A Revisit to the Ordered State of Cu-spins in La_2CuO_4

A Quantum Approach to the Muon Sites

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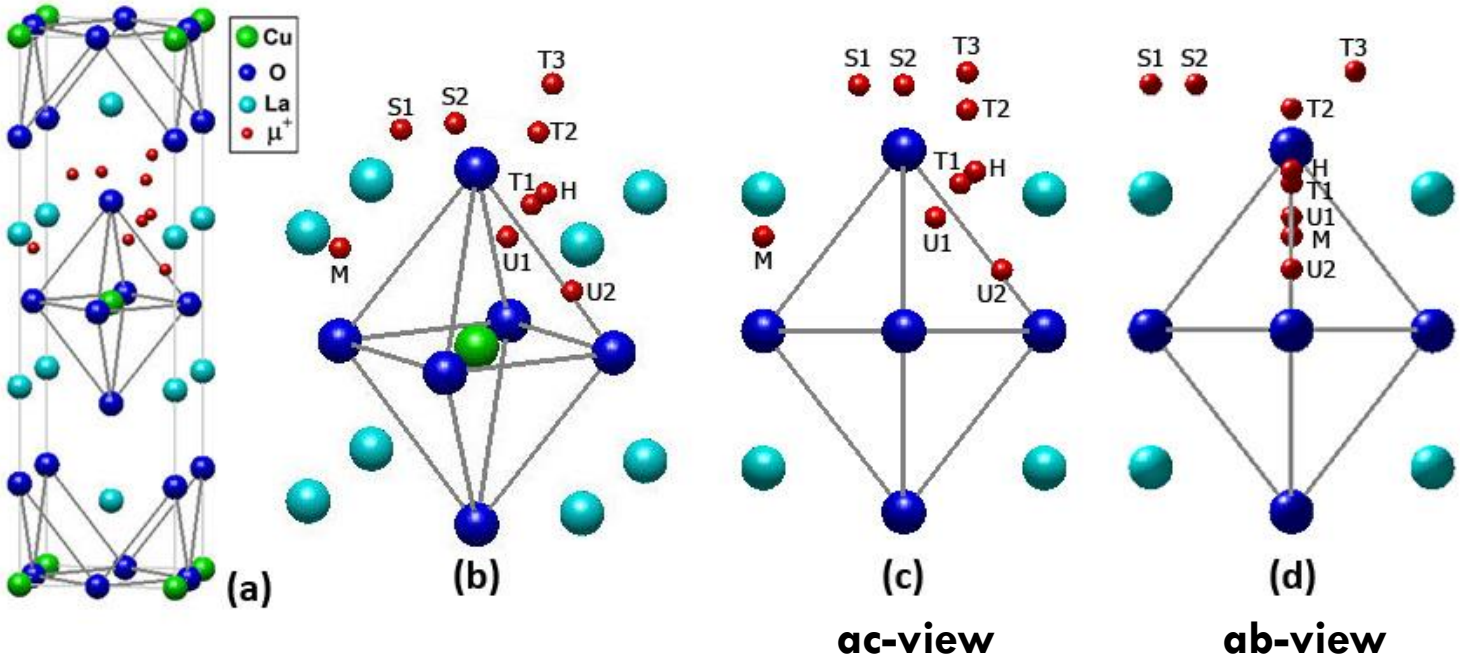
Why do we need to reconsider muon sites?

La_2CuO_4 (LCO)



