How muon senses ordered Cu spin in $YBa_2Cu_3O_6$? - A supercell approach by DFT calculations-

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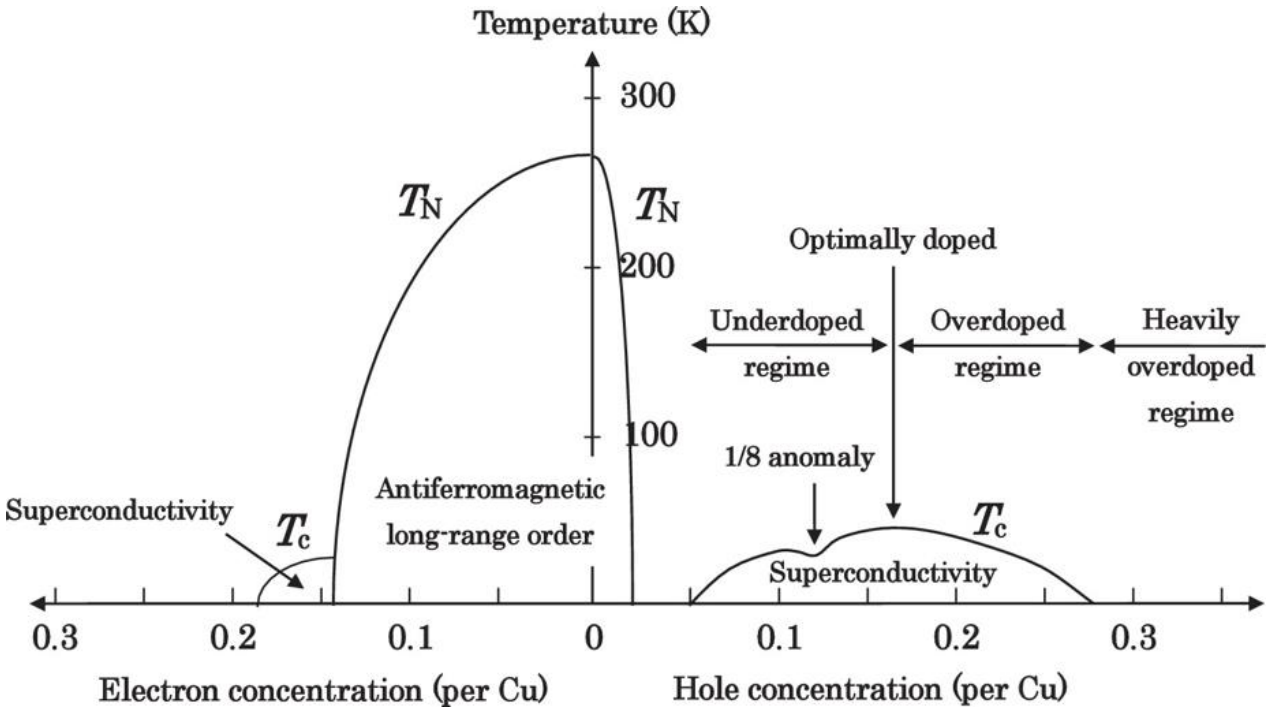
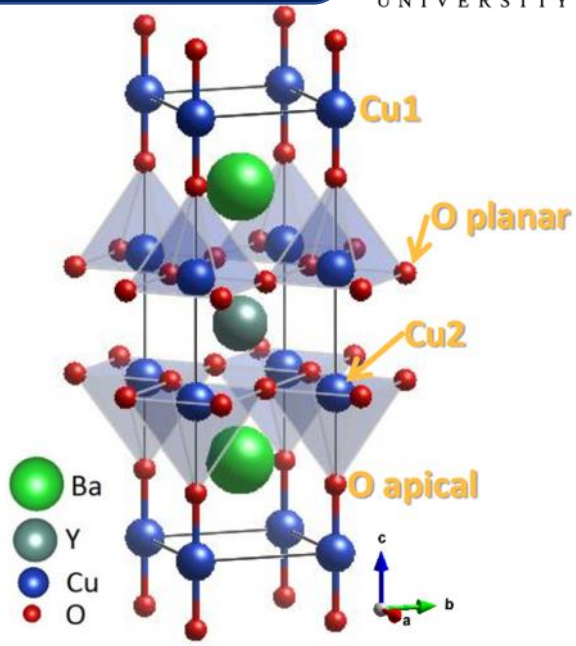
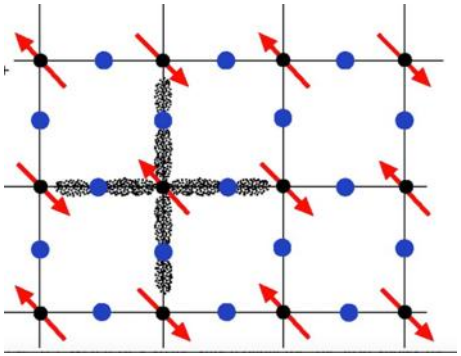
Basic properties of $YBa_2Cu_3O_{6+x}$





