

Determination of muon sites on metal-organic hybrids of $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ and $(C_2H_5NH_3)_2CuCl_4^\dagger$

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Hybrid materials consisting of metal and organic components have recently attracted considerable attention because they have lots of possibilities for tailoring their functionalities and physical properties by adjusting their metal and/or organic building blocks [1]. The organic component can be used not only to bind the metal components but also to control the connectivity between the metal components and to manipulate their dimensionality [2]. One of the interesting type of hybrid materials is the magnetic hybrid with perovskite-type transition metal salt with a chemical formula such as $(C_2H_5NH_3)_2CuCl_4$ (EA) and $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (PEA) [3]. We have carried out μ SR measurements on both materials at the RIKEN-RAL muon facilities. The results revealed the appearance of clear muon spin precession under the zero-field condition in magnetically ordered states. This observation provided evidence of the formation of long-range magnetic ordering of Cu spins. The internal field at the muon site was determined from the muon-spin precession frequency to be approximately 200 G at 4 K in both systems. In the case of PEA, a fast-depolarized component in an earlier time region was observed from room temperature down to 4 K. This fast depolarized component was not decoupled even in fields of a couple of Tesla, showing the existence of a possible muon state that is strongly coupled with the surrounding electrons via radical formation. Such a state was not observed in EA. The dipole-dipole interaction is too weak to trigger the 3D magnetic ordered state because of the large distance between the $CuCl_6$ layers.

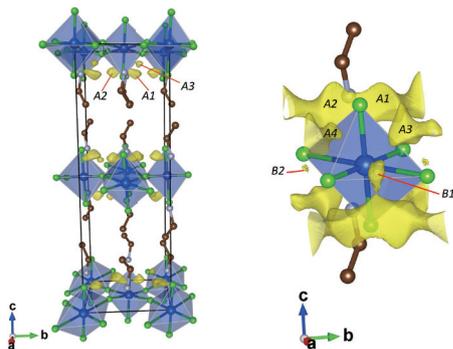


Fig. 1. Crystal structure of EA is shown with Cu ions represented by blue balls and Cl ions by green balls. The isosurface of the electrostatic potential for 455 meV (right) represents the localization volume for muon site positions.

In order to gain an understanding of the magnetic properties of EA and PEA, we are now attempting to reveal the muon positions. We determine the spin alignment by comparing the experimental results with the muon positions estimated using the computational techniques on the basis of the assumption that internal fields at the muon site are caused by dipole fields from surrounding magnetic moments. We present the results of the first trial to apply density functional theory (DFT) method [4] to EA and PEA in order to reveal the minimum energy positions that could facilitate muon injection. The estimation of the potential minimum positions was carried within the DFT framework as implemented in the Vienna ab-initio simulation package (VASP) [5] using the RICC supercomputer.

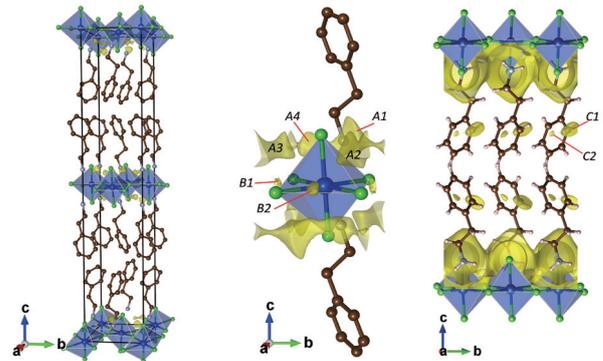


Fig. 2. Crystal structure (left) and DFT calculation results on PEA. The isosurfaces of the electrostatic potentials for 425 meV (center) and 1.025 meV (right) show possible muon sites.

We found six potential minimum positions around $CuCl_6$ in EA as well as in PEA, as shown in Figs. 1 and 2. Four of them (A1 - 4) were around the apical Cl^- ions and two of them (B1 and 2) were in between in-plane Cl^- ions on the $CuCl_4$ plane. These muon positions can be candidates to show muon-spin precession behavior under the zero-field condition in magnetically ordered states in both EA and PEA. Two more minimum potential positions (C1 and 2) were found in PEA in and on the phenyl ring of the organic part, causing possible muon states bound with the surrounding electrons via radical formation with large hyperfine fields.

References

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[†] Condensed from the article in Journal of Physics: Conference Series **551**, 012054 (2014)

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