9-Positions

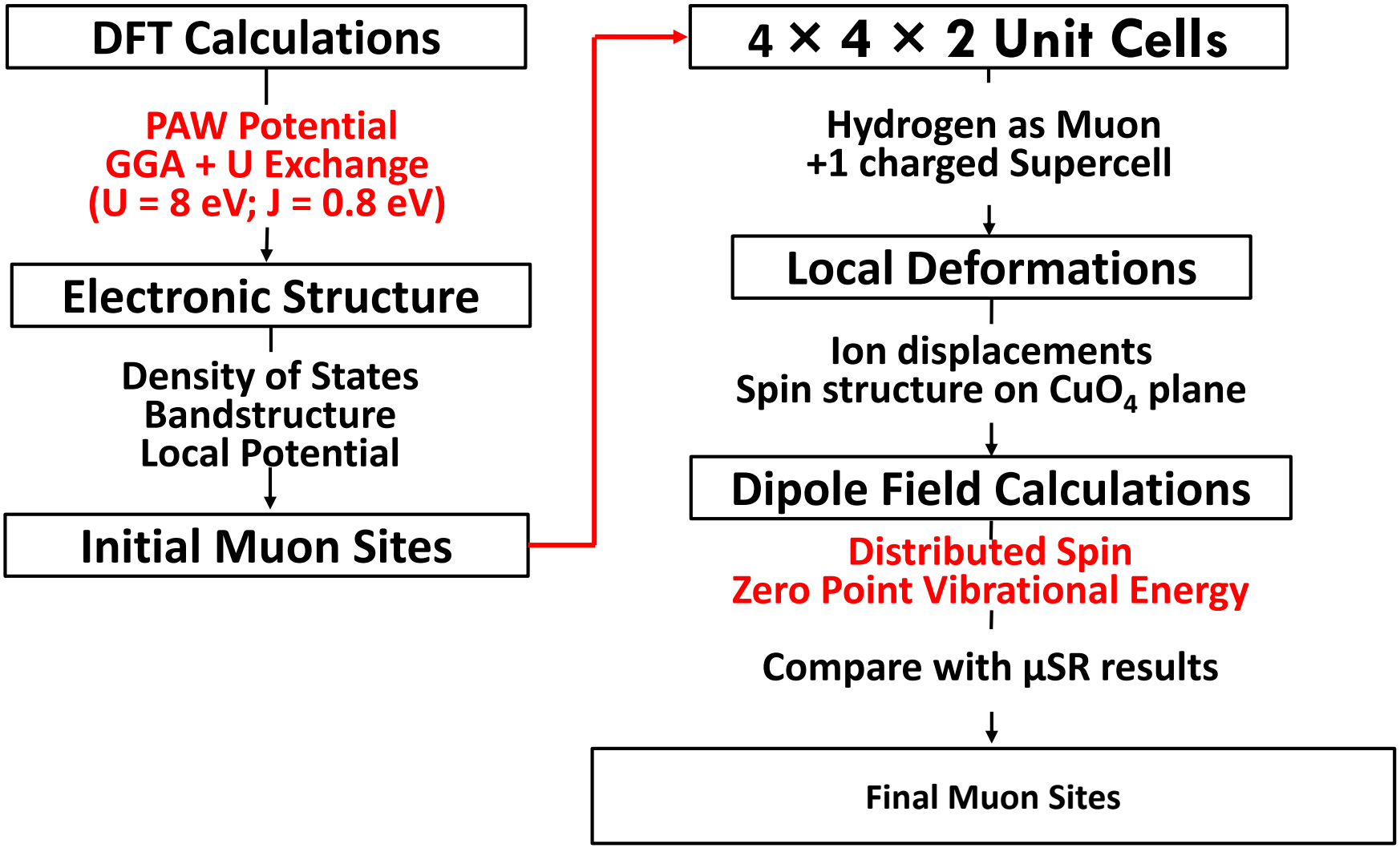
Dipole :
H, T1, T2, T3

Ab-initio :
M, U1, U2, S1, S2

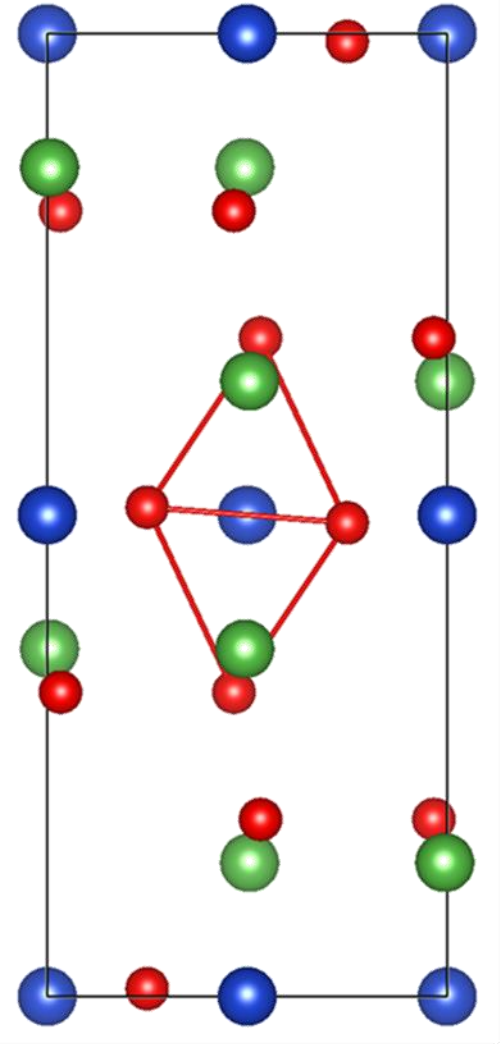
References:
1) H → Hitti *et al.* (1990)
2) M → McMullen *et al.* (1991)
3) T → Torikai *et al.* (1993)
4) U → Sulaiman *et al.* (1993)
5) S → Saito *et al.* (1991)

No unified method to find muon sites yet!!

