

Project Title:

Computational Studies of muon location, electronic structure and hyperfine interactions in high Tc Superconductors, Organic and Organometallic System

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1. Background

Muon Spin Rotation (μ SR) technique is an excellent method to study magnetic properties and electronic structures of materials. It can be applied to diverse class of materials such as high Tc superconductors and organic magnets. There are only a few μ SR facilities in the world and one of them at Rutherford Appleton Laboratory is operated by Advanced Meson Science Laboratory RIKEN. There is a need for a close collaboration between experimental efforts and computational works so that the underlying science of the materials of interest could be unraveled. One of the main objectives for the computational works is to study the stopping sites for muon and muonium. Knowledge about the muon and muonium stopping sites could pave a way to enhance our understanding about the materials.

The computational effort requires excellent computing power such as the ones provided by RICC.

2. Specific usage.

We have used two main software to conduct our computational studies. They are

- i) Gaussian 09 which is available at RICC
- ii) VASP software for band structure and supercell calculation. This software is owned by Advanced Meson Science Laboratory.

3. Result

We have continued to study the stopping sites and related hyperfine interactions for positive muon in La_2CuO_4 system. One of the PhD students in our research group (Budi Adiperdana) has completed his doctoral studies. We have also started work on other systems such as muon $\text{YBa}_2\text{Cu}_3\text{O}_6$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ which are materials related to high Tc superconductors. Additionally, preliminary works have been initiated for muon in $\text{V}_4\text{S}_9\text{Br}_4$ and $\text{CeRu}_2\text{Al}_{10}$.

4. Conclusion

We have been able to carry out computational works that form the basis of our endeavor for studying muon in materials. The facilities at RICC have enable us to conduct such studies.

5. Schedule and prospect for the future

We will need and would like to continue using the RICC computing facilities in the future for our studies on muon in materials.

RICC Usage Report for Fiscal Year 2013

Fiscal Year 2013 List of Publications Resulting from the Use of RICC

[Proceedings, etc.]

Budi Adiperdana, Irwan Ary Dharmawan, Rustam Efendi Siregar, Shukri Sulaiman, Mohamed Ismail Mohamed-Ibrahim and Isao Watanabe, "*Muon Site Estimation on La₂CuO₄ using Dipole Field and Density Functional Theory Calculation*", Padjadjaran International Physics Symposium 2013 (PIPS-2013), AIP Conf. Proc. 1554, 214 (2013)