Project Title:

Computatioanal 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 (μSR) 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 μSR facilities in the world and one of them at Rutherford Appleton Laboratory is operated by Advanced Meson Science Laboratory RIKEN. The 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 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 continued to study the stopping sites and related hyperfine interactions for positive muon in La_2CuO_4 and $YBa_2Cu_3O_6$ systems. We also continued to further performed our investigations on muon in $V_4S_9Br_4$ and $CeRu_2Al_{10}$. We have started working on a new problem, which is muon in organic magnets. Specifically, we performed first principle computational studies on the muon locations and the electronic structures of β′-X $[Pd(dmit)_2]_2$ in the antiferromagnetic state.

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. Our future computing efforts would require more powerful computing facilites to enable us to include periodic boundary conditions in the computation of the electronic structures.

Fiscal Year 2014 List of Publications Resulting from the Use of RICC

[Publication]

1. B. Adiperdana, E. Suprayoga, N. Adam, S.S. Mohd-Tajudin, A.F. Rozlan, S. Sulaiman, M. I. Mohamed-Ibrahim, T. Kawamata, T. Adachi, I. A. Dharmawan, R. E. Siregar, Y. Koike, and I. Watanabe, 2014, *An Effect of the Supercell Calculations on Muon Positions and Local Deformation of Crystal Structures in La_2CuO_4,* Journal of Physics: Conference Series, 551, 012051.
2. S.S. Mohd-Tajudin, S. N. A. Ahmad, D. F. Hasan-Baseri, E. Suprayoga, N. Adam, A.F. Rozlan, S. Sulaiman, M. I. Mohamed-Ibrahim and I. Watanabe, 2014, *An investigation of muon sites in $YBa_2Cu_3O_6$ by using Density Functional Theory*, Journal of Physics: Conference Series, 551, 012052.
3. N. Adam, E. Suprayoga, B. Adiperdana, H. Guo, H. Taneda, S.S. Mohd-Tajudin, R. Kobayashi, M. Sera, T. Nishioka, M. Matsumura, S. Sulaiman, M. I. Mohamed-Ibrahim, and I. Watanabe, 2014, *Muon Sites in $Ce(Ru, Rh)_2Al_{10}$ investigated by Density Functional Theory from the view point of electronic potential,* Journal of Physics: Conference Series, 551, 012053.