Flowchart of Our Calculations

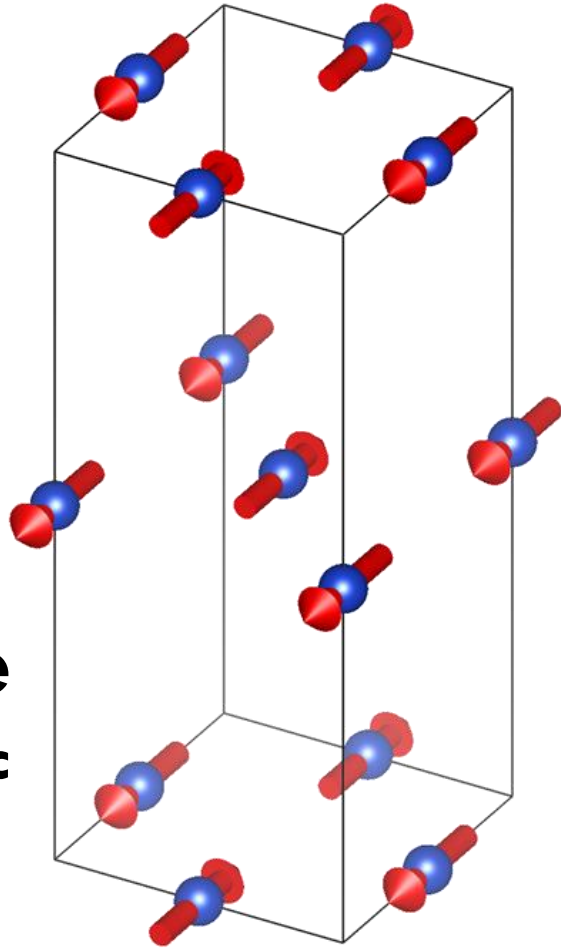


Initial Conditions, Crystal and Spin Structure



Crystal Structure

- Orthorhombhic La_2CuO_4
- Single Crystal
  - a = 5.333
  - b = 5.419
  - c = 13.095



Spin Structure

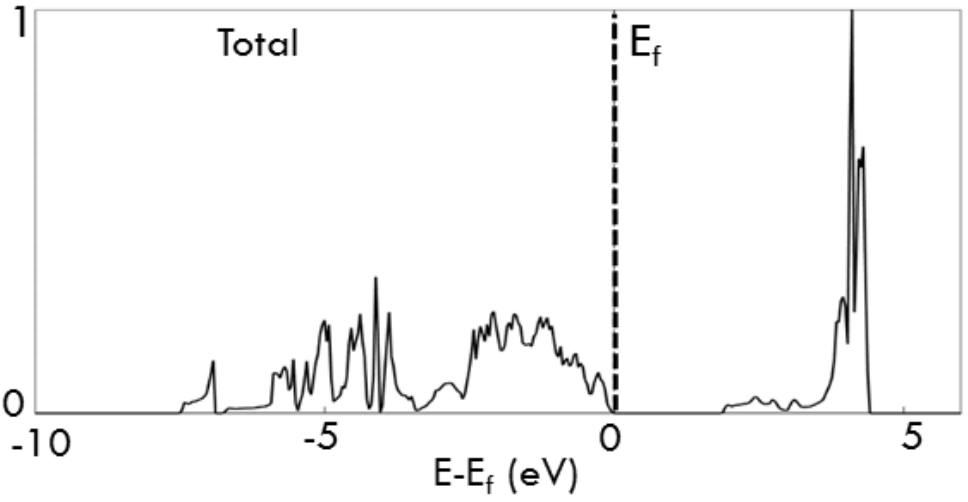
- Antiferromagnetic
- 0.5 μ_B/Cu-atom
- Spin aligned to *b*-direction