Crystal structure of YBCO



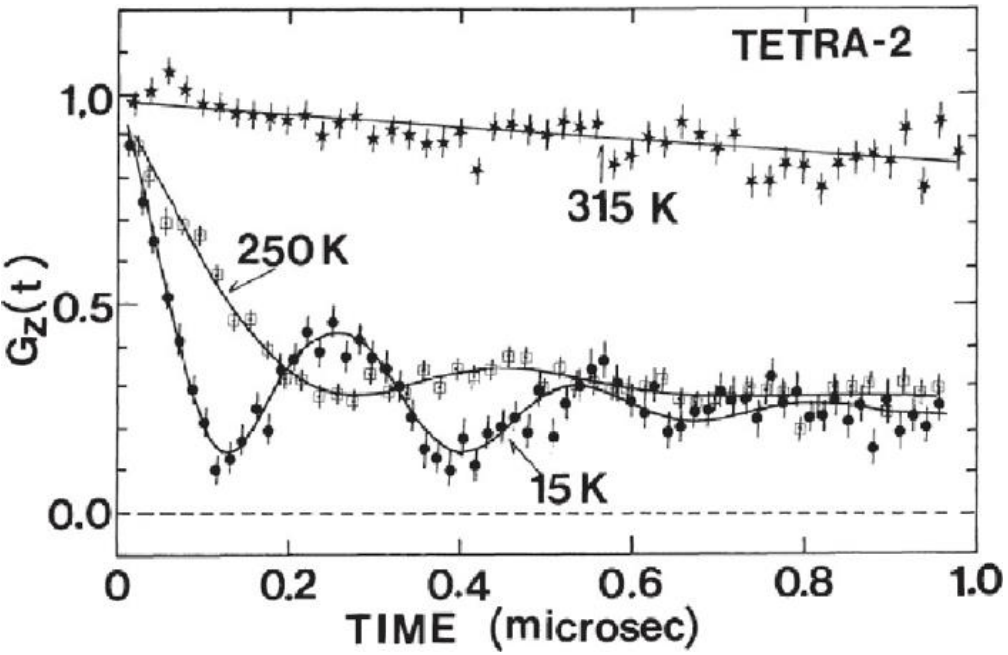
Ordered Spin Structure

⇒The mother compound is *Antiferromagnetic ordering*

⇒This AF ordering disappears with doping and superconductivity appears

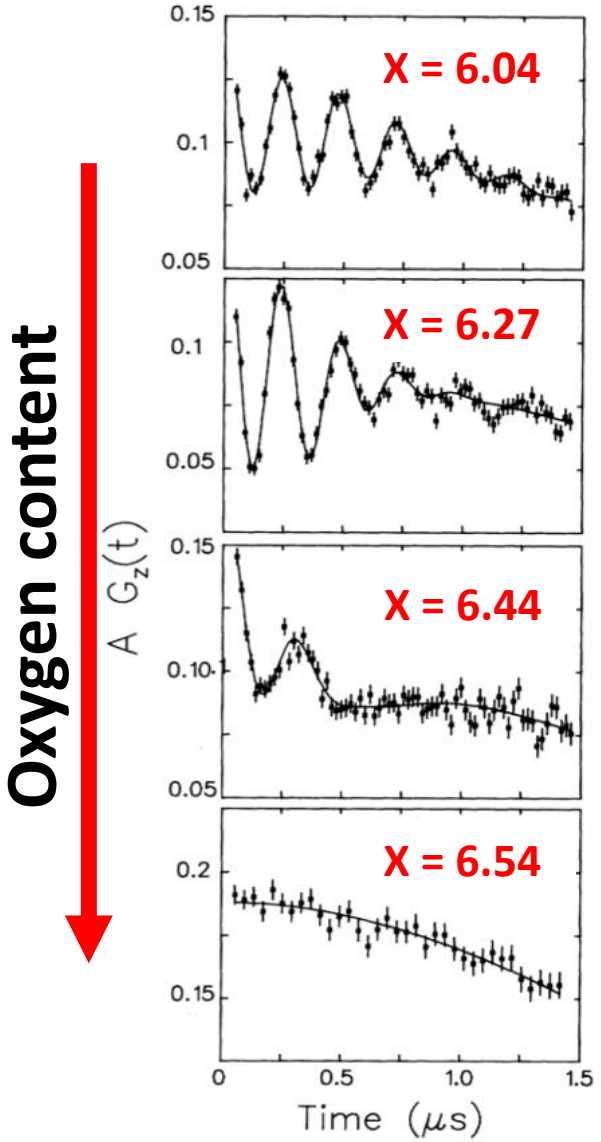
Early μSR experiments of YBCOx

First evidence AF ordering in YBCOx



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

Internal field at the muon site : 250 ~ 300 G



R.F. Kiefl *et al.*, Phys. Rev. Lett. **63**, 2136 (1989)

