How muon senses ordered Cu spin in YBa$_2$Cu$_3$O$_6$?
- A supercell approach by DFT calculations-

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Basic properties of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$

Crystal structure of YBCO

The mother compound is **Antiferromagnetic ordering**

This AF ordering disappears with doping and superconductivity appears
Early $\mu$SR experiments of YBCO$_x$

First evidence AF ordering in YBCO$_x$

Internal field at the muon site: 250 ~ 300 G

N. Nishida et. al, Jap. J. Appl. Phys. 26 (11), 1987

Oxygen content

$X = 6.04$

$X = 6.27$

$X = 6.44$

$X = 6.54$

Questions

Where does the muon stop in the system?

How the muon senses the internal fields in the system and how much does the muon perturb the host system?

- Local deformations caused by muon?
- Spatial distribution of the Cu-spin density?
- Zero-point energy motion of the muon?
μSR and DFT

μSR Experiment

Fourier transform of μSR time spectra

Internal Fields

Muon state

DFT calculations

Muon position and local perturbation of muon

Dipole fields calculations (ZPE, Spin distribution)

Internal Fields at muon sites

Spin state
1. Optimize Parameter
   - Energy cut
   - Hubbard value, U
   - Mott insulator of YBCO

2. Calculate potential
   - Unperturbed system
   - No muon,
   - supercell 4x4x2
   - Initial muon position

3. Relaxation
   - Supercell + One No muon,
   - Charge supercell
   - Final muon position
   - Ionic Relaxation, Spin density

4. Internal fields
   - Dipolar interaction
   - Zero point energy motion
   - Spin density
Band structure and DOS

- Energy cut = 500 eV
- GGA + U
- Antiferromagnetic ordering
- Hubbard, \( U = 9.0 \) eV
Initial muon positions

Isosurface at 500 meV
Unperturbed system
Supercell calculations

Calculation conditions
- Energy cut = 500 eV
- Non-collinear calculation
- AF ordering of Cu(II)
- Muon as light isotope of Hydrogen
- Charge of supercell +1
Quantum effect corrections

**Zero-point energy (ZPE) vibration energy**

\[ V_0 + E_{ZPE} \]

\[ V_0 \]

\[ E_{ZPE} \]

Solving Schrödinger equation for muon

\[
\left[ -\frac{\hbar^2}{2m_\mu} \left( \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \right) + V_\mu(x, y, z) \right] \psi_\mu(x, y, z) = E_{ZPE} \psi_\mu(x, y, z)
\]

- Zero point energy
- Muon probability density \( \rightarrow \langle \psi_\mu | \psi_\mu \rangle \)
Muon probability density

Muon Position M1

Muon Position M2

Muon Position M3
Thank you very much for your attention