Band Structure

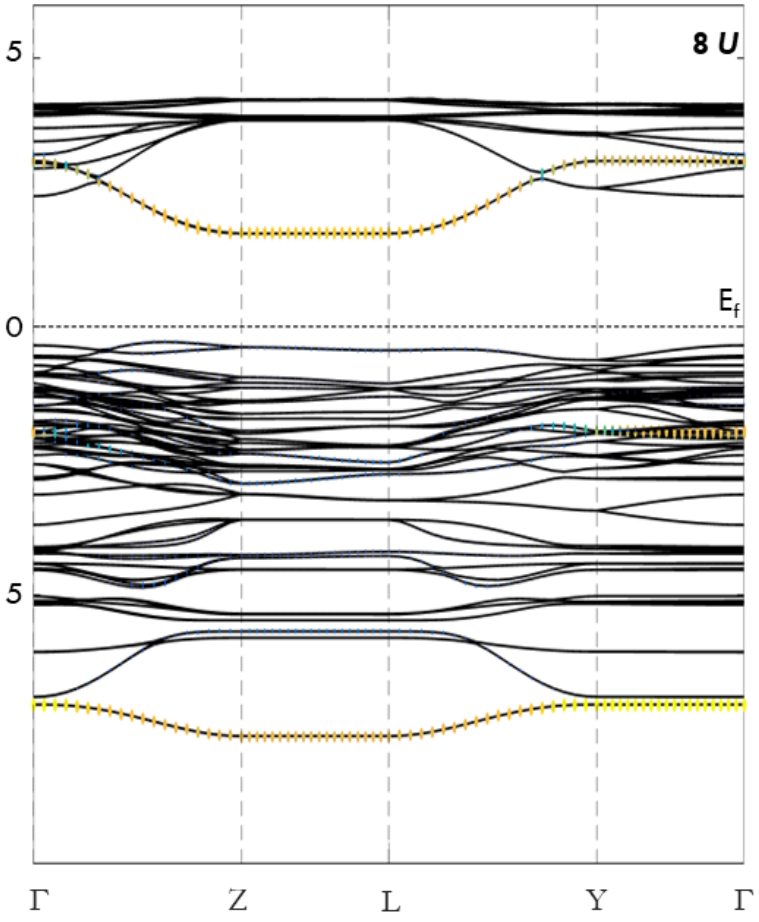
Magnetic Moment of Cu atoms

	s	p	d	f	total
1	-0.013	-0.014	0.637	0.000	0.610
2	0.013	0.014	-0.637	0.000	-0.610
3	-0.013	-0.014	0.637	0.000	0.610
4	0.013	0.014	-0.637	0.000	-0.610