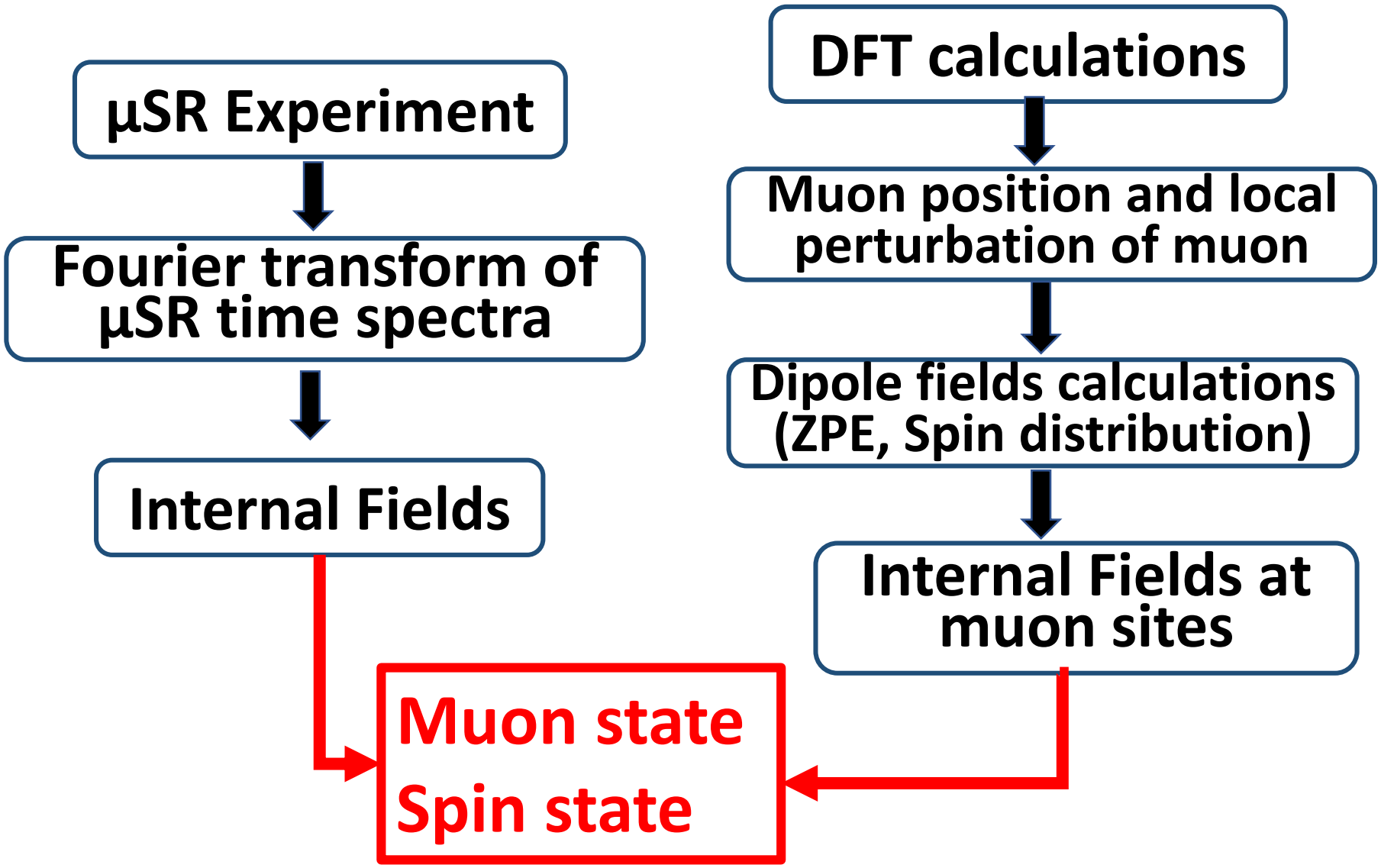
Questions

⇒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
DFT calculations
Muon position and local perturbation of muon
Dipole fields calculations (ZPE, Spin distribution)
Internal Fields at muon sites
Muon state
Spin state

