Materials with strong electron correlation and strong electron-phonon interaction

H. Koizumi
Institute of materials science, U. of Tsukuba

Research Directions

1. Anomalous electric conductivity phenomena in transition metal oxides.

a) High temperature superconductivity in cuprates (copper oxides).

b) Colossal magnetoresistance in manganites (manganese oxides).

2. Role of transition metals in biological systems

(not started, yet).

Current central topic:

High temperature superconductivity in hole-doped cuprates.

(it was found in 1986, but its mechanism is not elucidated, yet)

Two major challenges for theoretical treatment

1. Strong correlation: the parent compound is a Mott insulator.

Calculations based on the local density approximation predicts it as a metal.

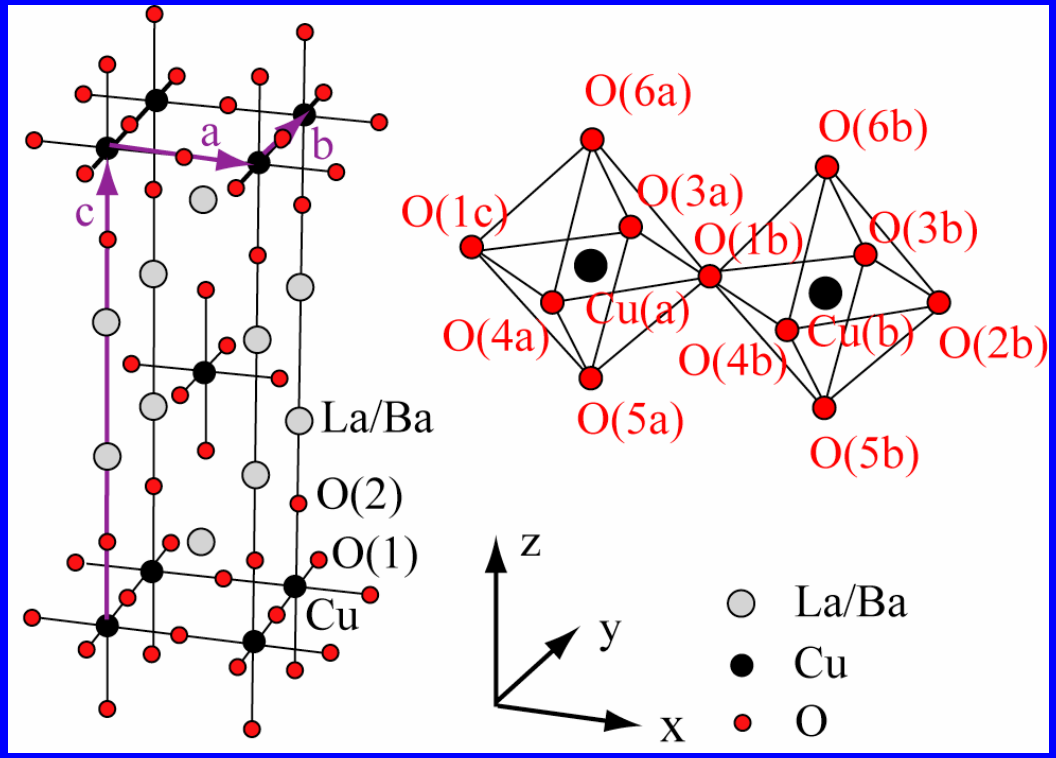
2. Strong doped hole - lattice interaction: EXAFS and other experimental data indicates strong doped hole - lattice interaction.

Then, doped holes become small polarons, that are not good charge carriers at low temperature; yet, superconductivity occurs.

To deal with strong correlation

Molecular orbital cluster calculations：apply molecular orbital method to a part of a solid (“cluster”).

Crystal environment is mimicked by an effective potential.