Density of States

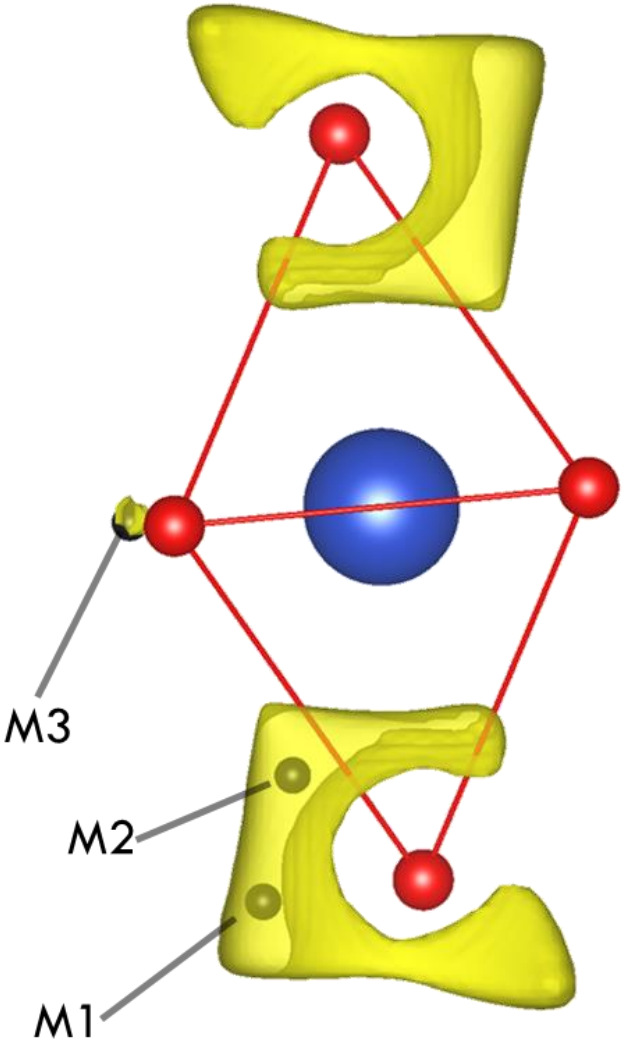


Bandstructure

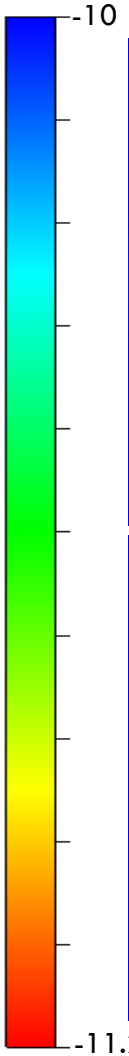


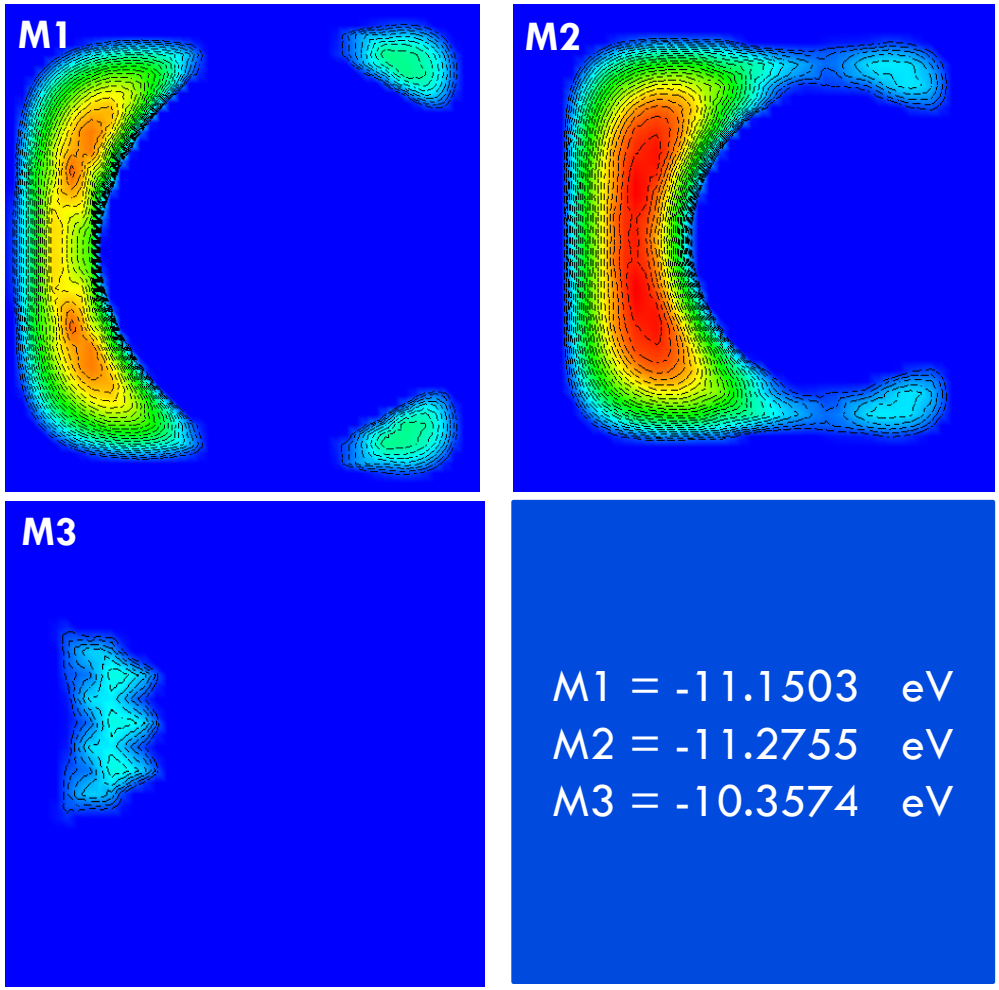
- Antiferromagnetic with 0.61 μB/ Cu atom
- 1.8 eV gap