Calculation Method

1. Optimize Parameter

⇒ Energy cut
⇒ Hubbard value, U
⇒ Mott insulator of YBCO

2. Calculate potential

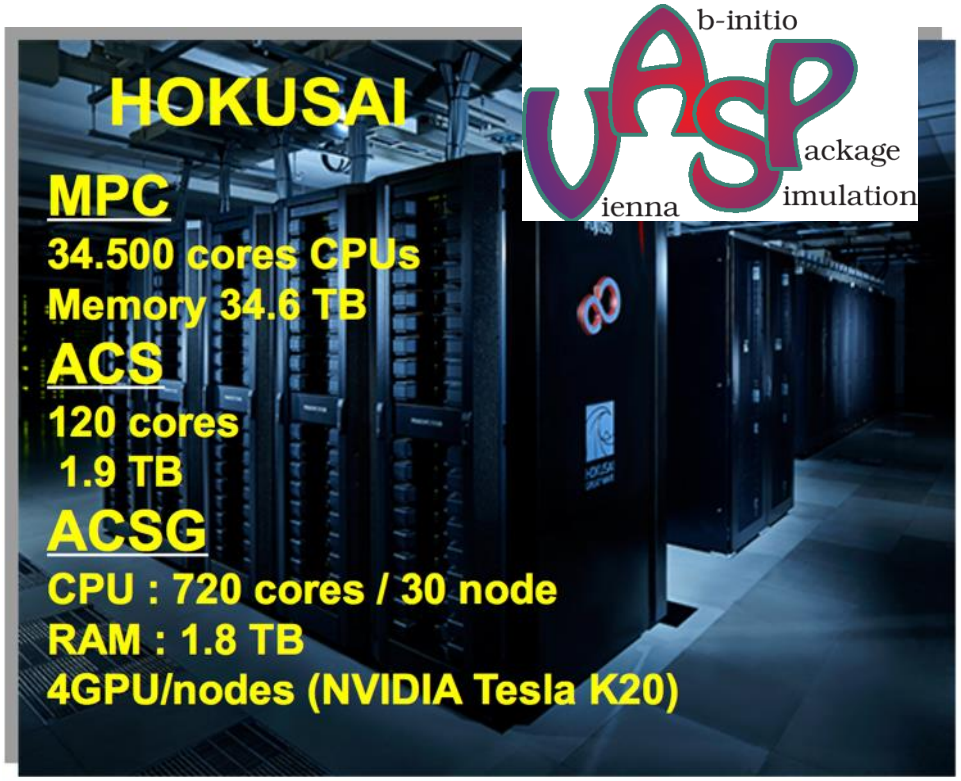
⇒ Unperturbed system
⇒ No muon,
⇒ supercell4x4x2
⇒ Initial muon position

