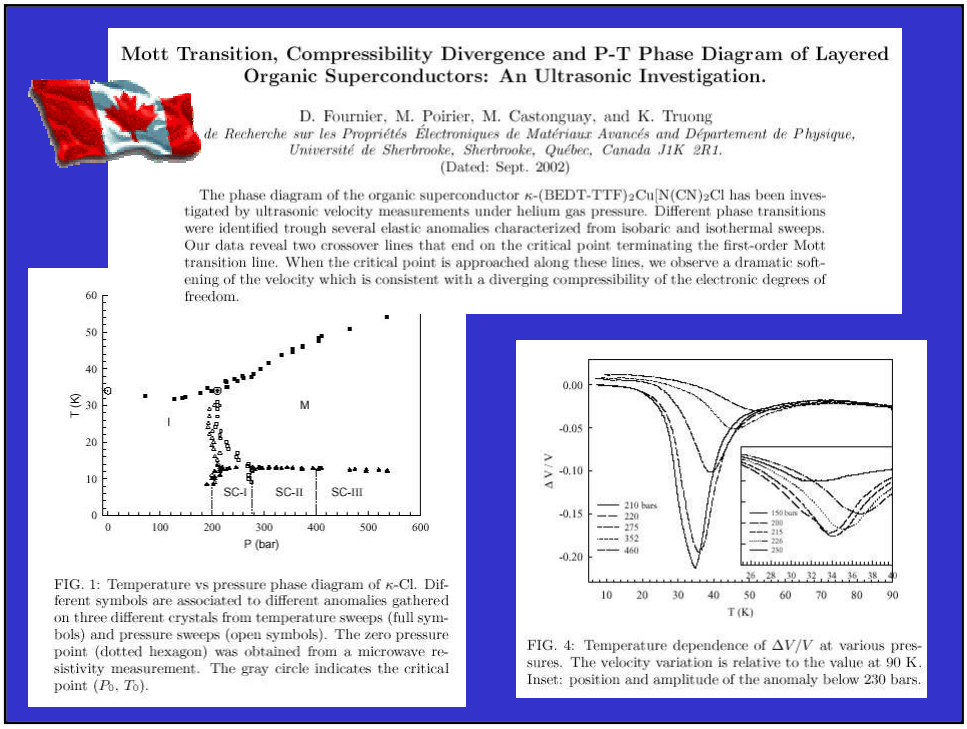
FIG. 2 (color). Density plot of the dHvA spectrum of $CaVO_3$ as a function of the direction of B (grey shaded). The main panel uses the high-field (18 → 15 T) sections of each sweep, while the lower inset uses all available data (18 → 10 T), with higher-frequency resolution at the expense of signal to noise. The right inset shows a blowup around the a axis for fields in the a-c plane. Superposed are the frequency predictions from LDA band structure calculations, for both the orthorhombic (thin dashed lines) and the hypothetical cubic (thick solid lines) unit cells—the color code corresponds to Fig. 3.

Work at the workshop on this topic by:
A.Poteryaev, E. Pavarini, S. Biermann, A. Lichtenstein et al.



J. Allen (et al.) Talk@KITP on V2O3





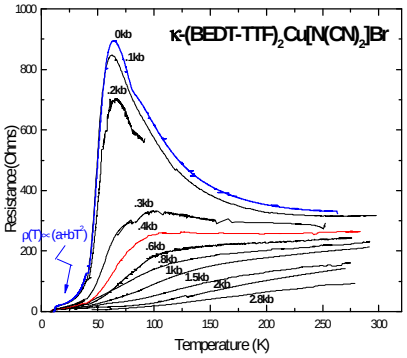
Mott Transition, Compressibility Divergence and P-T Phase Diagram of Layered Organic Superconductors: An Ultrasonic Investigation.