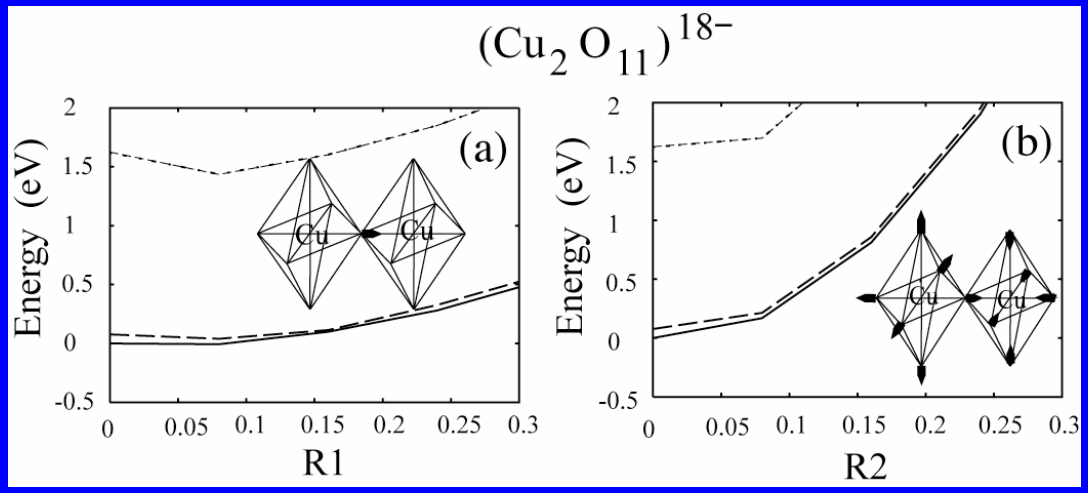
Complete active space self-consistent filed method (CASSCF method)

Package programs are used to obtain wave functions: GAMESS, MOLCAS

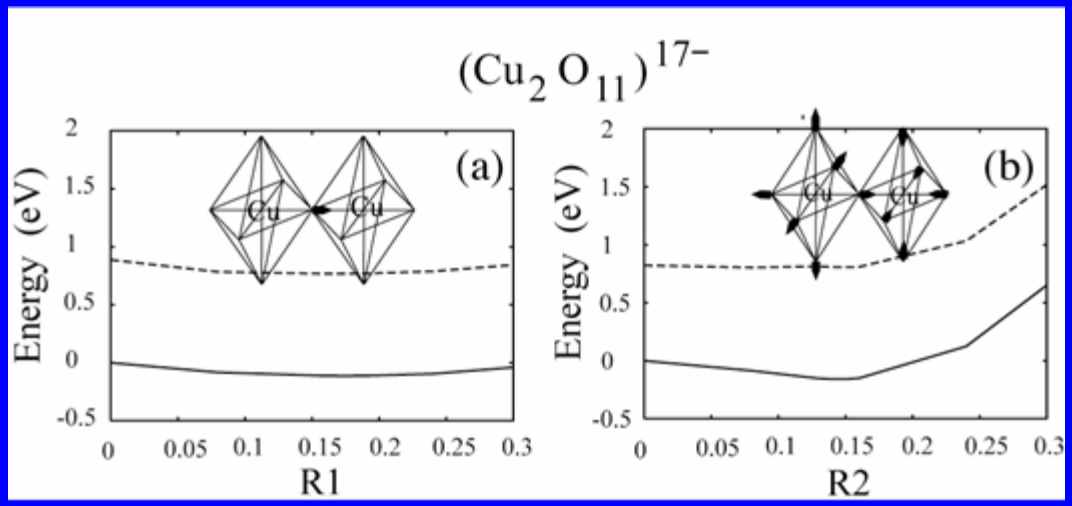
To see strong doped hole - lattice interaction:

total energy is calculated with deforming the cluster.

Excited states are also calculated to compare with experiments.



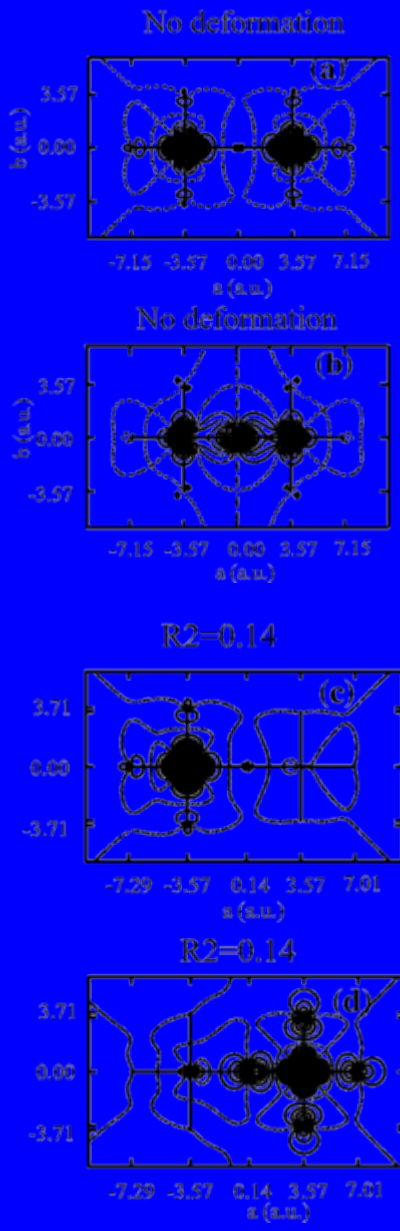
Parent cluster does not show lattice instability. The excitation energy agrees with that obtained by experiment.