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



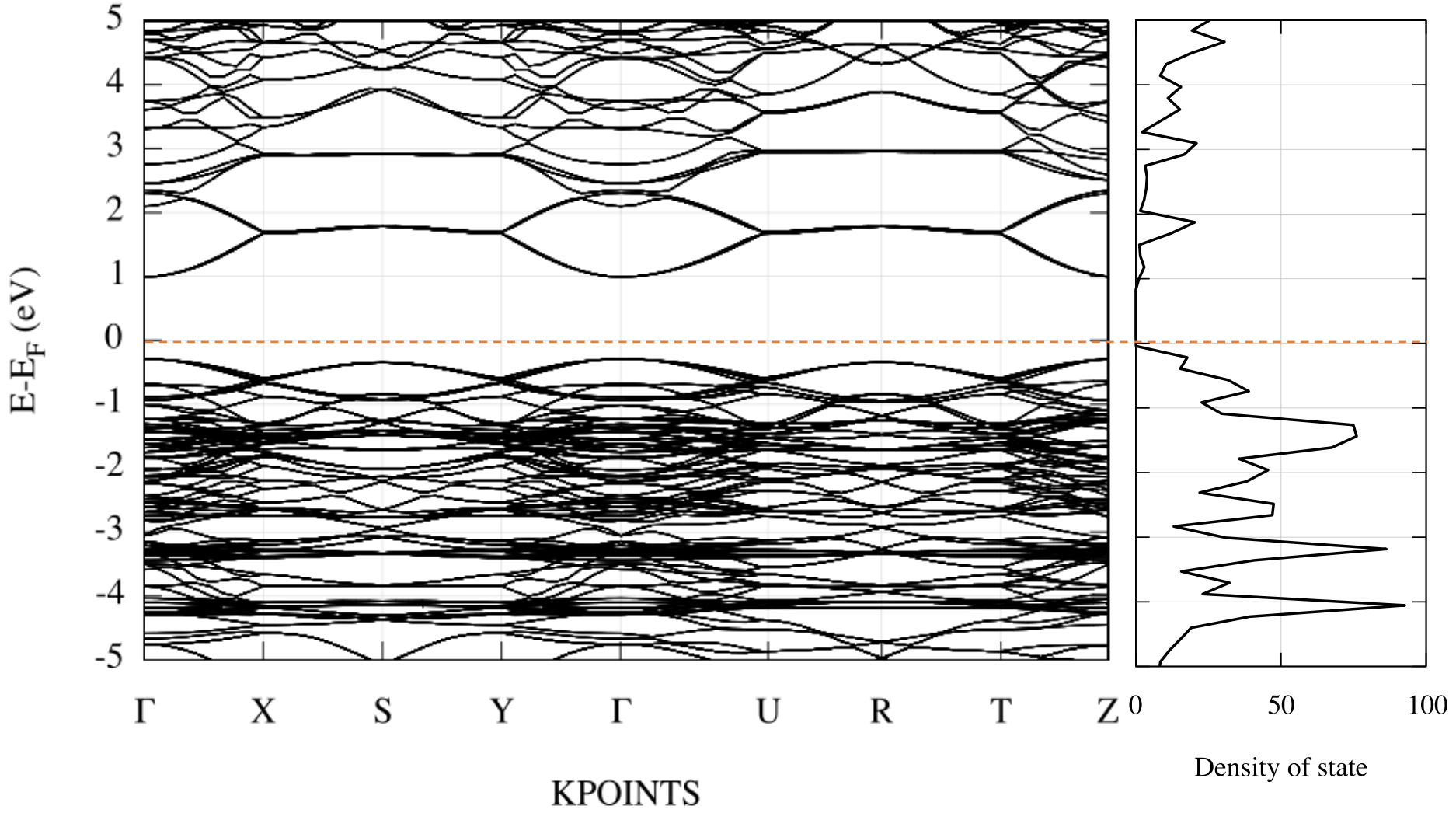
Band structure and DOS

⇒Energy cut = 500 eV

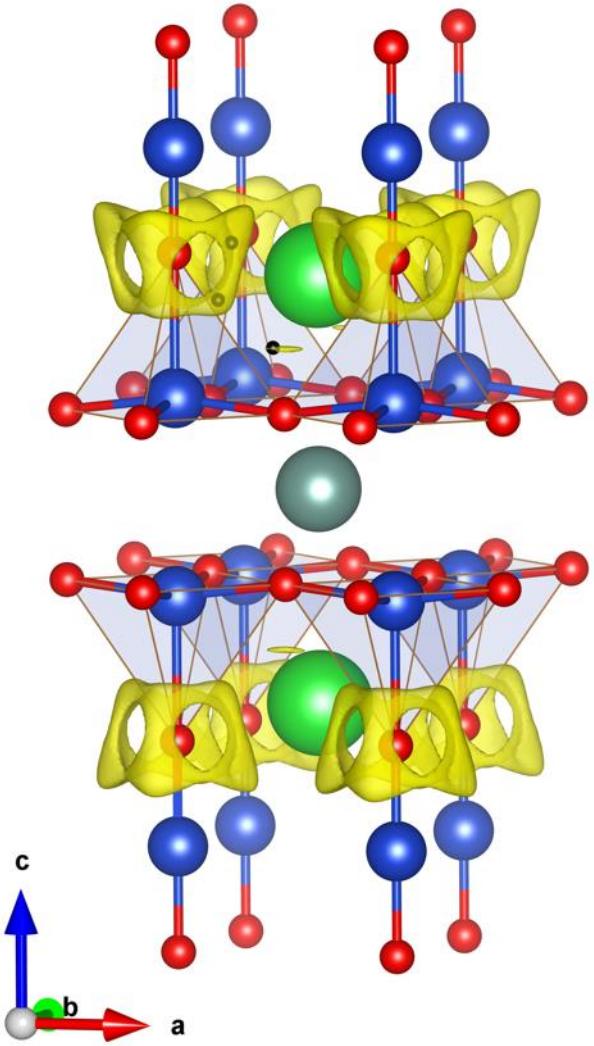
⇒GGA + U

⇒Antiferromagnetic ordering