Electrostatic Potential



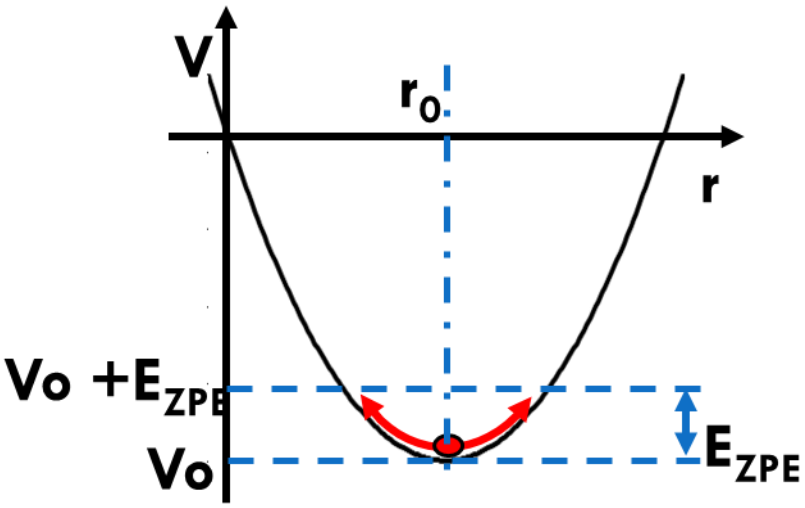
Isoruface at 1000 meV

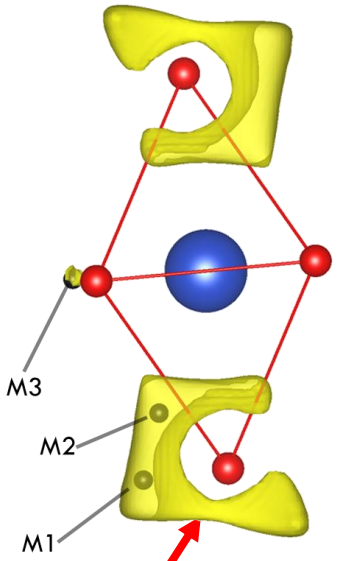


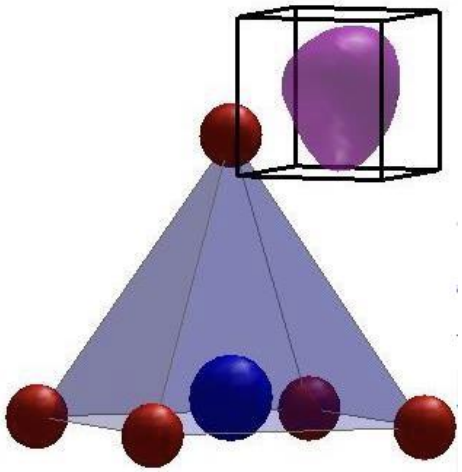


AB slice on each site

Zero-Point Vibrational Energy of μ







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 vibrational energy**
- **Muon probability density** → $\langle\psi_\mu|\psi_\mu\rangle$

Conclusions

- **M2 (nearest to the apical oxygen) and M3 (near planar oxygen) already shows a good agreement to the experimental results**

- **M1 has slight difference (~25 %). The reason is still on discussion**