Hole-doped cluster shows lattice instability. The magnitude of the deformation agrees with the one obtained by EXAFS experiment. The excitation

energy seems to agree with the peak in the energy loss function.

Plots of natural orbitals



The lattice instability is a pseudo Jahn-Teller type; antisymmetric orbital and symmetric orbital couple with antisymmetric deformation.

Doped-hole is mostly in the bridging oxygen when the cluster is not deformed. When the deformation is taken into account the hole-occupied orbital becomes the one constructed from a central copper d-orbital and surrounding four oxygen p-orbitals. This orbital is a molecular orbital-like, in contrast to the Zhan-Rice singlet state.

Doped holes become small polarons, that are not good charge carriers at low temperature; yet, superconductivity occurs.

Need new current flow mechanism !

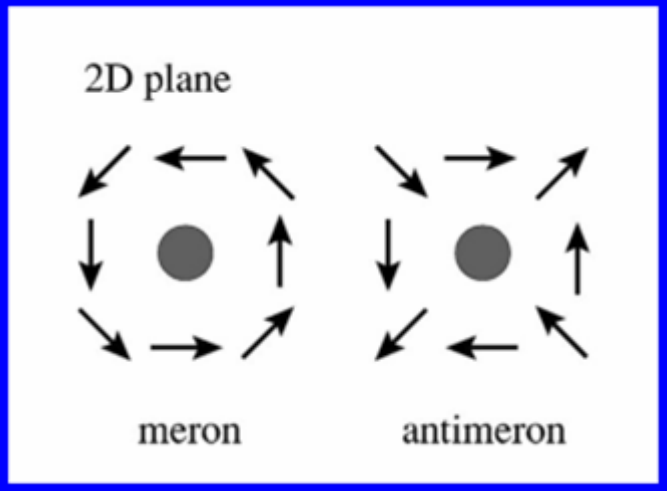
A novel current flow mechanism is currently under construction.

Main ingredient is a fictitious magnetic field from a Berry phase that acts as a magnetic field applied to electrons. It appears when spin vortices are created.

Calculations are done with a Hubbard model; since

in order to describe many spin vortices,

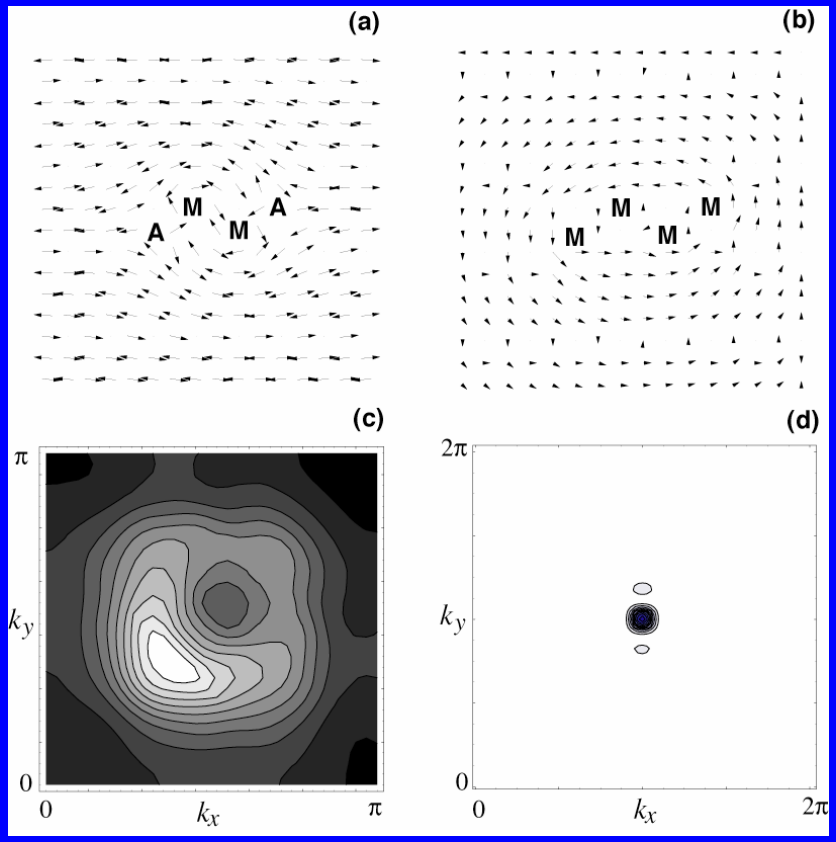
a large number of clusters have to be included.