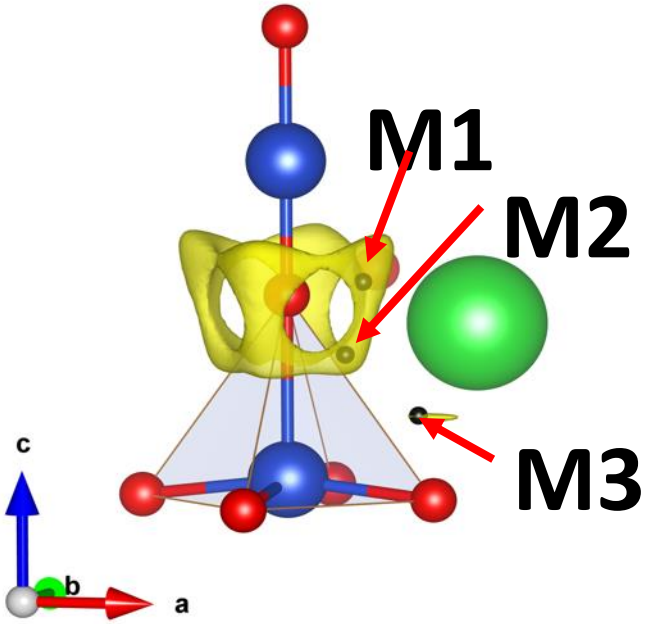
⇒Hubbard ,U = 9.0 eV

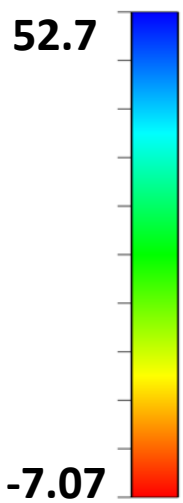


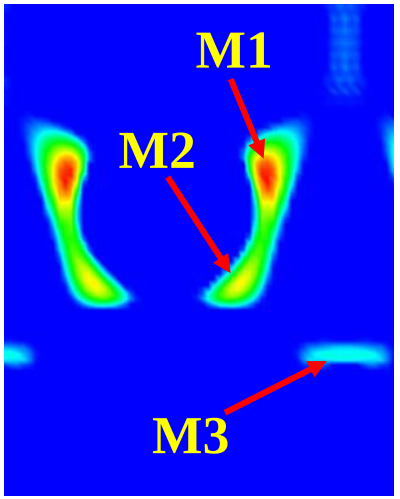
Initial muon positions



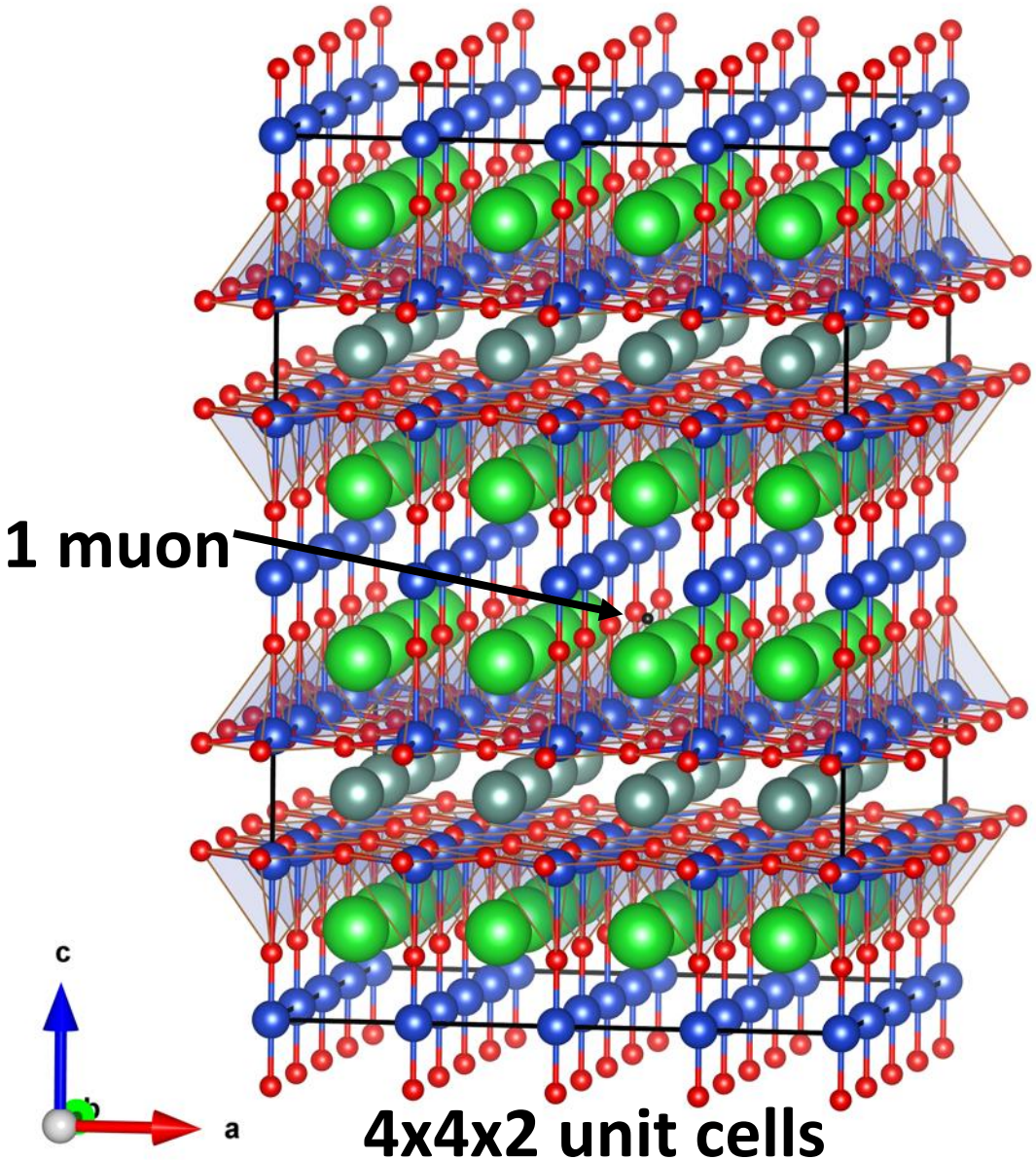
Isosurface at 500 meV
Unperturbed system







