

Muon Sites in La_2CuO_4

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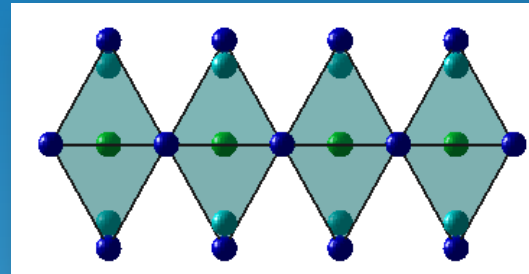
USM/Malaysia



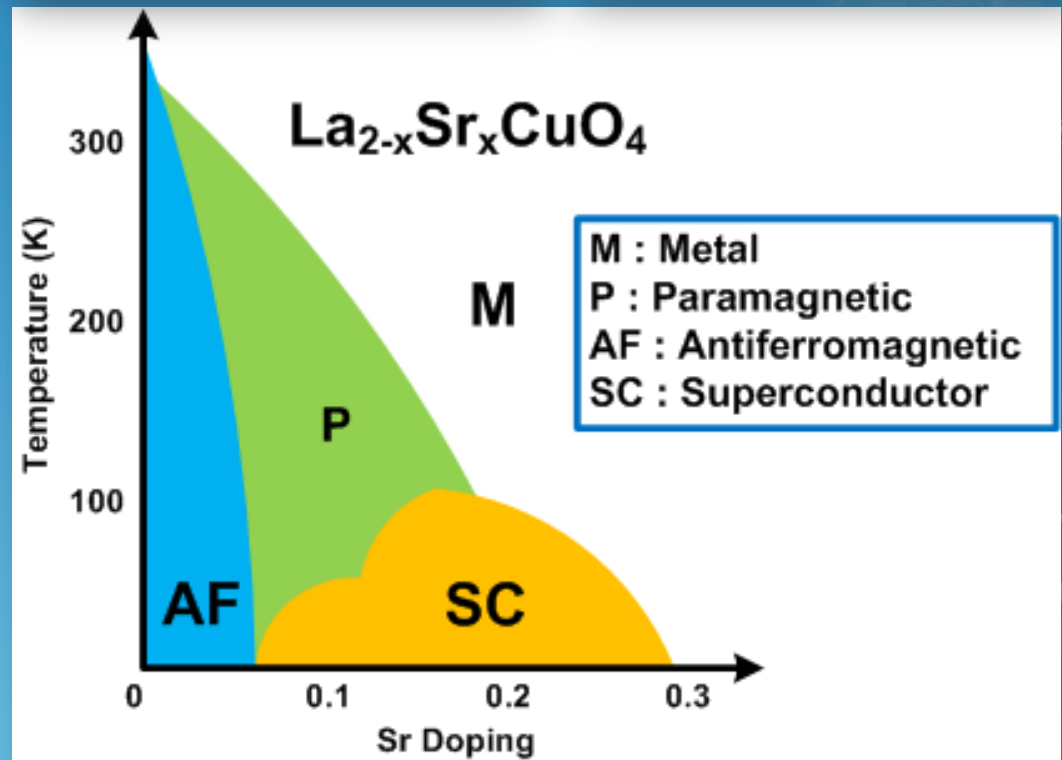
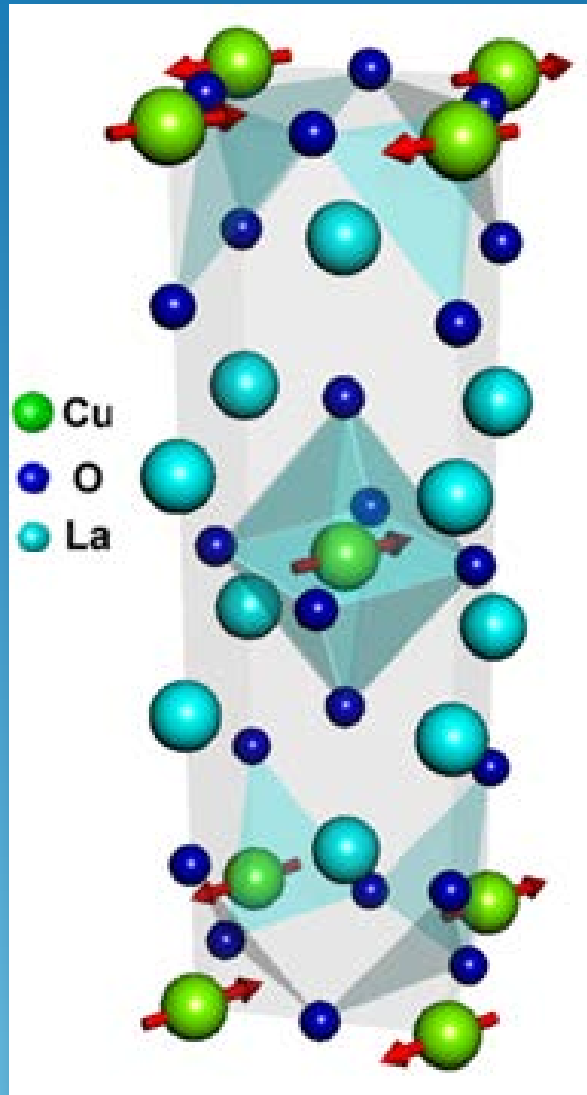
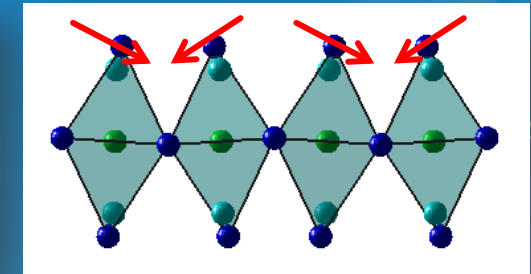
La₂CuO₄