Meron: spin vortex with winding number +1 is called “meron”.

Antimeron: spin vortex with winding number -1 is called “antimeron”.

So far, mean field calculations have been done.

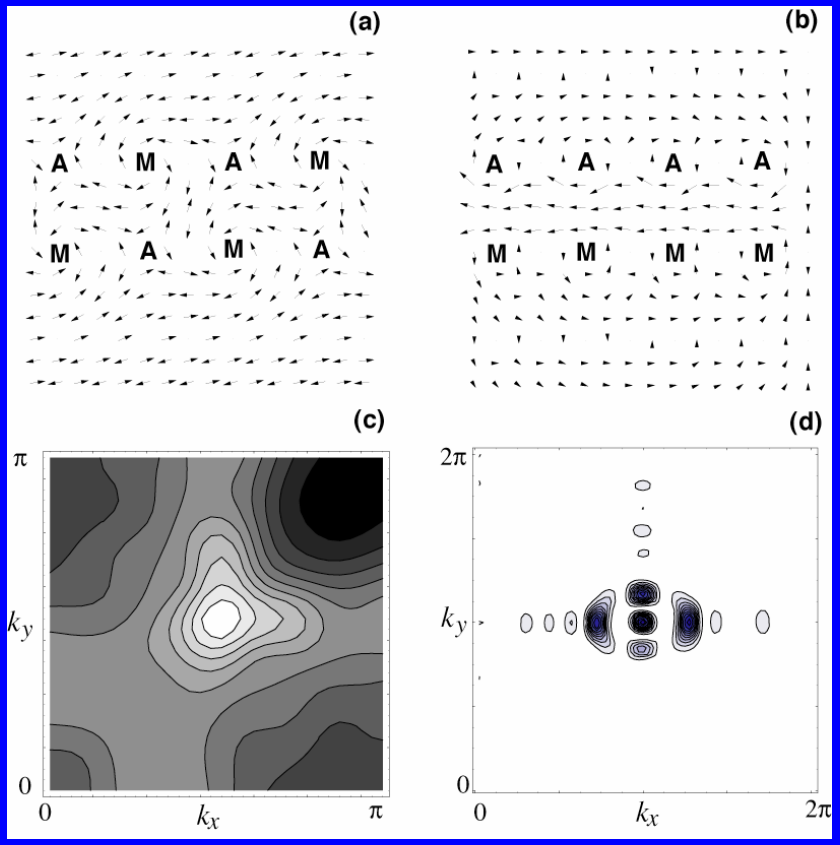


(a) Spin configuration with two merons and two antimerons.

(b) Current distribution; it shows an extended current flow region generated by the fictitious magnetic field from a Berry phase.

(c) The simulated angle-resolved photoemission spectrum. It shows an arc-like fermi-surface region.

(d) The simulated inelastic neutron scattering profile. The central peak is due to the antiferromagnetic spin order.



(a) Spin configuration with four merons and four antimerons.

(b) Current distribution; it shows a river of current .

(c) The simulated angle-resolved photoemission spectrum.

(d) The simulated inelastic neutron scattering profile; the splitting of the antiferromagnetic peak is seen, which agrees with experiment.

Future plans

1. CASSCF calculations for a larger clusters; include more than 4 coppers.

2. Variational Monte Carlo calculations for a Hubbard model that includes small polarons (holes with surrounding lattice distortion) and spin vortices.

By further increase of the cluster size, stability of spin vortices will be examined in terms of molecular orbital calculations. We believe that spin vortices and fictitious magnetic field are the key ingredients to elucidate cuprate superconductivity.

3. Application of new current flow mechanism to manganites.

4. Application of new current flow mechanism to biological systems.