

**Project Title:**

**Computational Studies of muon location, electronic structure and hyperfine interactions in high  $T_c$  Superconductor, Organic and Organometallic Systems**

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1. Background

$\mu$ SR is a powerful technique for probing the magnetic properties and electronic structures of matters such as high  $T_c$  superconductors, organic and organometallic systems. The interpretation of  $\mu$ SR results and the understanding of the properties of the muonated systems often requires the knowledge of the muon location(s) in the system and the electronic structures especially in the immediate vicinity of the muon site. The knowledge about the muon stable sites would also enable the study of the magnetic structure in certain systems.

In this project, the studies of the muon location and the electronic structures of the muonated systems were performed computationally by applying the ab initio Hartree-Fock and post Hartree-Fock methods as well as the Density Functional Theory.

2. Specific Usage

We have mainly used two software for our research investigation using the RICC computing facility. They are:

- i) Gaussian 09 software which is readily available on RICC.
- ii) VASP software which is owned by the Advanced Meson Science Laboratory under the supervision of Dr. Isao Watanabe. We have installed it on the RICC computers for our computational studies.

One of the major objectives when we applied for the Quick User account is to understand the capacity and capabilities of the computing facilities at RICC with respect to the size of our computational jobs.

3. Result

Two different systems were studied using the RICC facilities:

- i) Location of muon in  $\text{La}_2\text{CuO}_4$ .
- ii) Location of muonium in substituted benzenes.

The results from our studies on the location of muon in  $\text{La}_2\text{CuO}_4$  were presented at the International Conference on  $\mu$ SR: Theory and Application at Universiti Sains Malaysia, Penang, Malaysia on 1 – 3 November 2012. For our work on muonium in substituted benzenes, the results will be presented at the The 17th International Annual Symposium on Computational Science and Engineering ANSCSE 17, to be held from March 27, 2013 – March 29, 2013 at Khon Kaen University, Thailand.

4. Conclusion

The computing facility offered at RICC is excellent because it provides us with additional and more powerful computing resources for our computational work on muon science. Additionally the available software at RICC, specifically Gaussian 09, does meet our requirement.

## RICC Usage Report for Fiscal Year 2012

### 5. Schedule and prospect for the future

We would like to continue to be users of RICC to support our research efforts on muon science. This is also crucial so that the current collaborations between RIKEN (Advanced Meson Science Laboratory), Universiti Sains Malaysia, and Universitas Padjadjaran Indonesia can continue. We expect to have more members in our collaborative effort in the Fiscal Year 2013.

**Fiscal Year 2012 List of Publications Resulting from the Use of RICC**

**[Others]**

1. Poster Presentation at the International Conference on  $\mu$ SR: Theory and Applications at Universiti Sains Malaysia, Penang, Malaysia on 1 – 3 November 2012.

B. Adiperdana, I. A. Dharmawan, R. E. Siregar , S. Sulaiman, M. I. M. Ibrahim , I. Kawasaki, H. Guo and I. Watanabe *“Determining muon site in  $La_2CuO_4$  using ab-initio and dipole field calculation”*

2. Accepted for oral presentation at The 17th International Annual Symposium on Computational Science and Engineering (ANSCSE 17), to be held from March 27, 2013 – March 29, 2013 at Khon Kaen University, Thailand (to appear in the conference proceeding).

Ang Lee Sin, Dang Fatihah Hasan Baseri, Shukri Sulaiman and Mohamed Ismail Mohamed-Ibrahim *“Ab Initio and DFT Calculations of the Electronic Properties on Muonium in Substituted Benzene”*