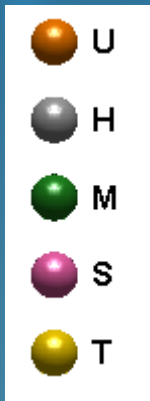
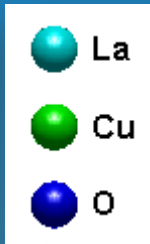
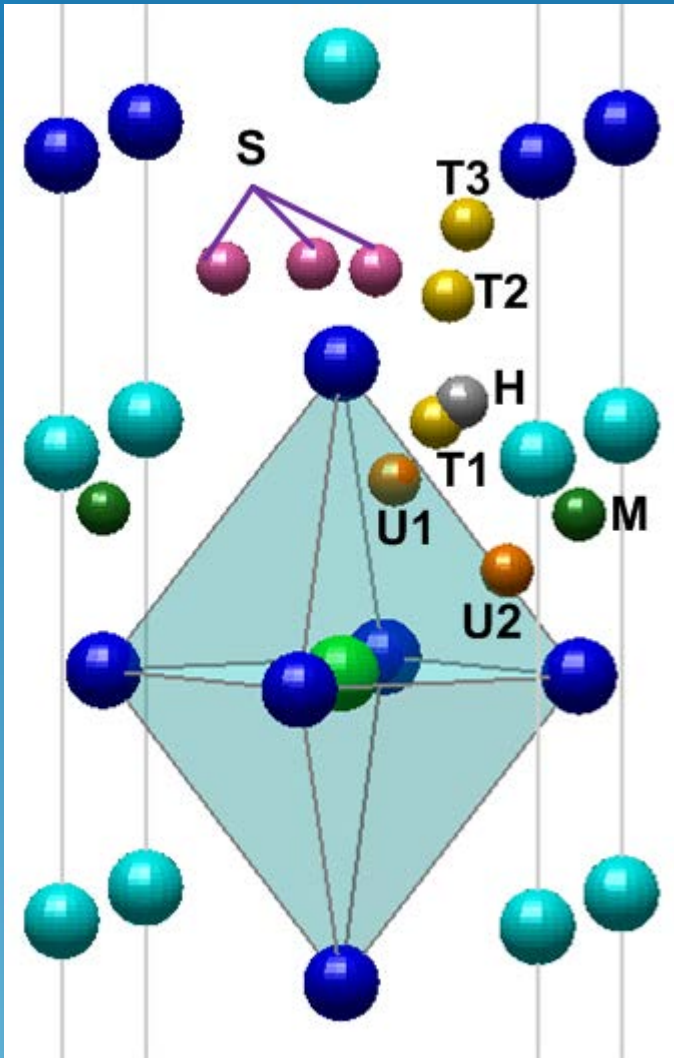
T-Structure ($>T_N$)