Supercell calculations

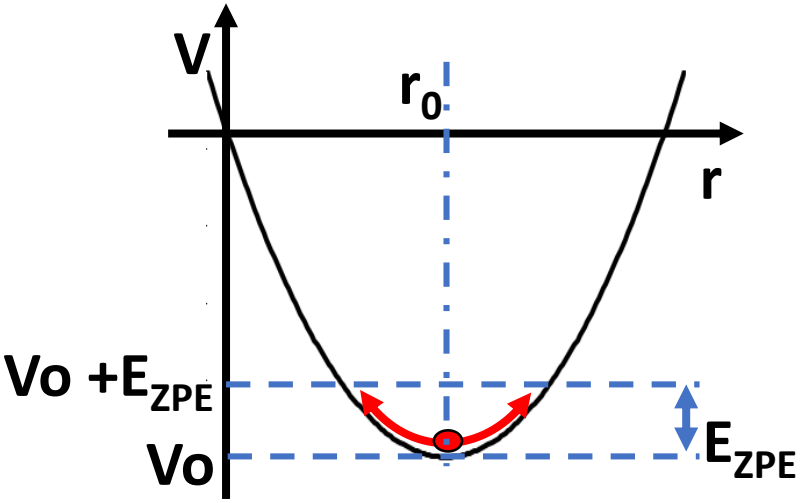


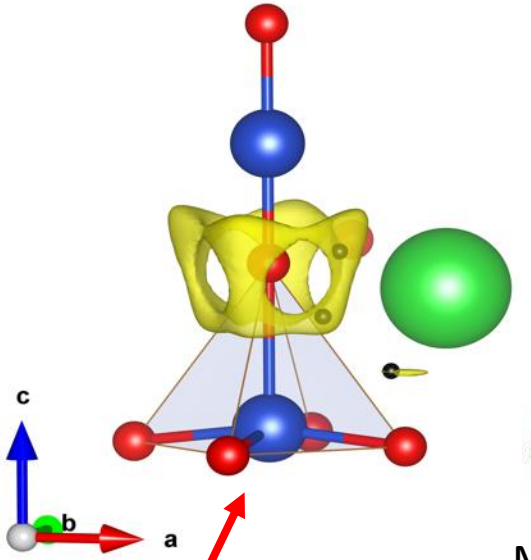
Calculation conditions

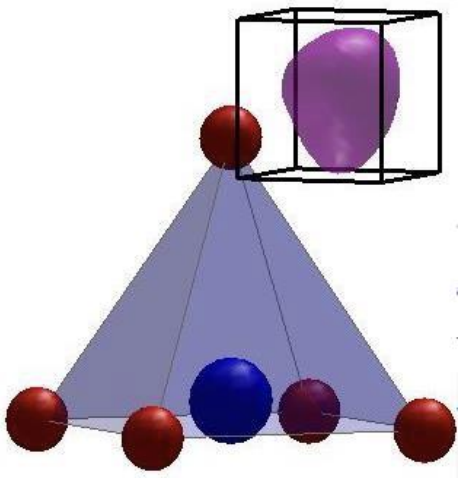
- Energy cut = 500 eV
- Non-collinear calculation
- AF ordering of Cu(II)
- Muon as light isotope of Hydrogen
- Charge of supercell +1