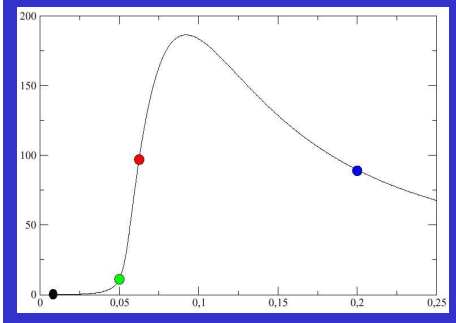
D. Fournier, M. Poirier, M. Castonguay, and K. Truong
de Recherche sur les Propriétés Électroniques de Matériaux Avancés and Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1.
(Dated: Sept. 2002)

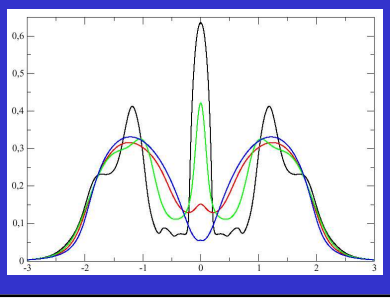
The phase diagram of the organic superconductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$Cl has been investigated by ultrasonic velocity measurements under helium gas pressure. Different phase transitions were identified trough several elastic anomalies characterized from isobaric and isothermal sweeps. Our data reveal two crossover lines that end on the critical point terminating the first-order Mott transition line. When the critical point is approached along these lines, we observe a dramatic softening of the velocity which is consistent with a diverging compressibility of the electronic degrees of freedom.

FIG. 1: Temperature vs pressure phase diagram of κ-Cl. Different symbols are associated to different anomalies gathered on three different crystals from temperature sweeps (full symbols) and pressure sweeps (open symbols). The zero pressure point (dotted hexagon) was obtained from a microwave resistivity measurement. The gray circle indicates the critical point (P_0, T_0).

FIG. 4: Temperature dependence of $\Delta V/V$ at various pressures. The velocity variation is relative to the value at 90 K. Inset: position and amplitude of the anomaly below 230 bars.

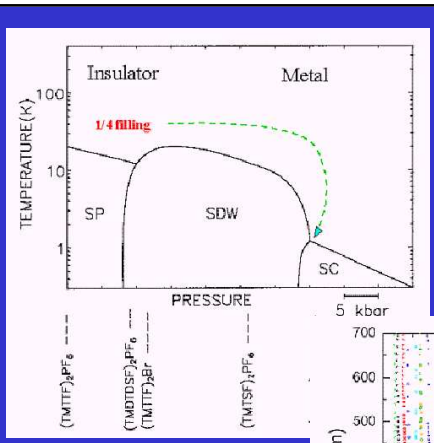




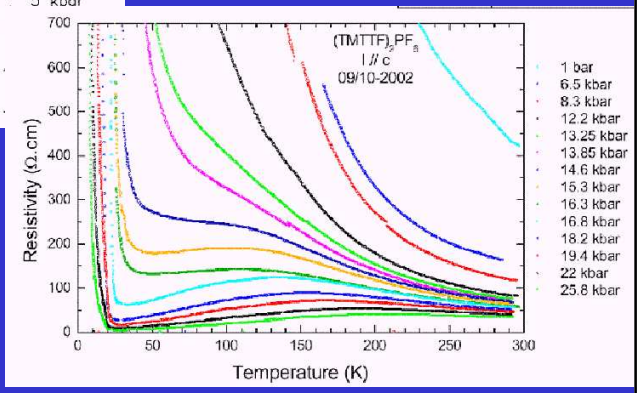


Model transport calculations were performed at this workshop (S. Florens et al.)

Cf. Mc Kenzie et al.



Proximity to Mott transition plays a key role in quasi-1D organics (Bechgaard salts)
Cf. **D. Jerome (KITP 2002)**



Other experimental highlights:

* Strong spatial inhomogeneities in cuprates revealed by STM (S. Davis, A. Kapitulnik)

* New optical data on FeSi, on Ce (van der Marel)

* Role of local clusters in frustrated magnets (SW Cheong)

* Intriguing aspects of obital fluctuations in d1 perovskites (B.Keimer)

* AND MANY MORE…

Some **collaborative work** started or completed during the workshop

(Just a few examples…)

New Frontiers…

Materials- related issues:

• I already mentioned several works on specific materials:
d1 transition metal oxides, organics etc…

In addition, several collaborations took place
on f-electron systems:

- Mc Mahan, Held, Scalettar on Cerium (including SO, etc…)
alpha/gamma transition

- Savrasov and Kotliar on the role of phonons in Plutonium

- …

•**Increasing evidence for key role played by:**

- Spatial **inhomogeneities** meso/nano-scale
- Coupling to **lattice** degrees of freedom

(Note: Many phases in close competition in SCEMs)

•Orbital **fluctuations** and orbital **ordering** raise intriguing questions:

- Exotic phases (spin/orbital liquids) ?
- Frustration
- But also: underlying rationale for some of the successes of DMFT…

* Common methods to handle interactions in the field of mesoscopic conductors (Coulomb blockade, etc…)

Advances on Methods:

Combining DMFT w/ different approaches to electronic structure:

-**Downfolding** ('NMTO') + DMFT
(Biermann, Lichtenstein, Pavarini, Saha-Dasgupta)

-**PAW + DMFT** (Alouani and Bloechl)

-**Multiple kappa's (FP-LMTO)** S. Savrasov

(Projects initiated/completed @workshop)

Code for realistic calculations of optical spectra (Oudovenko, Palsson, Savrasov, Kotliar)

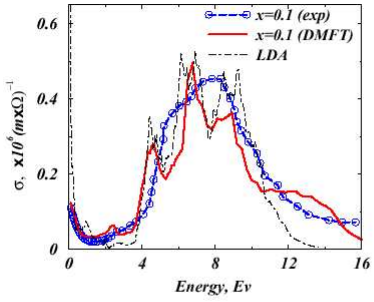


FIG. 3. Calculated optical conductivity spectrum for $La_{1-x}Sr_xTiO_3$, $x = 0.1$, at large frequency interval using DMFT method (full line) as compared with the experimental data (symbols) and the results of the corresponding LDA only calculations (dashed line).

Project completed @ workshop

Cond-mat 0209336

Other active topics at workshop: / Methods

•**Progress in QMC techniques** : S. Zhang

(A lot more is expected to come, including applications cf. M. Scheffler's talk)

* Other **Numerical algorithms**: S. White, M. Imada, M. Troyer,…

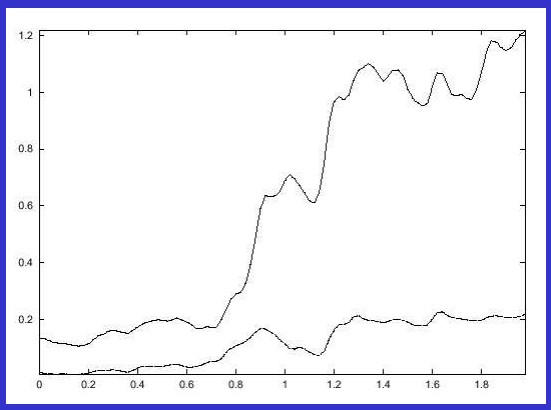
*** Renormalization group** techniques were the subject of very active discussions/joint work among a group of participants

Screening, electronic structure and DMFT…

* Start from RPA treatment of screening:
the **GW approximation**
(quite successful: e.g semiconductors)

* For CEMs: improve on local components of BOTH the self-energy and the effective interaction
using extended versions of DMFT
with a frequency-dependent U, calculated from first principles

A number of people involved in such work @ workshop:
F. Aryasetiawan, S. Biermann, S. Florens,A.G,
A. Lichtenstein, G. Kotliar, P.Sun



Local and n.n components of effective screened interaction for Nickel (F. Aryasetiawan@workshop)

REPRESENTABILITY in terms of impurity model ?

Perhaps not
`` A LIFE WITHOUT U `` **?**

But hopefully…
`` A BETTER LIFE WITH U ``
(with lots of energy-dependence)

Spatial correlations, J,
and **cluster extensions**
of DMFT…

DMFT has energy gain from ORDERING but
Does not have the feedback of local correlations into G
In a disordered environment.

Needed if strong k-dependence, e.g OF THE QUASIPARTICLE COHERENCE SCALE

A number of people involved in such work @ workshop:
G. Biroli, O. Parcollet, M. Capone, G. Kotliar,
A. Lichtenstein, A. Poteryaev, etc…