O-Structure ($<T_N$)



Muon Sites in La_2CuO_4



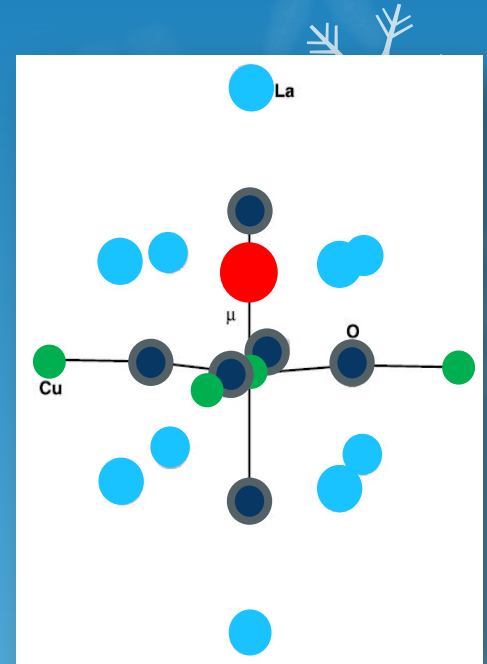
Sulaiman *et al.* (1994)

Hitti *et al.* (1990)

McMullen *et al.* (1990)

Saito *et al.* (1990)

Torikai *et al.* (1993)



● Suter *et al.* (2003)

Muon Site Estimation in La_2CuO_4

Previous Methods

Hitti *et al.* (1990) – Electric Dipole Field

Torikai *et al.* (1993) – Nuclear Dipole Field

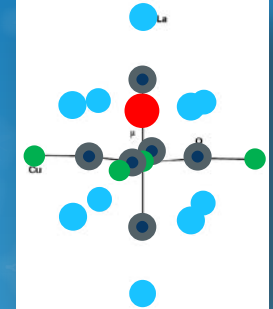
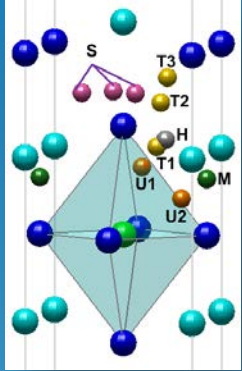
Saito *et al.* (1990) – Electrostatic Potential

McMullen *et al.* (1990) – Modified Electrostatic Potential

Sulaiman *et al.* (1994) – Minimum Energy Search

Suter *et al.* (2003) – Partial Relaxation

Huang *et al.* (2013) – Time Dependent Schrodinger Equations



[-] Tetragonal Structure (High Temperature Structure)

[-] Relaxation degree of Freedom,

[-] Spherical-Wave (Molecules/Ion), and

[-] Relationship with μSR data

Muon Site Estimation in La_2CuO_4

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Hitti *et al.* (1990) – Electric Dipole Field