Quantum effect corrections

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







Muon probability density

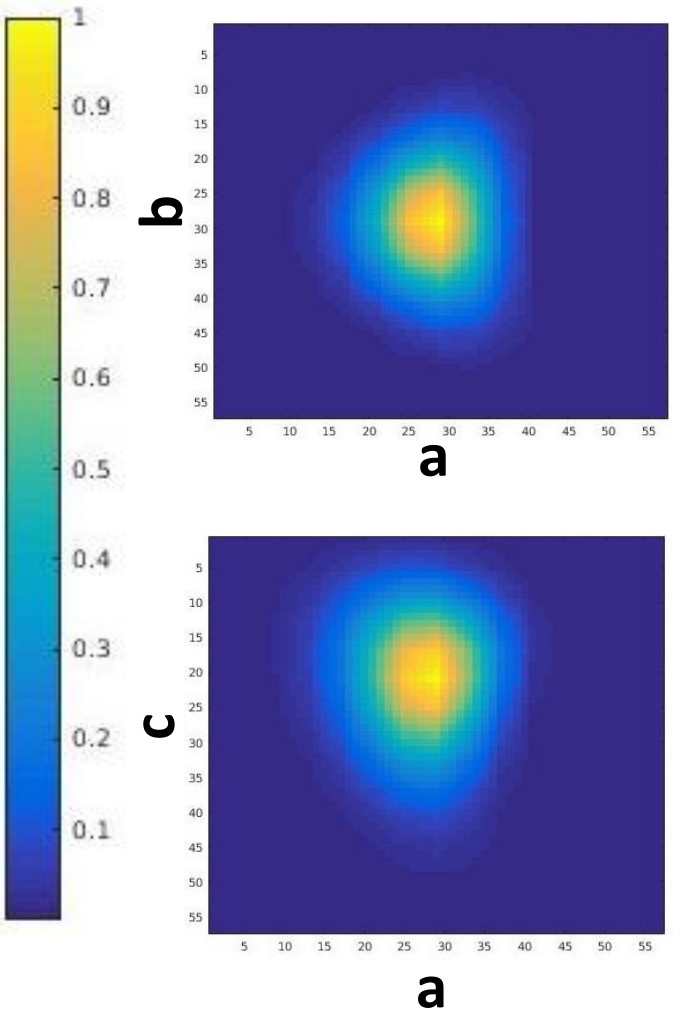
Solving Schrodinger equation for muon

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

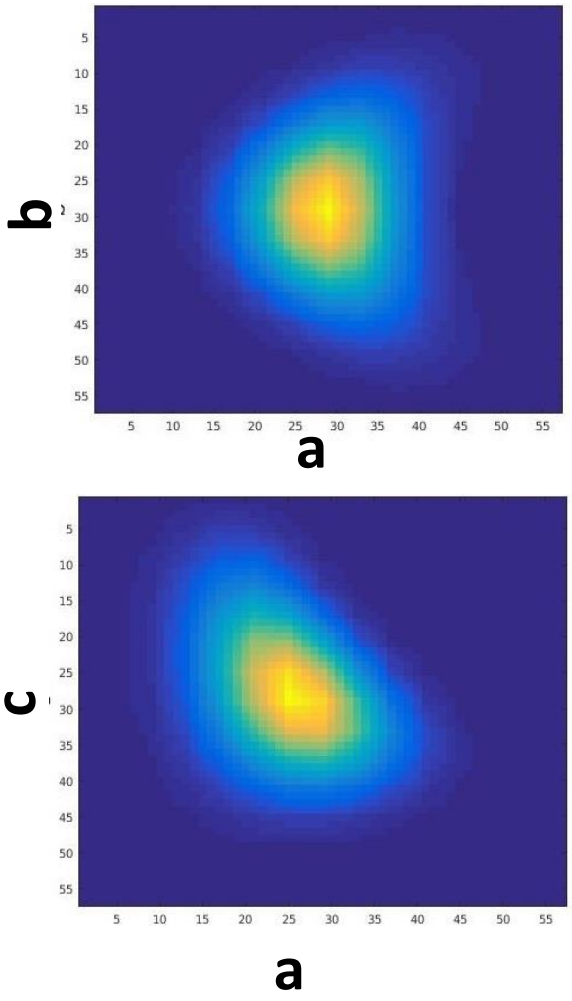
- **Zero point energy**
- **Muon probability density** $\rightarrow\langle\psi_\mu|\psi_\mu\rangle$

Muon probability density

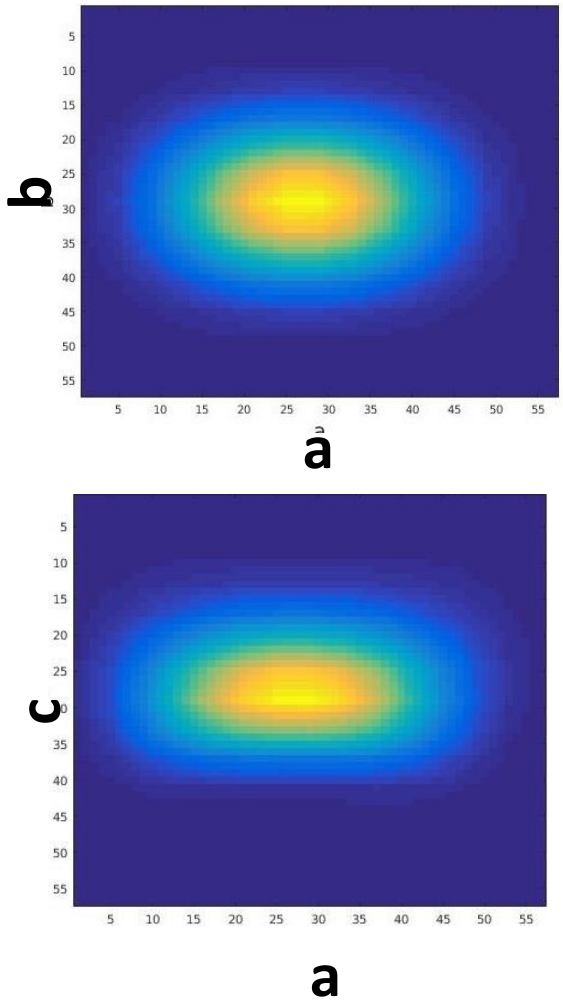
Muon Position M1



Muon Position M2



Muon Position M3



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Thank you very much for your attention