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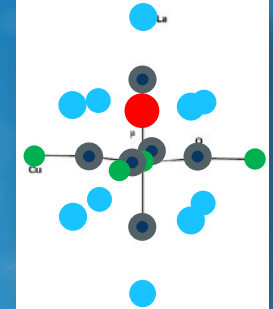
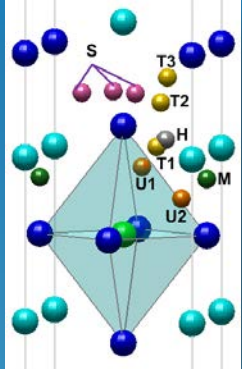
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[+] Orthorombic Structure

[+] Relaxation (lattice and muon position)

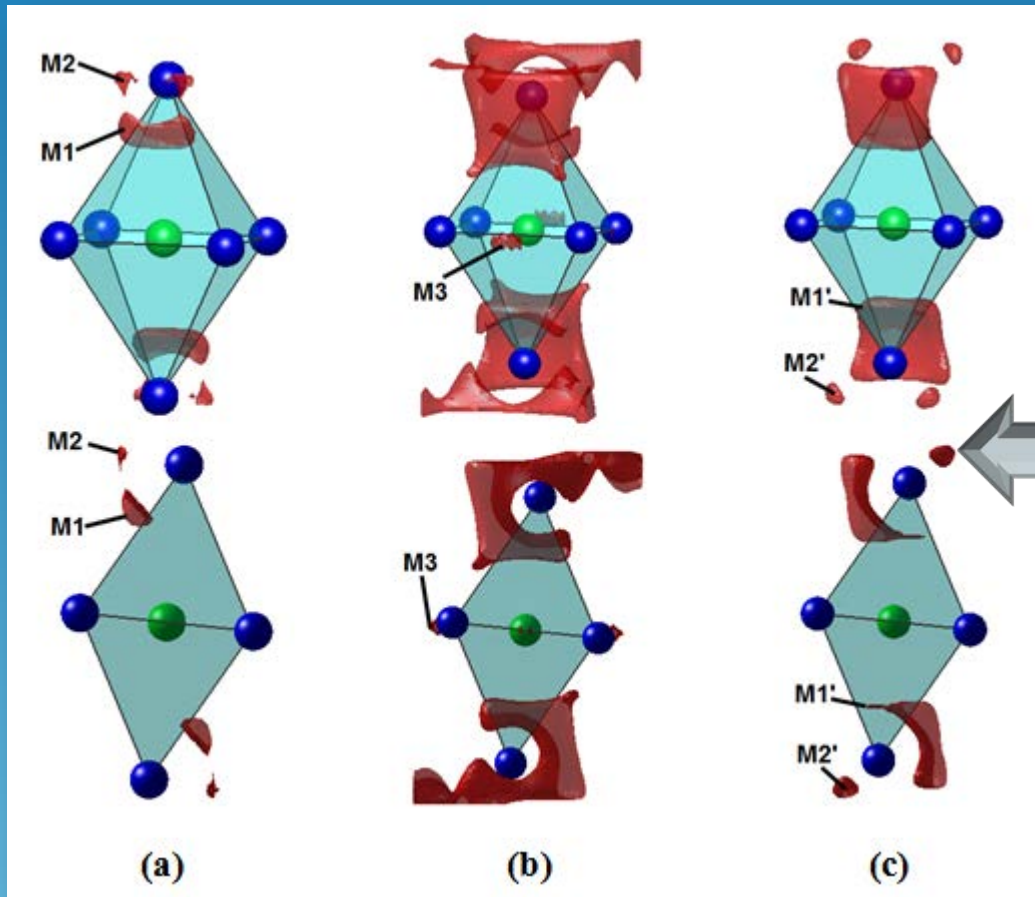
[+] appropriate correction function

[+] Relationship with μSR data

[+] Supercell (3x3) calculations

DFT Calculations by VASP

for one unit cell



RIKEN RICC Cluster



Retry μ SR on La_2CuO_4

@ RIKEN-RAL and PSI

Thin Film of La_2CuO_4

PHYSICAL REVIEW B 88, 064419 (2013)

Magnetic phase diagram of low-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ thin films studied by low-energy muon-spin rotation

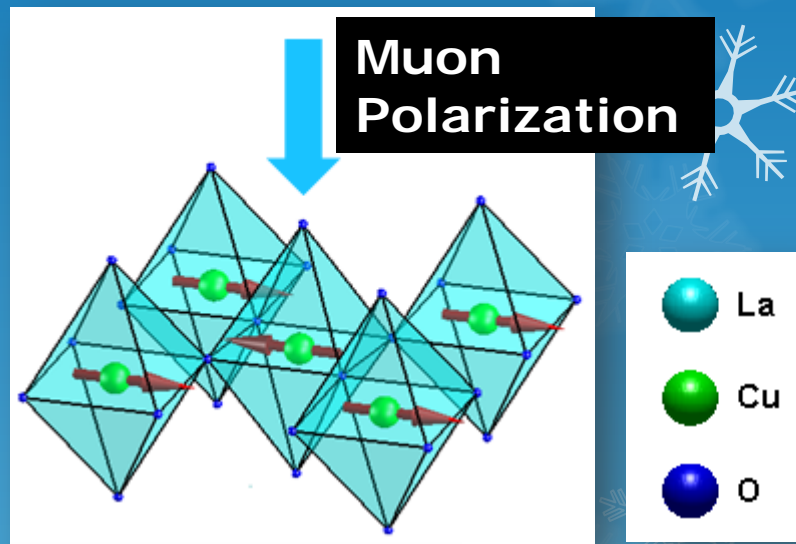
E. Stulp,^{1,2} A. Suter,¹ T. Prokscha,¹ E. Morenzoni,¹ H. Keller,² B. M. Wojek,^{1,2,*} H. Luetkens,¹ A. Gozar,³ G. Logvenov,^{3,†} and I. Božović³

¹Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

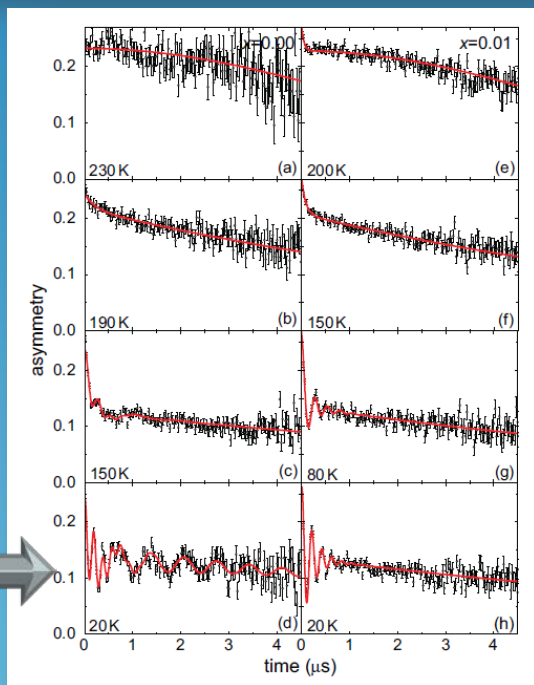
²Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

³Brookhaven National Laboratory, Upton, New York 11973-5000, USA

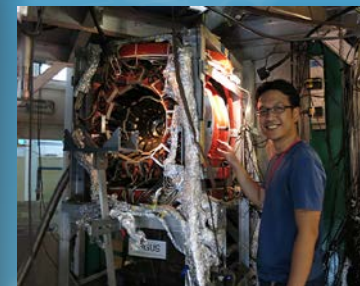
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PSI



2-sites



Sample provided from
Koike Lab., Tohoku Univ.

Summary

- 1) We have retry to estimate muon sites in La_2CuO_4 .
- 2) From DFT calculations, we estimated three muon positions.
- 3) We have observed three muon sites. Two of them are newly observed.
- 4) Dipole-field calculations do not reproduce experimental results.